intel

Intel[®] Math Kernel Library

Reference Manual

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Intel[®] Math Kernel Library Reference Manual

Revision	Revision History	Date
-001	Original Issue.	11/94
-002	Added functions crotg, zrotg. Documented versions of functions ?her2k, ?symm, ?syrk, and ?syr2k not previously described. Pagination revised.	5/95
-003	Changed the title; former title: "Intel BLAS Library for the Pentium [®] Processor Reference Manual." Added functions ?rotm,?rotmg and updated Appendix C.	1/96
-004	Documents Intel Math Kernel library release 2.0 with the parallelism capability. Information on parallelism has been added in Chapter 1 and in section "BLAS Level 3 Routines" in Chapter 2.	11/96
-005	Two-dimensional FFTs have been added. C interface has been added to both one- and two-dimensional FFTs.	8/97
-006	Documents Intel Math Kernel Library release 2.1. Sparse BLAS section has been added in Chapter 2.	1/98
-007	Documents Intel Math Kernel Library release 3.0. Descriptions of LAPACK routines (Chapters 4 and 5) and CBLAS interface (Appendix C) have been added. Quick Reference has been excluded from the manual; MKL 3.0 Quick Reference is now available in HTML format.	1/99
-008	Documents Intel Math Kernel Library release 3.2. Description of FFT routines have been revised. In Chapters 4 and 5 NAG names for LAPACK routines have been excluded.	6/99
-009	New LAPACK routines for eigenvalue problems have been added inchapter 5.	11/99
-010	Documents Intel Math Kernel Library release 4.0. Chapter 6 describing the VML functions has been added.	06/00
-011	Documents Intel Math Kernel Library release 5.1. LAPACK section has been extended to include the full list of computational and driver routines .	04/01
-6001	Documents Intel Math Kernel Library release 6.0 beta. New DFT interface (chapter 8) and Vector Statistical Library functions (chapter 7) have been added.	07/02
-6002	Documents Intel Math Kernel Library 6.0 beta update. DFT functions description (chapter 8) has been updated. CBLAS interface description was extended.	12/02
-6003	Documents Intel Math Kernel Library 6.0 gold. DFT functions have been updated. Auxiliary LAPACK routines' descriptions were added to the manual.	03/03
-6004	Documents Intel Math Kernel Library release 6.1.	07/03

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Overview



The Intel[®] Math Kernel Library (Intel[®] MKL) provides Fortran routines and functions that perform a wide variety of operations on vectors and matrices. The library also includes fast Fourier transform functions and new discrete Fourier transform functions, as well as vector mathematical and vector statistical functions with Fortran and C interfaces. The Intel MKL enhances performance of the programs that use it because the library has been optimized for Intel[®] processors.

This chapter introduces the Intel Math Kernel Library and provides information about the organization of this manual.

About This Software

The Intel Math Kernel Library includes the following groups of routines:

- Basic Linear Algebra Subprograms (BLAS): -vector operations
 -matrix-vector operations
 -matrix-matrix operations
- Sparse BLAS (basic vector operations on sparse vectors)
- Fast Fourier transform routines (with Fortran and C interfaces)
- LAPACK routines for solving systems of linear equations
- LAPACK routines for solving least-squares problems, eigenvalue and singular value problems, and Sylvester's equations
- Auxiliary LAPACK routines
- Vector Mathematical Library (VML) functions for computing core mathematical functions on vector arguments (with Fortran and C interfaces)
- Vector Statistical Library (VSL) functions for generating vectors of pseudorandom numbers with different types of statistical distributions
- Advanced Discrete Fourier Transform Functions (DFT).

For specific issues on using the library, please refer to the *MKL Release Notes*.

Technical Support

Intel MKL provides a product web site that offers timely and comprehensive product information, including product features, white papers, and technical articles. For the latest information, check: <u>http://developer.intel.com/software/products/</u>

Intel also provides a support web site that contains a rich repository of self help information, including getting started tips, known product issues, product errata, license information, user forums, and more (visit http://support.intel.com/support/).

Registering your product entitles you to one year of technical support and product updates through Intel® Premier Support. Intel Premier Support is an interactive issue management and communication web site providing these services:

- Submit issues and review their status.
- Download product updates anytime of the day.

To register your product, contact Intel, or seek product support, please visit: http://www.intel.com/software/products/support

BLAS Routines

BLAS routines and functions are divided into the following groups according to the operations they perform:

- <u>BLAS Level 1 Routines and Functions</u> perform operations of both addition and reduction on vectors of data. Typical operations include scaling and dot products.
- <u>BLAS Level 2 Routines</u> perform matrix-vector operations, such as matrix-vector multiplication, rank-1 and rank-2 matrix updates, and solution of triangular systems.
- <u>BLAS Level 3 Routines</u> perform matrix-matrix operations, such as matrix-matrix multiplication, rank-k update, and solution of triangular systems.

Sparse BLAS Routines

<u>Sparse BLAS Routines and Functions</u> operate on sparse vectors (that is, vectors in which most of the elements are zeros). These routines perform vector operations similar to BLAS Level 1 routines. Sparse BLAS routines take advantage of vectors' sparsity: they allow you to store only non-zero elements of vectors.

Fast Fourier Transforms

<u>Fast Fourier Transforms</u> (FFTs) are used in digital signal processing and image processing and in partial differential equation (PDE) solvers. Combined with the BLAS routines, the FFTs contribute to the portability of the programs and provide a simplified interface between your program and the available library. To obtain more functionality and ease of use, consider also using the new DFT functions described in <u>Chapter 9</u>.

LAPACK Routines

The Intel Math Kernel Library covers the full set of the LAPACK computational and driver routines. These routines can be divided into the following groups according to the operations they perform:

- Routines for solving systems of linear equations, factoring and inverting matrices, and estimating condition numbers (see <u>Chapter 4</u>).
- Routines for solving least-squares problems, eigenvalue and singular value problems, and Sylvester's equations (see <u>Chapter 5</u>).
- Auxiliary routines used to perform certain subtasks or common low-level computation (see <u>Chapter 6</u>).

VML Functions

VML functions (see <u>Chapter 7</u>) include a set of highly optimized implementations of certain computationally expensive core mathematical functions (power, trigonometric, exponential, hyperbolic etc.) that operate on real vector arguments.

VSL Functions

Vector Statistical Library (VSL) functions (see <u>Chapter 8</u>) include a set of pseudorandom number generator subroutines implementing basic continuous and discrete distributions. To provide best performance, VSL subroutines use calls to highly optimized Basic Random Number Generators and the library of vector mathematical functions, VML.

DFT Functions

The newly developed Discrete Fourier Transform functions (see <u>Chapter 9</u>) provide uniformity of DFT computation and combine functionality with ease of use. Both Fortran and C interface specification are given. Users are encouraged to migrate to the new interface in their application programs.

Performance Enhancements

The Intel Math Kernel Library has been optimized by exploiting both processor and system features and capabilities. Special care has been given to those routines that most profit from cache-management techniques. These especially include matrix-matrix operation routines such as dgemm().

In addition, code optimization techniques have been applied to minimize dependencies of scheduling integer and floating-point units on the results within the processor.

The major optimization techniques used throughout the library include:

- Loop unrolling to minimize loop management costs.
- Blocking of data to improve data reuse opportunities.
- Copying to reduce chances of data eviction from cache.
- Data prefetching to help hide memory latency.
- Multiple simultaneous operations (for example, dot products in dgemm) to eliminate stalls due to arithmetic unit pipelines.
- Use of hardware features such as the SIMD arithmetic units, where appropriate.

These are techniques from which the arithmetic code benefits the most.

Parallelism

In addition to the performance enhancements discussed above, the Intel MKL offers performance gains through parallelism provided by the symmetric multiprocessing performance (SMP) feature. You can obtain improvements from SMP in the following ways:

- One way is based on user-managed threads in the program and further distribution of the operations over the threads based on data decomposition, domain decomposition, control decomposition, or some other parallelizing technique. Each thread can use any of the Intel MKL functions because the library has been designed to be thread-safe.
- Another method is to use the FFT and BLAS level 3 routines. They have been parallelized and require no alterations of your application to gain the performance enhancements of multiprocessing. Performance using multiple processors on the level 3 BLAS shows excellent scaling. Since the threads are called and managed within the library, the application does not need to be recompiled thread-safe (see also <u>BLAS</u> <u>Level 3 Routines</u> in Chapter 2).
- Yet another method is to use *tuned LAPACK routines*. Currently these include the single- and double precision flavors of routines for *QR* factorization of general matrices, triangular factorization of general and symmetric positive-definite matrices, solving systems of equations with such matrices, as well as solving symmetric eigenvalue problems.

For instructions on setting the number of available processors for the BLAS level 3 and LAPACK routines, see the *Release Notes*.

Platforms Supported

The Intel Math Kernel Library includes Fortran routines and functions optimized for Intel[®] processor-based computers running operating systems that support multiprocessing. In addition to the Fortran interface, the Intel MKL includes a C-language interface for the fast Fourier transform functions, new discrete Fourier transform API, as well as for the Vector Mathematical Library and Vector Statistical Library functions.

About This Manual

This manual describes the routines of the Intel Math Kernel Library. Each reference section describes a routine group consisting of routines used with four basic data types: single-precision real, double-precision real, single-precision complex, and double-precision complex.

Each routine group is introduced by its name, a short description of its purpose, and the calling sequence for each type of data with which each routine of the group is used. The following sections are also included:

Discussion	Describes the operation performed by routines of the group based on one or more equations. The data types of the arguments are defined in general terms for the group.
Input Parameters	Defines the data type for each parameter on entry, for example:
	a REAL for saxpy DOUBLE PRECISION for daxpy
Output Parameters	Lists resultant parameters on exit.

Audience for This Manual

The manual addresses programmers proficient in computational linear algebra and assumes a working knowledge of linear algebra and Fourier transform principles and vocabulary.

Manual Organization

The manual contains the following chapters and appendixes:

Chapter 1	<u>Overview</u> . Introduces the Intel Math Kernel Library software, provides information on manual organization, and explains notational conventions.
Chapter 2	<u>BLAS and Sparse BLAS Routines</u> . Provides descriptions of BLAS and Sparse BLAS functions and routines.

Chapter 3	<u>Fast Fourier Transforms</u> . Provides descriptions of fast Fourier transforms (FFT).
Chapter 4	LAPACK Routines: Linear Equations. Provides descriptions of LAPACK routines for solving systems of linear equations and performing a number of related computational tasks: triangular factorization, matrix inversion, estimating the condition number of matrices.
Chapter 5	<u>LAPACK Routines: Least Squares and Eigenvalue</u> <u>Problems</u> . Provides descriptions of LAPACK routines for solving least-squares problems, standard and generalized eigenvalue problems, singular value problems, and Sylvester's equations.
Chapter 6	<u>LAPACK Auxiliary Routines</u> . Describes auxiliary LAPACK routines that perform certain subtasks or common low-level computation.
Chapter 7	<u>Vector Mathematical Functions</u> . Provides descriptions of VML functions for computing elementary mathematical functions on vector arguments.
Chapter 8	<u>Vector Generators of Statistical Distributions</u> . Provides descriptions of VSL functions for generating vectors of pseudorandom numbers.
Chapter 9	<u>Advanced DFT Functions</u> . Describes new functions for computing the Discrete Fourier Transform.
Appendix A	<u>Routine and Function Arguments</u> . Describes the major arguments of the BLAS routines and VML functions: vector and matrix arguments.
Appendix B	<u>Code Examples</u> . Provides code examples of calling BLAS functions and routines.
Appendix C	<u>CBLAS Interface to the BLAS</u> . Provides the C interface to the BLAS.

The manual also includes a Glossary and an Index.

Notational Conventions

This manual uses the following notational conventions:

- Routine name shorthand (?ungqr instead of cungqr/zungqr).
- Font conventions used for distinction between the text and the code.

Routine Name Shorthand

For shorthand, character codes are represented by a question mark "?" in names of routine groups. The question mark is used to indicate any or all possible varieties of a function; for example:

?swap

Refers to all four data types of the vector-vector ?swap routine: sswap, dswap, cswap, and zswap.

Font Conventions

The following font conventions are used:

UPPERCASE COURIER	Data type used in the discussion of input and output parameters for Fortran interface. For example, CHARACTER*1.
lowercase courier	<pre>Code examples: a(k+i,j) = matrix(i,j) and data types for C interface, for example, const float*</pre>
lowercase courier mixed with UpperCase courier	Function names for C interface, for example, vmlSetMode
lowercase courier italic	Variables in arguments and parameters discussion. For example, <i>incx</i> .
*	Used as a multiplication symbol in code examples and equations and where required by the Fortran syntax.

Related Publications

For more information about the BLAS, Sparse BLAS, LAPACK, VML, VSL, and DFT routines, refer to the following publications:

• BLAS Level 1

C. Lawson, R. Hanson, D. Kincaid, and F. Krough. *Basic Linear Algebra Subprograms for Fortran Usage*, ACM Transactions on Mathematical Software, Vol.5, No.3 (September 1979) 308-325.

• BLAS Level 2

J. Dongarra, J. Du Croz, S. Hammarling, and R. Hanson. *An Extended Set of Fortran Basic Linear Algebra Subprograms*, ACM Transactions on Mathematical Software, Vol.14, No.1 (March 1988) 1-32.

• BLAS Level 3

J. Dongarra, J. DuCroz, I. Duff, and S. Hammarling. *A Set of Level 3 Basic Linear Algebra Subprograms*, ACM Transactions on Mathematical Software (December 1989).

• Sparse BLAS

D. Dodson, R. Grimes, and J. Lewis. *Sparse Extensions to the FORTRAN Basic Linear Algebra Subprograms*, ACM Transactions on Mathematical Software, Vol.17, No.2 (June 1991).

D. Dodson, R. Grimes, and J. Lewis. *Algorithm 692: Model Implementation and Test Package for the Sparse Basic Linear Algebra Subprograms*, ACM Transactions on Mathematical Software, Vol.17, No.2 (June 1991).

LAPACK

E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel,J. Donagarra, J. Du Croz, A. Greenbaum, S. Hammarling,A. McKenney, and D. Sorensen. *LAPACK Users' Guide*, Third Edition,Society for Industrial and Applied Mathematics (SIAM), 1999.

G. Golub and C. Van Loan. *Matrix Computations*, Johns Hopkins University Press, 1989.

• VML

J.M.Muller. *Elementary functions: algorithms and implementation*, Birkhauser Boston, 1997.

IEEE Standard for Binary Floating-Point Arithmetic. ANSI/IEEE Std 754-1985.

• VSL	
[Bratley87]	Bratley P., Fox B.L., and Schrage L.E. <i>A Guide to</i> <i>Simulation</i> . 2nd edition. Springer-Verlag, New York, 1987.
[Coddington94]	Coddington, P. D. Analysis of Random Number Generators Using Monte Carlo Simulation. Int. J. Mod. Phys. C-5, 547, 1994.
[Gentle98]	Gentle, James E. <i>Random Number Generation and</i> <i>Monte Carlo Methods</i> , Springer-Verlag New York, Inc., 1998.
[L'Ecuyer94]	L'Ecuyer, Pierre. <i>Uniform Random Number Generation</i> . Annals of Operations Research, 53, 77–120, 1994.
[L'Ecuyer99]	L'Ecuyer, Pierre. <i>Tables of Linear Congruential Generators of Different Sizes and Good Lattice Structure</i> . Mathematics of Computation, 68, 225, 249-260, 1999.
[L'Ecuyer99a]	L'Ecuyer, Pierre. <i>Good Parameter Sets for Combined</i> <i>Multiple Recursive Random Number Generators.</i> Operations Research, 47, 1, 159-164, 1999.
[L'Ecuyer01]	L'Ecuyer, Pierre. <i>Software for Uniform Random Number</i> <i>Generation: Distinguishing the Good and the Bad.</i> Proceedings of the 2001 Winter Simulation Conference, IEEE Press, 95–105, Dec. 2001.
[Kirkpatrick81]	Kirkpatrick, S., and Stoll, E. <i>A Very Fast Shift-Register</i> <i>Sequence Random Number Generatory</i> . Journal of Computational Physics, V. 40. 517–526, 1981.
[Knuth81]	Knuth, Donald E. <i>The Art of Computer Programming,</i> <i>Volume 2, Seminumerical Algorithms</i> . 2nd edition, Addison-Wesley Publishing Company, Reading, Massachusetts, 1981.
[NAG]	NAG Numerical Libraries. http://www.nag.co.uk/numeric/numerical libraries.asp

• DFT

[1] E. Oran Brigham, *The Fast Fourier Transform and Its Applications*, Prentice Hall, New Jersey, 1988.

[2] Athanasios Papoulis, *The Fourier Integral and its Applications*, 2nd edition, McGraw-Hill, New York, 1984.

[3] Ping Tak Peter Tang, *DFTI*, a New API for DFT: Motivation, Design, and Rationale, July 2002.

[4] Charles Van Loan, *Computational Frameworks for the Fast Fourier Transform*, SIAM, Philadelphia, 1992

For a reference implementation of BLAS, sparse BLAS, and LAPACK packages (without platform-specific optimizations) visit <u>www.netlib.org</u>.

BLAS and Sparse BLAS Routines



This chapter contains descriptions of the BLAS and Sparse BLAS routines of the Intel[®] Math Kernel Library. The routine descriptions are arranged in four sections according to the BLAS level of operation:

- <u>BLAS Level 1 Routines and Functions</u> (vector-vector operations)
- <u>BLAS Level 2 Routines</u> (matrix-vector operations)
- <u>BLAS Level 3 Routines</u> (matrix-matrix operations)
- <u>Sparse BLAS Routines and Functions</u>.

Each section presents the routine and function group descriptions in alphabetical order by routine or function group name; for example, the **?asum** group, the **?axpy** group. The question mark in the group name corresponds to different character codes indicating the data type (s, d, c, and z or their combination); see *Routine Naming Conventions* on the next page.

When BLAS routines encounter an error, they call the error reporting routine XERBLA. To be able to view error reports, you must include XERBLA in your code. A copy of the source code for XERBLA is included in the library.

In BLAS Level 1 groups i?amax and i?amin, an "i" is placed before the character code and corresponds to the index of an element in the vector. These groups are placed in the end of the BLAS Level 1 section.

Routine Naming Conventions

s

d

BLAS routine names have the following structure:

<character code> <name> <mod> ()

The *<character code>* is a character that indicates the data type:

- real, single precision c complex, single precision
- real, double precision z complex, double precision

Some routines and functions can have combined character codes, such as sc or dz. For example, the function scasum uses a complex input array and returns a real value.

The <name> field, in BLAS level 1, indicates the operation type. For example, the BLAS level 1 routines ?dot, ?rot, ?swap compute a vector dot product, vector rotation, and vector swap, respectively.

In BLAS level 2 and 3, <*name*> reflects the matrix argument type:

- ge general matrix
- gb general band matrix
- sy symmetric matrix
- sp symmetric matrix (packed storage)
- sb symmetric band matrix
- he Hermitian matrix
- hp Hermitian matrix (packed storage)
- hb Hermitian band matrix
- triangular matrix
- tp triangular matrix (packed storage)
- tb triangular band matrix.

The *<mod>* field, if present, provides additional details of the operation. BLAS level 1 names can have the following characters in the *<mod>* field:

- c conjugated vector
- u unconjugated vector
- g Givens rotation.

BLAS level 2 names can have the following characters in the <mod> field:

- mv matrix-vector product
- sv solving a system of linear equations with matrix-vector operations
- **r** rank-1 update of a matrix
- r2 rank-2 update of a matrix.

BLAS level 3 names can have the following characters in the <mod> field:

- mm matrix-matrix product
- sm solving a system of linear equations with matrix-matrix operations
- **rk** rank-*k* update of a matrix
- r2k rank-2k update of a matrix.

The examples below illustrate how to interpret BLAS routine names:

<d><dot></dot></d>	ddot: double-precision real vector-vector dot product
<c> <dot> <c></c></dot></c>	cdotc: complex vector-vector dot product, conjugated
<sc> <asum></asum></sc>	scasum: sum of magnitudes of vector elements, single precision real output and single precision complex input
<c> <dot> <u></u></dot></c>	cdotu: vector-vector dot product, unconjugated, complex
<s><ge> <mv></mv></ge></s>	sgemv: matrix-vector product, general matrix, single precision
<z> <mm></mm></z>	ztrmm: matrix-matrix product, triangular matrix, double-precision complex.

Sparse BLAS naming conventions are similar to those of BLAS level 1. For more information, see *Naming conventions in Sparse BLAS*.

Matrix Storage Schemes

Matrix arguments of BLAS routines can use the following storage schemes:

- *Full storage*: a matrix *A* is stored in a two-dimensional array *a*, with the matrix element *a_{ii}* stored in the array element *a*(*i*, *j*).
- *Packed storage* scheme allows you to store symmetric, Hermitian, or triangular matrices more compactly: the upper or lower triangle of the matrix is packed by columns in a one-dimensional array.
- *Band storage*: a band matrix is stored compactly in a two-dimensional array: columns of the matrix are stored in the corresponding columns of the array, and *diagonals* of the matrix are stored in rows of the array.

For more information on matrix storage schemes, see <u>Matrix Arguments</u> in Appendix A.

BLAS Level 1 Routines and Functions

BLAS Level 1 includes routines and functions, which perform vector-vector operations. Table 2-1 lists the BLAS Level 1 routine and function groups and the data types associated with them.

Table 2-1 BLAS Level 1 Routine Groups and Their Data Types

Routine or Function		
Group	Data Types	Description
?asum	s, d, sc, dz	Sum of vector magnitudes (functions)
?axpy	s, d, c, z	Scalar-vector product (routines)
?copy	s, d, c, z	Copy vector (routines)
?dot	s, d	Dot product (functions)
?sdot	sd, d	Dot product with extended precision (functions)
?dotc	C, Z	Dot product conjugated (functions)
?dotu	C, Z	Dot product unconjugated (functions)
?nrm2	s, d, sc, dz	Vector 2-norm (Euclidean norm) a normal or null vector (functions)
?rot	s, d, cs, zd	Plane rotation of points (routines)
?rotg	s, d, c, z	Givens rotation of points (routines)
?rotm	s, d	Modified plane rotation of points
?rotmg	s, d	Givens modified plane rotation of points
?scal	s, d, c, z, cs, zd	Vector scaling (routines)
?swap	s, d, c, z	Vector-vector swap (routines)
<u>i?amax</u>	s, d, c, z	Vector maximum value, absolute largest element of a vector where i is an index to this value in the vector array (functions)
<u>i?amin</u>	s, d, c, z	Vector minimum value, absolute smallest element of a vector where i is an index to this value in the vector array (functions)

?asum

Computes the sum of magnitudes of the vector elements.

```
res = sasum ( n, x, incx )
res = scasum ( n, x, incx )
res = dasum ( n, x, incx )
res = dzasum ( n, x, incx )
```

Discussion

Given a vector x, ?asum functions compute the sum of the magnitudes of its elements or, for complex vectors, the sum of magnitudes of the elements' real parts plus magnitudes of their imaginary parts:

 $res = |\operatorname{Rex}(1)| + |\operatorname{Imx}(1)| + |\operatorname{Rex}(2)| + |\operatorname{Imx}(2)| + ...+ |\operatorname{Rex}(n)| + |\operatorname{Imx}(n)|$

where x is a vector of order n.

Input Parameters

n	INTEGER. Specifies the order of vector \mathbf{x} .
x	REAL for sasum
	DOUBLE PRECISION for dasum
	COMPLEX for scasum
	DOUBLE COMPLEX for dzasum
	Array, DIMENSION at least $(1 + (n-1)*abs(incx))$.
incx	INTEGER. Specifies the increment for the elements of x .

Output Parameters

res REAL for sasum DOUBLE PRECISION for dasum REAL for scasum DOUBLE PRECISION for dzasum

Contains the sum of magnitudes of all elements' real parts plus magnitudes of their imaginary parts.

?axpy

Computes a vector-scalar product and adds the result to a vector.

call saxpy (n, a, x, incx, y, incy)
call daxpy (n, a, x, incx, y, incy)
call caxpy (n, a, x, incx, y, incy)
call zaxpy (n, a, x, incx, y, incy)

Discussion

The ?axpy routines perform a vector-vector operation defined as

```
y := a^*x + y
```

where:

a is a scalar

x and y are vectors of order n.

n	INTEGER. Specifies the order of vectors \mathbf{x} and \mathbf{y} .
a	REAL for saxpy DOUBLE PRECISION for daxpy COMPLEX for caxpy DOUBLE COMPLEX for zaxpy
	Specifies the scalar a.
x	REAL for saxpy DOUBLE PRECISION for daxpy COMPLEX for caxpy DOUBLE COMPLEX for zaxpy
	Array, DIMENSION at least (1 + (n-1)*abs(incx)).
incx	INTEGER . Specifies the increment for the elements of <i>x</i> .

2	REAL for saxpy DOUBLE PRECISION for daxpy
	COMPLEX for caxpy
	DOUBLE COMPLEX for zaxpy
	Array, DIMENSION at least $(1 + (n-1)*abs(incy))$.
incy	INTEGER. Specifies the increment for the elements of y .
Output Parameters	

y Contains the updated vector *y*.

?copy

Copies vector to another vector.

call scopy (n, x, incx, y, incy)
call dcopy (n, x, incx, y, incy)
call ccopy (n, x, incx, y, incy)
call zcopy (n, x, incx, y, incy)

Discussion

The ?copy routines perform a vector-vector operation defined as

y = x

where \mathbf{x} and \mathbf{y} are vectors.

п	INTEGER. Specifies the order of vectors \mathbf{x} and \mathbf{y} .
x	REAL for scopy
	DOUBLE PRECISION for dcopy
	COMPLEX for ccopy
	DOUBLE COMPLEX for zcopy
	Array, DIMENSION at least (1 + (n-1)*abs(incx)).
incx	INTEGER. Specifies the increment for the elements of \mathbf{x} .

У	REAL for scopy DOUBLE PRECISION for dcopy COMPLEX for ccopy DOUBLE COMPLEX for zcopy		
	Array, DIMENSION at least $(1 + (n-1)*abs(incy))$.		
incy	INTEGER. Specifies the increment for the elements of <i>y</i> .		
Output Pa	Output Parameters		
У	Contains a copy of the vector \mathbf{x} if \mathbf{n} is positive.		
	Otherwise, parameters are unaltered.		

?dot

Computes a vector-vector dot product.

res = sdot (n, x, incx, y, incy) res = ddot (n, x, incx, y, incy)

Discussion

The ?dot functions perform a vector-vector reduction operation defined as $res = \sum (x^*y)$

where x and y are vectors.

п	INTEGER. Specifies the order of vectors \mathbf{x} and \mathbf{y} .
x	REAL for sdot DOUBLE PRECISION for ddot
	Array, DIMENSION at least $(1+(n-1)*abs(incx))$.
incx	INTEGER . Specifies the increment for the elements of x .

У	REAL for sdot
	DOUBLE PRECISION for ddot
	Array, DIMENSION at least $(1+(n-1)*abs(incy))$.
incy	INTEGER. Specifies the increment for the elements of y .
Output Pa	arameters
res	REAL for sdot
	DOUBLE PRECISION for ddot
	Contains the result of the dot product of x and y , if n is positive. Otherwise, <i>res</i> contains 0.

?sdot

Computes a vector-vector dot product with extended precision.

res = sdsdot (n, sb, sx, incx, sy, incy)
res = dsdot (n, sx, incx, sy, incy)

Discussion

The ?sdot functions compute the inner product of two vectors with extended precision. Both functions use extended precision accumulation of the intermediate results, but the function sdsdot outputs the final result in single precision, whereas the function dsdot outputs the double precision result. The function sdsdot also adds scalar value *sb* to the inner product.

n	INTEGER . Specifies the number of elements in the input
	vectors sx and sy.
sb	REAL . Single precision scalar to be added to inner
	product (for the function sdsdot only).

sx, sy	REAL. Arrays, DIMENSION at least $(1+(n-1)*abs(incx))$ and $(1+(n-1)*abs(incy))$, respectively. Contain the input single precision vectors.
incx	INTEGER. Specifies the increment for the elements of <i>sx</i> .
incy	INTEGER. Specifies the increment for the elements of <i>sy</i> .
Outrast Dam	

res	REAL for sdsdot DOUBLE PRECISION for dsdot
	Contains the result of the dot product of sx and sy (with sb added for $sdsdot$), if n is positive. Otherwise, res contains sb for $sdsdot$ and 0 for $dsdot$.

?dotc

Computes a dot product of a conjugated vector with another vector.

res = cdotc (n, x, incx, y, incy)res = zdotc (n, x, incx, y, incy)

Discussion

The ?dotc functions perform a vector-vector operation defined as

 $res = \sum (conjg(x)^*y)$

where *x* and *y* are *n*-element vectors.

Input Parameters

n

INTEGER. Specifies the order of vectors \mathbf{x} and \mathbf{y} .

x	COMPLEX for cdotc DOUBLE COMPLEX for zdotc
	Array, DIMENSION at least $(1 + (n-1)*abs(incx))$.
incx	INTEGER. Specifies the increment for the elements of x .
У	COMPLEX for cdotc DOUBLE COMPLEX for zdotc
	Array, DIMENSION at least $(1 + (n-1)*abs(incy))$.
incy	INTEGER . Specifies the increment for the elements of <i>y</i> .
Output Par	rameters
res	COMPLEX for cdotc DOUBLE COMPLEX for zdotc
	Contains the result of the dot product of the conjugated x and unconjugated y , if n is positive. Otherwise, <i>res</i> contains 0.

?dotu

Computes a vector-vector dot product.

res = cdotu (n, x, incx, y, incy)
res = zdotu (n, x, incx, y, incy)

Discussion

The ?dotu functions perform a vector-vector reduction operation defined as $res = \sum (x^*y)$

where x and y are *n*-element complex vectors.

Input Parameters

n

INTEGER. Specifies the order of vectors x and y.

x	COMPLEX for cdotu DOUBLE COMPLEX for zdotu
	Array, DIMENSION at least $(1 + (n-1)*abs(incx))$.
incx	INTEGER. Specifies the increment for the elements of x .
У	COMPLEX for cdotu DOUBLE COMPLEX for zdotu
	Array, DIMENSION at least $(1 + (n-1)*abs(incy))$.
incy	INTEGER. Specifies the increment for the elements of <i>y</i> .
Output Parameters	
res	COMPLEX for cdotu

DOUBLE COMPLEX for zdotu	
Contains the result of the dot product of x and y , if n positive. Otherwise, <i>res</i> contains 0.	is

?nrm2

Computes the Euclidean norm of a vector.

res = snrm2 (n, x, incx)
res = dnrm2 (n, x, incx)
res = scnrm2 (n, x, incx)
res = dznrm2 (n, x, incx)

Discussion

The ?nrm2 functions perform a vector reduction operation defined as

res = ||x||

where:

x is a vector

res is a value containing the Euclidean norm of the elements of **x**.

Input Parameters	
n	INTEGER . Specifies the order of vector x .
x	REAL for snrm2
	DOUBLE PRECISION for dnrm2
	COMPLEX for scnrm2
	DOUBLE COMPLEX for dznrm2
	Array, DIMENSION at least $(1 + (n-1)*abs(incx))$.
incx	INTEGER. Specifies the increment for the elements of \mathbf{x} .
Output Parame	ters
res	REAL for snrm2
	DOUBLE PRECISION for dnrm2
	REAL for scnrm2
	DOUBLE PRECISION for dznrm2

Contains the Euclidean norm of the vector **x**.

?rot

Performs rotation of points in the plane.

call srot (n, x, incx, y, incy, c, s)
call drot (n, x, incx, y, incy, c, s)
call csrot (n, x, incx, y, incy, c, s)
call zdrot (n, x, incx, y, incy, c, s)

Discussion

Given two complex vectors \mathbf{x} and \mathbf{y} , each vector element of these vectors is replaced as follows:

 $x(i) = c^*x(i) + s^*y(i)$ $y(i) = c^*y(i) - s^*x(i)$

Input Parameters

n	INTEGER. Specifies the order of vectors x and y .
x	REAL for srot DOUBLE PRECISION for drot COMPLEX for csrot DOUBLE COMPLEX for zdrot
	Array, DIMENSION at least $(1 + (n-1)*abs(incx))$.
incx	INTEGER. Specifies the increment for the elements of x .
У	REAL for srot DOUBLE PRECISION for drot COMPLEX for csrot DOUBLE COMPLEX for zdrot
	Array, DIMENSION at least $(1 + (n-1)*abs(incy))$.
incy	INTEGER. Specifies the increment for the elements of <i>y</i> .
С	REAL for srot DOUBLE PRECISION for drot REAL for csrot DOUBLE PRECISION for zdrot
	A scalar.
\$	REAL for srot DOUBLE PRECISION for drot REAL for csrot DOUBLE PRECISION for zdrot A scalar.
	A scalal.

Output Parameters

X	Each element is replaced by $c^*x + s^*y$.
Y	Each element is replaced by $c * y - s * x$.

?rotg

Computes the parameters for a Givens rotation.

call srotg (a, b, c, s)
call drotg (a, b, c, s)
call crotg (a, b, c, s)
call zrotg (a, b, c, s)

Discussion

Given the cartesian coordinates (a, b) of a point p, these routines return the parameters a, b, c, and s associated with the Givens rotation that zeros the y-coordinate of the point.

Input Parameters

a	REAL for srotg DOUBLE PRECISION for drotg
	COMPLEX for crotg
	DOUBLE COMPLEX for zrotg
	Provides the x-coordinate of the point p.
b	REAL for srotg
b	DOUBLE PRECISION for drotg
Ь	DOUBLE PRECISION for drotg COMPLEX for crotg
b	DOUBLE PRECISION for drotg

Output Parameters

a	Contains the parameter r associated with the Givens rotation.
b	Contains the parameter z associated with the Givens rotation.

 c
 REAL for srotg

 DOUBLE PRECISION for drotg

 REAL for crotg

 DOUBLE PRECISION for zrotg

 Contains the parameter c associated with the Givens rotation.

 s

 REAL for srotg

 DOUBLE PRECISION for drotg

 COMPLEX for crotg

 DOUBLE COMPLEX for zrotg

 Contains the parameter s associated with the Givens rotation.

?rotm

Performs rotation of points in the modified plane.

call srotm (n, x, incx, y, incy, param)
call drotm (n, x, incx, y, incy, param)

Discussion

Given two complex vectors x and y, each vector element of these vectors is replaced as follows:

 $x(i) = H^*x(i) + H^*y(i)$ $y(i) = H^*y(i) - H^*x(i)$

where:

H is a modified Givens transformation matrix whose values are stored in the *param(2)* through *param(5)* array. See discussion on the *param* argument.

Input Parameters

n	INTEGER. Specifies the order of vectors x and y .
x	REAL for srotm DOUBLE PRECISION for drotm
	Array, DIMENSION at least $(1 + (n-1)*abs(incx))$.
incx	INTEGER. Specifies the increment for the elements of \mathbf{x} .
У	REAL for srotm
	DOUBLE PRECISION for drotm
	Array, DIMENSION at least $(1 + (n-1)*abs(incy))$.
incy	INTEGER . Specifies the increment for the elements of <i>y</i> .
param	REAL for srotm
	DOUBLE PRECISION for drotm
	Array, DIMENSION 5.
	The elements of the <i>param</i> array are:
	<pre>param(1) contains a switch, flag.</pre>
	param(2-5) contain h11, h21, h12, and h22,
	respectively, the components of the array H.
	Depending on the values of $flag$, the components of H
	are set as follows:
	flag = -1.: H = h11 h12 h21 h22
	$flag = 0.: H = \begin{bmatrix} 1. & h12 \\ h21 & 1. \end{bmatrix}$
	$flag = 1.: H = \begin{bmatrix} h11 & 1. \\ -1. & h22 \end{bmatrix}$
	$flag = -2.: H = \begin{bmatrix} 1. & 0. \\ 0. & 1. \end{bmatrix}$

In the above cases, the matrix entries of 1., -1., and 0. are assumed based on the last three values of *flag* and are not actually loaded into the *param* vector.

x	Each element is replaced by $h11*x + h12*y$.
У	Each element is replaced by $h21*x + h22*y$.
Н	Givens transformation matrix updated.

?rotmg

Computes the modified parameters for a Givens rotation.

call srotmg (*d1*, *d2*, *x1*, *y1*, *param*) call drotmg (*d1*, *d2*, *x1*, *y1*, *param*)

Discussion

Given cartesian coordinates (x1, y1) of an input vector, these routines compute the components of a modified Givens transformation matrix *H* that zeros the *y*-component of the resulting vector:



d1	REAL for srotmg DOUBLE PRECISION for drotmg Provides the scaling factor for the <i>x</i> -coordinate of the input vector (sqrt(d1)x1).
d2	REAL for srotmg DOUBLE PRECISION for drotmg Provides the scaling factor for the <i>y</i> -coordinate of the input vector (sqrt(d2)y1).

x1	REAL for srotmg
	DOUBLE PRECISION for drotmg
	Provides the x-coordinate of the input vector.
y1	REAL for srotmg
	DOUBLE PRECISION for drotmg
	Provides the <i>y</i> -coordinate of the input vector.

param

REAL for srotmg DOUBLE PRECISION for drotmg Array, DIMENSION 5.

The elements of the *param* array are:

param(1) contains a switch, flag.

param(2-5) contain h11, h21, h12, and h22,

respectively, the components of the array *H*.

Depending on the values of *flag*, the components of *H* are set as follows:

 $flag = -1.: H = \begin{bmatrix} h11 & h12 \\ h21 & h22 \end{bmatrix}$ $flag = 0.: H = \begin{bmatrix} 1. & h12 \\ h21 & 1. \end{bmatrix}$ $flag = 1.: H = \begin{bmatrix} h11 & 1. \\ -1. & h22 \end{bmatrix}$ $flag = -2.: H = \begin{bmatrix} 1. & 0. \\ 0. & 1. \end{bmatrix}$

In the above cases, the matrix entries of 1., -1., and 0. are assumed based on the last three values of *flag* and are not actually loaded into the *param* vector.

?scal

Computes a vector by a scalar product.

```
call sscal ( n, a, x, incx )
call dscal ( n, a, x, incx )
call cscal ( n, a, x, incx )
call zscal ( n, a, x, incx )
call csscal ( n, a, x, incx )
call zdscal ( n, a, x, incx )
```

Discussion

The ?scal routines perform a vector-vector operation defined as

 $x = a^*x$

where:

a is a scalar, x is an *n*-element vector.

n	INTEGER . Specifies the order of vector x .
a	REAL for sscal and csscal DOUBLE PRECISION for dscal and zdscal COMPLEX for cscal DOUBLE COMPLEX for zscal
	Specifies the scalar a.
x	REAL for sscal DOUBLE PRECISION for dscal COMPLEX for cscal and csscal DOUBLE COMPLEX for zscal and csscal
	Array, DIMENSION at least $(1 + (n-1)*abs(incx))$.
incx	INTEGER . Specifies the increment for the elements of <i>x</i> .

x Overwritten by the updated vector **x**.

?swap

Swaps a vector with another vector.

call	sswap	(n,	х,	incx,	Y'	incy)
call	dswap	(n,	x,	incx,	Y'	incy)
call	cswap	(n,	x,	incx,	Y'	incy)
call	zswap	(n,	x,	incx,	Y'	incy)

Discussion

Given the two complex vectors x and y, the ?swap routines return vectors y and x swapped, each replacing the other.

n	INTEGER. Specifies the order of vectors x and y .
x	REAL for sswap DOUBLE PRECISION for dswap COMPLEX for cswap DOUBLE COMPLEX for zswap
	Array, DIMENSION at least (1 + (n-1)*abs(incx)).
incx	INTEGER. Specifies the increment for the elements of \mathbf{x} .
У	REAL for sswap DOUBLE PRECISION for dswap COMPLEX for cswap DOUBLE COMPLEX for zswap
	Array, DIMENSION at least $(1 + (n-1)*abs(incy))$.
incy	INTEGER. Specifies the increment for the elements of <i>y</i> .

x	Contains the resultant vector \mathbf{x} .
У	Contains the resultant vector <i>y</i> .

i?amax

Finds the element of a vector that has the largest absolute value.

```
index = isamax ( n, x, incx )
index = idamax ( n, x, incx )
index = icamax ( n, x, incx )
index = izamax ( n, x, incx )
```

Discussion

Given a vector \mathbf{x} , the i?amax functions return the position of the vector element $\mathbf{x}(i)$ that has the largest absolute value or, for complex flavors, the position of the element with the largest sum $|\operatorname{Re} \mathbf{x}(i)| + |\operatorname{Im} \mathbf{x}(i)|$.

If n is not positive, 0 is returned.

If more than one vector element is found with the same largest absolute value, the index of the first one encountered is returned.

n	INTEGER. Specifies the order of the vector \mathbf{x} .
x	REAL for isamax
	DOUBLE PRECISION for idamax
	COMPLEX for icamax
	DOUBLE COMPLEX for izamax
	Array, DIMENSION at least $(1+(n-1)*abs(incx))$.
incx	INTEGER. Specifies the increment for the elements of x .

index **INTEGER.** Contains the position of vector element **x** that has the largest absolute value.

i?amin

Finds the element of a vector that has the smallest absolute value.

```
index = isamin ( n, x, incx )
index = idamin ( n, x, incx )
index = icamin ( n, x, incx )
index = izamin ( n, x, incx )
```

Discussion

Given a vector \mathbf{x} , the i?amin functions return the position of the vector element $\mathbf{x}(i)$ that has the smallest absolute value or, for complex flavors, the position of the element with the smallest sum $|\operatorname{Rex}(i)| + |\operatorname{Imx}(i)|$.

If n is not positive, 0 is returned.

If more than one vector element is found with the same smallest absolute value, the index of the first one encountered is returned.

n	INTEGER. On entry, n specifies the order of the vector
	х.
x	REAL for isamin
	DOUBLE PRECISION for idamin
	COMPLEX for icamin
	DOUBLE COMPLEX for izamin
	Array, DIMENSION at least $(1+(n-1)*abs(incx))$.
incx	INTEGER. Specifies the increment for the elements of \mathbf{x} .

index

INTEGER. Contains the position of vector element \mathbf{x} that has the smallest absolute value.

BLAS Level 2 Routines

This section describes BLAS Level 2 routines, which perform matrix-vector operations. Table 2-2 lists the BLAS Level 2 routine groups and the data types associated with them.

Table 2-2 BLAS Level 2 Routine Groups and Their Data Types

Routine Groups	Data Types	Description
?gbmv	s, d, c, z	Matrix-vector product using a general band matrix
?gemv	s, d, c, z	Matrix-vector product using a general matrix
?ger	s, d	Rank-1 update of a general matrix
?gerc	C, Z	Rank-1 update of a conjugated general matrix
?geru	C, Z	Rank-1 update of a general matrix, unconjugated
?hbmv	C, Z	Matrix-vector product using a Hermitian band matrix
?hemv	C, Z	Matrix-vector product using a Hermitian matrix
?her	C, Z	Rank-1 update of a Hermitian matrix
?her2	C, Z	Rank-2 update of a Hermitian matrix
?hpmv	C, Z	Matrix-vector product using a Hermitian packed matrix
?hpr	C, Z	Rank-1 update of a Hermitian packed matrix
?hpr2	C, Z	Rank-2 update of a Hermitian packed matrix
?sbmv	s, d	Matrix-vector product using symmetric band matrix
?spmv	s, d	Matrix-vector product using a symmetric packed matrix
?spr	s, d	Rank-1 update of a symmetric packed matrix
?spr2	s, d	Rank-2 update of a symmetric packed matrix
?symv	s, d	Matrix-vector product using a symmetric matrix
?syr	s, d	Rank-1 update of a symmetric matrix
?syr2	s, d	Rank-2 update of a symmetric matrix

continued *

BEAU ECV		Cioups and men bata types (continued)
Routine Groups	Data Types	Description
?tbmv	s, d, c, z	Matrix-vector product using a triangular band matrix
?tbsv	s, d, c, z	Linear solution of a triangular band matrix
?tpmv	s, d, c, z	Matrix-vector product using a triangular packed matrix
?tpsv	s, d, c, z	Linear solution of a triangular packed matrix
?trmv	s, d, c, z	Matrix-vector product using a triangular matrix
?trsv	s, d, c, z	Linear solution of a triangular matrix

Table 2-2 BLAS Level 2 Routine Groups and Their Data Types (continued)

?gbmv

Computes a matrix-vector product using a general band matrix

Discussion

The ?gbmv routines perform a matrix-vector operation defined as

y := alpha*a*x + beta*y
or
y := alpha*a'*x + beta*y,
or
y := alpha*conjg(a')*x + beta*y,

where:

alpha and beta are scalars

x and **y** are vectors

a is an m by n band matrix, with k1 sub-diagonals and ku super-diagonals.

Input Parameters

transCHARACTER*1. Specifies the operation to be performed,
as follows:

trans value	Operation to be Performed
N or n	y:= alpha*a*x + beta*y
T or t	y:= alpha*a'*x + beta*y
C or c	y:= alpha*conjg(a')*x +beta*y
m	INTEGER. Specifies the number of rows of the matrix a . The value of m must be at least zero.
п	INTEGER. Specifies the number of columns of the matrix a . The value of n must be at least zero.
kl	INTEGER. Specifies the number of sub-diagonals of the matrix a . The value of kl must satisfy $0 \leq kl$.
ku	INTEGER. Specifies the number of super-diagonals of the matrix a . The value of ku must satisfy $0 \leq ku$.
alpha	REAL for sgbmv DOUBLE PRECISION for dgbmv COMPLEX for cgbmv DOUBLE COMPLEX for zgbmv
	Specifies the scalar alpha.
a	REAL for sgbmv DOUBLE PRECISION for dgbmv COMPLEX for cgbmv DOUBLE COMPLEX for zgbmv

Array, DIMENSION (1da, n). Before entry, the leading (kl + ku + 1) by *n* part of the array *a* must contain the matrix of coefficients. This matrix must be supplied column-by-column, with the leading diagonal of the matrix in row (ku + 1) of the array, the first super-diagonal starting at position 2 in row ku, the first sub-diagonal starting at position 1 in row (ku + 2), and so on. Elements in the array *a* that do not correspond to elements in the band matrix (such as the top left ku by ku triangle) are not referenced.

The following program segment transfers a band matrix from conventional full matrix storage to band storage:

```
do 20, j = 1, n
    k = ku + 1 - j
    do 10, i = max(1, j-ku), min(m, j+kl)
    a(k+i, j) = matrix(i,j)
    10 continue
    20 continue
```

INTEGER. Specifies the first dimension of *a* as declared in the calling (sub)program. The value of lda must be at least (kl + ku + 1).

REAL for sgbmv DOUBLE PRECISION for dgbmv COMPLEX for cgbmv DOUBLE COMPLEX for zgbmv

Array, DIMENSION at least (1 + (n - 1)*abs(incx))when trans = 'N' or 'n' and at least (1 + (m - 1)*abs(incx)) otherwise. Before entry, the incremented array x must contain the vector x.

INTEGER. Specifies the increment for the elements of *x*. *incx* must not be zero.

REAL for sgbmv DOUBLE PRECISION for dgbmv COMPLEX for cgbmv DOUBLE COMPLEX for zgbmv

lda

х

beta

incx

Specifies the scalar beta. When beta is supplied as zero, then y need not be set on input.

Y	REAL for sgbmv
	DOUBLE PRECISION for dgbmv
	COMPLEX for cgbmv
	DOUBLE COMPLEX for zgbmv
	Array, DIMENSION at least $(1 + (m - 1)*abs(incy))$ when <i>trans</i> = 'N' or 'n' and at least (1 + (n - 1)*abs(incy)) otherwise. Before entry, the
	incremented array y must contain the vector y.
incy	INTEGER . Specifies the increment for the elements of <i>y</i> .
	The value of <i>incy</i> must not be zero.
Output Para	notors

Output Parameters

y Overwritten by the updated vector *y*.

?gemv

Computes a matrix-vector product using a general matrix

call sgemv (trans, m, n, alpha, a, lda, x, incx, beta, y, incy) call dgemv (trans, m, n, alpha, a, lda, x, incx, beta, y, incy) call cgemv (trans, m, n, alpha, a, lda, x, incx, beta, y, incy) call zgemv (trans, m, n, alpha, a, lda, x, incx, beta, y, incy)

Discussion

The ?gemv routines perform a matrix-vector operation defined as

 $y := alpha^*a^*x + beta^*y$,

```
or
y := alpha*a'*x + beta*y,
or
y := alpha*conjg(a')*x + beta*y,
where:
alpha and beta are scalars
x and y are vectors
a is an m by n matrix.
```

trans	CHARACTER*1. Specifies the operation to be performed,
	as follows:

trans value	Operation to be Performed
N or n	y:= alpha*a*x + beta*y
T or t	y:= alpha*a'*x + beta*y
C or c	y:= alpha*conjg(a')*x +beta*y
m	INTEGER. Specifies the number of rows of the matrix a . <i>m</i> must be at least zero.
п	INTEGER. Specifies the number of columns of the matrix a . The value of n must be at least zero.
alpha	REAL for sgemv DOUBLE PRECISION for dgemv COMPLEX for cgemv DOUBLE COMPLEX for zgemv
	Specifies the scalar alpha.
a	REAL for sgemv DOUBLE PRECISION for dgemv COMPLEX for cgemv DOUBLE COMPLEX for zgemv

	Array, DIMENSION $(1da, n)$. Before entry, the leading <i>m</i> by <i>n</i> part of the array <i>a</i> must contain the matrix of coefficients.
lda	INTEGER. Specifies the first dimension of a as declared in the calling (sub)program. The value of <i>lda</i> must be at least max(1, m).
x	REAL for sgemv DOUBLE PRECISION for dgemv COMPLEX for cgemv DOUBLE COMPLEX for zgemv
	<pre>Array, DIMENSION at least (1+(n-1)*abs(incx)) when trans = 'N' or 'n' and at least (1+(m-1)*abs(incx)) otherwise. Before entry, the incremented array x must contain the vector x.</pre>
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
beta	REAL for sgemv DOUBLE PRECISION for dgemv COMPLEX for cgemv DOUBLE COMPLEX for zgemv
	Specifies the scalar $beta$. When $beta$ is supplied as zero, then y need not be set on input.
У	REAL for sgemv DOUBLE PRECISION for dgemv COMPLEX for cgemv DOUBLE COMPLEX for zgemv
	Array, DIMENSION at least $(1 + (m - 1)*abs(incy))$ when $trans = 'N'$ or 'n' and at least (1 + (n - 1)*abs(incy)) otherwise. Before entry with <i>beta</i> non-zero, the incremented array <i>y</i> must contain the vector <i>y</i> .
incy	INTEGER. Specifies the increment for the elements of <i>y</i> . The value of <i>incy</i> must not be zero.

y Overwritten by the updated vector *y*.

?ger

Performs a rank-1 update of a general matrix.

call sger (m, n, alpha, x, incx, y, incy, a, lda)
call dger (m, n, alpha, x, incx, y, incy, a, lda)

Discussion

The ?ger routines perform a matrix-vector operation defined as

a := alpha*x*y' + a,

where:

alpha is a scalar

x is an *m*-element vector

y is an *n*-element vector

a is an *m* by *n* matrix.

m	INTEGER. Specifies the number of rows of the matrix a . The value of m must be at least zero.
n	INTEGER. Specifies the number of columns of the matrix a . The value of n must be at least zero.
alpha	REAL for sger DOUBLE PRECISION for dger
	Specifies the scalar <i>alpha</i> .
x	REAL for sger DOUBLE PRECISION for dger

	Array, DIMENSION at least $(1 + (m - 1) * abs(incx))$. Before entry, the incremented array x must contain the <i>m</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
Y	REAL for sger DOUBLE PRECISION for dger
	Array, DIMENSION at least $(1 + (n - 1) * abs(incy))$. Before entry, the incremented array y must contain the <i>n</i> -element vector y.
incy	INTEGER. Specifies the increment for the elements of y . The value of <i>incy</i> must not be zero.
a	REAL for sger DOUBLE PRECISION for dger
	Array, DIMENSION $(1da, n)$. Before entry, the leading m by n part of the array a must contain the matrix of coefficients.
lda	INTEGER. Specifies the first dimension of a as declared in the calling (sub)program. The value of <i>lda</i> must be at least max(1, m).
Output Parameters	

а

Overwritten by the updated matrix.

?gerc

Performs a rank-1 update (conjugated) of a general matrix.

call cgerc (m, n, alpha, x, incx, y, incy, a, lda)
call zgerc (m, n, alpha, x, incx, y, incy, a, lda)

Discussion

The ?gerc routines perform a matrix-vector operation defined as

a := alpha*x*conjg(y') + a,

where:

alpha is a scalar

 \mathbf{x} is an *m*-element vector

y is an *n*-element vector

a is an m by n matrix.

m	INTEGER. Specifies the number of rows of the matrix a . The value of m must be at least zero.
n	INTEGER. Specifies the number of columns of the matrix \mathbf{a} . The value of n must be at least zero.
alpha	SINGLE PRECISION COMPLEX for cgerc DOUBLE PRECISION COMPLEX for zgerc
	Specifies the scalar <i>alpha</i> .
x	SINGLE PRECISION COMPLEX for cgerc DOUBLE PRECISION COMPLEX for zgerc
	Array, DIMENSION at least $(1 + (m - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>m</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
У	COMPLEX for cgerc DOUBLE COMPLEX for zgerc
	Array, DIMENSION at least $(1 + (n - 1)*abs(incy))$. Before entry, the incremented array y must contain the <i>n</i> -element vector y .
incy	INTEGER . Specifies the increment for the elements of <i>y</i> . The value of <i>incy</i> must not be zero.

a	COMPLEX for cgerc DOUBLE COMPLEX for zgerc
	Array, DIMENSION $(1da, n)$. Before entry, the leading <i>m</i> by <i>n</i> part of the array <i>a</i> must contain the matrix of coefficients.
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. The value of $1da$ must be at least max(1, m).
Output Parame	eters

а

Overwritten by the updated matrix.

?geru

Performs a rank-1 update (unconjugated) of a general matrix.

call cgeru (m, n, alpha, x, incx, y, incy, a, lda)
call zgeru (m, n, alpha, x, incx, y, incy, a, lda)

Discussion

The ?geru routines perform a matrix-vector operation defined as

a:= alpha*x*y' + a,

where:

alpha is a scalar

x is an *m*-element vector

y is an *n*-element vector

a is an m by n matrix.

Input Parameters

m	INTEGER. Specifies the number of rows of the matrix a . The value of m must be at least zero.
п	INTEGER. Specifies the number of columns of the matrix a . The value of n must be at least zero.
alpha	COMPLEX for cgeru DOUBLE COMPLEX for zgeru
	Specifies the scalar <i>alpha</i> .
x	COMPLEX for cgeru DOUBLE COMPLEX for zgeru
	Array, DIMENSION at least $(1 + (m - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>m</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
У	COMPLEX for cgeru DOUBLE COMPLEX for zgeru
	Array, DIMENSION at least $(1 + (n - 1)*abs(incy))$. Before entry, the incremented array y must contain the <i>n</i> -element vector y .
incy	INTEGER. Specifies the increment for the elements of <i>y</i> . The value of <i>incy</i> must not be zero.
a	COMPLEX for cgeru DOUBLE COMPLEX for zgeru
	Array, DIMENSION (<i>lda</i> , <i>n</i>). Before entry, the leading <i>m</i> by <i>n</i> part of the array <i>a</i> must contain the matrix of coefficients.
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. The value of $1da$ must be at least max(1, m).

Output Parameters

а	Overwritten by the updated matrix.
---	------------------------------------

?hbmv

Computes a matrix-vector product using a Hermitian band matrix.

call chbmv (uplo, n, k, alpha, a, lda, x, incx, beta, y, incy) call zhbmv (uplo, n, k, alpha, a, lda, x, incx, beta, y, incy)

Discussion

The ?hbmv routines perform a matrix-vector operation defined as

 $y := alpha^*a^*x + beta^*y$,

where:

alpha and beta are scalars

x and y are *n*-element vectors

a is an n by n Hermitian band matrix, with k super-diagonals.

Input Parameters

uplo CHARACTER*1. Specifies whether the upper or lower triangular part of the band matrix *a* is being supplied, as follows:

uplo value	Part of Matrix a Supplied
U or u	The upper triangular part of matrix a is being supplied.
L or l	The lower triangular part of matrix a is being supplied.
п	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.
k	INTEGER. Specifies the number of super-diagonals of the matrix a . The value of k must satisfy $0 \leq k$.

alpha
 COMPLEX for chbmv
 DOUBLE COMPLEX for zhbmv
 Specifies the scalar alpha.
 a
 COMPLEX for chbmv
 DOUBLE COMPLEX for zhbmv
 Array, DIMENSION (lda, n). Before entry with uplo = 'U' or 'u', the leading (k + 1) by n part of the array a must contain the upper triangular band part of the Hermitian matrix. The matrix must be supplied

column-by-column, with the leading diagonal of the matrix in row (k + 1) of the array, the first super-diagonal starting at position 2 in row k, and so on. The top left k by k triangle of the array a is not referenced.

The following program segment transfers the upper triangular part of a Hermitian band matrix from conventional full matrix storage to band storage:

```
do 20, j = 1, n
m = k + 1 - j
do 10, i = max(1, j - k), j
a(m + i, j) = matrix(i, j)
10 continue
20 continue
```

Before entry with uplo = 'L' or 'l', the leading (k + 1) by *n* part of the array *a* must contain the lower triangular band part of the Hermitian matrix, supplied column-by-column, with the leading diagonal of the matrix in row 1 of the array, the first sub-diagonal starting at position 1 in row 2, and so on. The bottom right *k* by *k* triangle of the array *a* is not referenced.

The following program segment transfers the lower triangular part of a Hermitian band matrix from conventional full matrix storage to band storage:

do 20, j = 1, n
 m = 1 - j
 do 10, i = j, min(n, j + k)

	a(m + i, j) = matrix(i, j) 10 continue 20 continue
	The imaginary parts of the diagonal elements need not be set and are assumed to be zero.
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. The value of $1da$ must be at least $(k + 1)$.
X	COMPLEX for chbmv DOUBLE COMPLEX for zhbmv
	Array, DIMENSION at least $(1 + (n - 1) * abs(incx))$. Before entry, the incremented array x must contain the vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
beta	COMPLEX for chbmv DOUBLE COMPLEX for zhbmv
	Specifies the scalar beta.
У	COMPLEX for chbmv DOUBLE COMPLEX for zhbmv
	Array, DIMENSION at least $(1 + (n - 1) * abs(incy))$. Before entry, the incremented array y must contain the vector y.
incy	INTEGER. Specifies the increment for the elements of y . The value of <i>incy</i> must not be zero.

y Overwritten by the updated vector *y*.

?hemv

Computes a matrix-vector product using a Hermitian matrix.

call chemv (uplo, n, alpha, a, lda, x, incx, beta, y, incy) call zhemv (uplo, n, alpha, a, lda, x, incx, beta, y, incy)

Discussion

The ?hemv routines perform a matrix-vector operation defined as

y := alpha*a*x + beta*y,

where:

uplo

alpha and beta are scalars

x and y are *n*-element vectors

a is an *n* by *n* Hermitian matrix.

Input Parameters

CHARACTER*1. Specifies whether the upper or lower triangular part of the array *a* is to be referenced, as follows:

uplo value	Part of Array a To Be Referenced
U or u	The upper triangular part of array a is to be referenced.
L or l	The lower triangular part of array <mark>a</mark> is to be referenced.
n	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.

alpha	COMPLEX for chemv DOUBLE COMPLEX for zhemv
	Specifies the scalar <i>alpha</i> .
a	COMPLEX for chemv DOUBLE COMPLEX for zhemv
	Array, DIMENSION (lda, n) . Before entry with uplo = 'U' or 'u', the leading <i>n</i> by <i>n</i> upper triangular part of the array <i>a</i> must contain the upper triangular part of the Hermitian matrix and the strictly lower triangular part of <i>a</i> is not referenced. Before entry with uplo = 'L' or '1', the leading <i>n</i> by <i>n</i> lower triangular part of the array <i>a</i> must contain the lower triangular part of the Hermitian matrix and the strictly upper triangular part of <i>a</i> is not referenced.
	The imaginary parts of the diagonal elements need not be set and are assumed to be zero.
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. The value of $1 da$ must be at least max(1, n).
x	COMPLEX for chemv DOUBLE COMPLEX for zhemv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
beta	COMPLEX for chemv DOUBLE COMPLEX for zhemv
	Specifies the scalar $beta$. When $beta$ is supplied as zero then y need not be set on input.

У	COMPLEX for chemv DOUBLE COMPLEX for zhemv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incy))$. Before entry, the incremented array y must contain the <i>n</i> -element vector y.
incy	INTEGER. Specifies the increment for the elements of <i>y</i> . The value of <i>incy</i> must not be zero.

Overwritten by the updated vector \mathbf{y} .

?her

Performs a rank-1 update of a Hermitian matrix.

 \boldsymbol{Y}

call cher (uplo, n, alpha, x, incx, a, lda)
call zher (uplo, n, alpha, x, incx, a, lda)

Discussion

The ?her routines perform a matrix-vector operation defined as

a := alpha*x*conjg(x') + a,
where:
alpha is a real scalar
x is an n-element vector
a is an n by n Hermitian matrix.

Input Parameters	
uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the array a is to be referenced, as follows:
uplo value	Part of Array a To Be Referenced
U or u	The upper triangular part of array a is to be referenced.
L or l	The lower triangular part of array <i>a</i> is to be referenced.
n	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.
alpha	REAL for cher DOUBLE PRECISION for zher
	Specifies the scalar alpha.
x	COMPLEX for cher DOUBLE COMPLEX for zher
	Array, dimension at least $(1 + (n - 1) * abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
a	COMPLEX for cher DOUBLE COMPLEX for zher
	Array, DIMENSION $(1da, n)$. Before entry with $uplo = 'U'$ or 'u', the leading <i>n</i> by <i>n</i> upper triangular part of the array <i>a</i> must contain the upper triangular part of the Hermitian matrix and the strictly lower triangular part of <i>a</i> is not referenced.
	Before entry with $uplo = 'L'$ or 'l', the leading <i>n</i> by <i>n</i> lower triangular part of the array <i>a</i> must contain the lower triangular part of the Hermitian matrix and the strictly upper triangular part of <i>a</i> is not referenced.

The imaginary parts of the diagonal elements need not be set and are assumed to be zero.

INTEGER. Specifies the first dimension of a as declared in the calling (sub)program. The value of 1da must be at least max(1, n).

Output Parameters

а

lda

With uplo = 'U' or 'u', the upper triangular part of the array **a** is overwritten by the upper triangular part of the updated matrix.

With uplo = 'L' or 'l', the lower triangular part of the array **a** is overwritten by the lower triangular part of the updated matrix.

The imaginary parts of the diagonal elements are set to zero.

?her2

Performs a rank-2 update of a Hermitian matrix.

call cher2 (uplo, n, alpha, x, incx, y, incy, a, lda)
call zher2 (uplo, n, alpha, x, incx, y, incy, a, lda)

Discussion

The ?her2 routines perform a matrix-vector operation defined as

a := alpha*x*conjg(y') + conjg(alpha)*y*conjg(x') + a,
where:

alpha is a scalar

- x and y are *n*-element vectors
- a is an *n* by *n* Hermitian matrix.

Input Parameters		
uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the array <i>a</i> is to be referenced, as follows:	
uplo value	Part of Array a To Be Referenced	
U or u	The upper triangular part of array a is to be referenced.	
L or l	The lower triangular part of array <u>a</u> is to be referenced.	
n	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.	
alpha	COMPLEX for cher2	
	DOUBLE COMPLEX for zher2	
	Specifies the scalar <i>alpha</i> .	
x	COMPLEX for cher2 DOUBLE COMPLEX for zher2	
	Array, DIMENSION at least $(1 + (n - 1) * abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.	
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.	
У	COMPLEX for cher2 DOUBLE COMPLEX for zher2	
	Array, DIMENSION at least $(1 + (n - 1)*abs(incy))$. Before entry, the incremented array y must contain the <i>n</i> -element vector y.	
incy	INTEGER. Specifies the increment for the elements of <i>y</i> . The value of <i>incy</i> must not be zero.	
a	COMPLEX for cher2 DOUBLE COMPLEX for zher2	

Array, DIMENSION (lda, n). Before entry with uplo = 'U' or 'u', the leading *n* by *n* upper triangular part of the array *a* must contain the upper triangular part of the Hermitian matrix and the strictly lower triangular part of *a* is not referenced.

Before entry with uplo = 'L' or 'l', the leading *n* by *n* lower triangular part of the array *a* must contain the lower triangular part of the Hermitian matrix and the strictly upper triangular part of *a* is not referenced.

The imaginary parts of the diagonal elements need not be set and are assumed to be zero.

INTEGER. Specifies the first dimension of a as declared in the calling (sub)program. The value of 1da must be at least max(1, n).

Output Parameters

а

lda

With uplo = 'U' or 'u', the upper triangular part of the array *a* is overwritten by the upper triangular part of the updated matrix.

With uplo = 'L' or 'l', the lower triangular part of the array **a** is overwritten by the lower triangular part of the updated matrix.

The imaginary parts of the diagonal elements are set to zero.

?hpmv

Computes a matrix-vector product using a Hermitian packed matrix.

call chpmv (uplo, n, alpha, ap, x, incx, beta, y, incy) call zhpmv (uplo, n, alpha, ap, x, incx, beta, y, incy)

Discussion

The ?hpmv routines perform a matrix-vector operation defined as

 $y := alpha^*a^*x + beta^*y$,

where:

alpha and beta are scalars

x and y are *n*-element vectors

a is an n by n Hermitian matrix, supplied in packed form.

Input Parameters

uplo CHARACTER*1. Specifies whether the upper or lower triangular part of the matrix *a* is supplied in the packed array *ap*, as follows:

uplo value	Part of Matrix a Supplied
U or u	The upper triangular part of matrix a is supplied in
	ap.
L or l	The lower triangular part of matrix a is supplied in
	ap.
п	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.
alpha	COMPLEX for chpmv
	DOUBLE COMPLEX for zhpmv
	Specifies the scalar <i>alpha</i> .
ap	COMPLEX for chpmv
	DOUBLE COMPLEX for zhpmv
	Array, DIMENSION at least $((n*(n+1))/2)$. Before entry with $uplo = 'U'$ or 'u', the array ap must contain the upper triangular part of the Hermitian matrix packed sequentially, column-by-column, so that $ap(1)$ contains $a(1, 1), ap(2)$ and $ap(3)$ contain $a(1, 2)$ and $a(2, 2)$ respectively, and so on. Before entry with uplo = 'L' or 'l', the array ap must contain the lower triangular part of the Hermitian matrix packed

	sequentially, column-by-column, so that $ap(1)$ contains $a(1, 1)$, $ap(2)$ and $ap(3)$ contain $a(2, 1)$ and $a(3, 1)$ respectively, and so on.
	The imaginary parts of the diagonal elements need not be set and are assumed to be zero.
x	COMPLEX for chpmv DOUBLE PRECISION COMPLEX for zhpmv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
beta	COMPLEX for chpmv DOUBLE COMPLEX for zhpmv
	Specifies the scalar <i>beta</i> . When <i>beta</i> is supplied as zero then <i>y</i> need not be set on input.
У	COMPLEX for chpmv DOUBLE COMPLEX for zhpmv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incy))$. Before entry, the incremented array y must contain the <i>n</i> -element vector y.
incy	INTEGER. Specifies the increment for the elements of <i>y</i> . The value of <i>incy</i> must not be zero.

Y	Overwritten by the updated vector y
---	--------------------------------------------

?hpr

Performs a rank-1 update of a Hermitian packed matrix.

call chpr (uplo, n, alpha, x, incx, ap)
call zhpr (uplo, n, alpha, x, incx, ap)

Discussion

The?hpr routines perform a matrix-vector operation defined as

a := alpha*x*conjg(x') + a,

where:

alpha is a real scalar

x is an *n*-element vector

a is an n by n Hermitian matrix, supplied in packed form.

Input Parameters

```
uplo CHARACTER*1. Specifies whether the upper or lower
triangular part of the matrix a is supplied in the packed
array ap, as follows:
```

uplo value	Part of Matrix a Supplied
U or u	The upper triangular part of matrix a is supplied in a <i>p</i> .
L or l	The lower triangular part of matrix <mark>a</mark> is supplied in ap.
п	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.
alpha	REAL for chpr DOUBLE PRECISION for zhpr
	Specifies the scalar alpha.

x	COMPLEX for chpr DOUBLE COMPLEX for zhpr
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . <i>incx</i> must not be zero.
ap	COMPLEX for chpr DOUBLE COMPLEX for zhpr
	Array, DIMENSION at least $((n*(n+1))/2)$. Before entry with $uplo = 'U'$ or 'u', the array ap must contain the upper triangular part of the Hermitian matrix packed sequentially, column-by-column, so that $ap(1)$ contains $a(1, 1)$, $ap(2)$ and $ap(3)$ contain $a(1, 2)$ and $a(2, 2)$ respectively, and so on.
	Before entry with $uplo = 'L'$ or 'l', the array ap must contain the lower triangular part of the Hermitian matrix packed sequentially, column-by-column, so that $ap(1)$ contains $a(1, 1), ap(2)$ and $ap(3)$ contain $a(2, 1)$ and $a(3, 1)$ respectively, and so on.
	The imaginary parts of the diagonal elements need not be set and are assumed to be zero.
Output Paramo	eters
ар	With $uplo = 'U'$ or 'u', overwritten by the upper triangular part of the updated matrix.

With *uplo* = 'L' or 'l', overwritten by the lower triangular part of the updated matrix.

The imaginary parts of the diagonal elements are set to zero.

?hpr2

Performs a rank-2 update of a Hermitian packed matrix.

call chpr2 (uplo, n, alpha, x, incx, y, incy, ap)
call zhpr2 (uplo, n, alpha, x, incx, y, incy, ap)

Discussion

The?hpr2 routines perform a matrix-vector operation defined as

a := alpha*x*conjg(y') + conjg(alpha)*y*conjg(x') + a,

where:

alpha is a scalar

x and y are *n*-element vectors

a is an n by n Hermitian matrix, supplied in packed form.

Input Parameters

```
uplo CHARACTER*1. Specifies whether the upper or lower
triangular part of the matrix a is supplied in the packed
array ap, as follows
```

uplo value	Part of Matrix a Supplied				
U or u	The upper triangular part of matrix a is supplied in app.				
L or l	The lower triangular part of matrix a is supplied in app.				
n	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.				
alpha	COMPLEX for chpr2 DOUBLE COMPLEX for zhpr2				
	Specifies the scalar alpha.				

x	COMPLEX for chpr2 DOUBLE COMPLEX for zhpr2
	Array, dimension at least $(1 + (n - 1) * abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
У	COMPLEX for chpr2 DOUBLE COMPLEX for zhpr2
	Array, DIMENSION at least $(1 + (n - 1)*abs(incy))$. Before entry, the incremented array y must contain the <i>n</i> -element vector y.
incy	INTEGER. Specifies the increment for the elements of <i>y</i> . The value of <i>incy</i> must not be zero.
ap	COMPLEX for chpr2 DOUBLE COMPLEX for zhpr2
	Array, DIMENSION at least $((n*(n+1))/2)$. Before entry with $uplo = 'U'$ or 'u', the array ap must contain the upper triangular part of the Hermitian matrix packed sequentially, column-by-column, so that $ap(1)$ contains $a(1, 1), ap(2)$ and $ap(3)$ contain $a(1, 2)$ and $a(2, 2)$ respectively, and so on.
	Before entry with $uplo = 'L'$ or 'l', the array ap must contain the lower triangular part of the Hermitian matrix packed sequentially, column-by-column, so that $ap(1)$ contains $a(1, 1), ap(2)$ and $ap(3)$ contain $a(2, 1)$ and $a(3, 1)$ respectively, and so on.
	The imaginary parts of the diagonal elements need not be set and are assumed to be zero.

ap With uplo = 'U' or 'u', overwritten by the upper triangular part of the updated matrix.

With *uplo* = 'L' or 'l', overwritten by the lower triangular part of the updated matrix.

The imaginary parts of the diagonal elements need are set to zero.

?sbmv

Computes a matrix-vector product using a symmetric band matrix.

call ssbmv (uplo, n, k, alpha, a, lda, x, incx, beta, y, incy) call dsbmv (uplo, n, k, alpha, a, lda, x, incx, beta, y, incy)

Discussion

The ?sbmv routines perform a matrix-vector operation defined as

 $y := alpha^*a^*x + beta^*y$,

where:

alpha and beta are scalars

x and y are *n*-element vectors

a is an *n* by *n* symmetric band matrix, with *k* super-diagonals.

Input Parameters

uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the band matrix <i>a</i> is being supplied, as follows:
uplo value	Part of Matrix a Supplied
U or u	The upper triangular part of matrix <i>a</i> is supplied.
L or l	The lower triangular part of matrix a is supplied.
п	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.
k	INTEGER. Specifies the number of super-diagonals of the matrix a . The value of k must satisfy $0 \leq k$.
alpha	REAL for ssbmv DOUBLE PRECISION for dsbmv
	Specifies the scalar <i>alpha</i> .
а	REAL for ssbmv
	DOUBLE PRECISION for dsbmv
	Array, DIMENSION $(1da, n)$. Before entry with uplo = 'U' or 'u', the leading $(k + 1)$ by n part of the array a must contain the upper triangular band part of the symmetric matrix, supplied column-by-column, with the leading diagonal of the matrix in row $(k + 1)$ of the array, the first super-diagonal starting at position 2 in row k , and so on. The top left k by k triangle of the array a is not referenced.
	The following program segment transfers the upper triangular part of a symmetric band matrix from conventional full matrix storage to band storage: do 20, $j = 1$, n

do 20, j = 1, n
m = k + 1 - j
do 10, i = max(1, j - k), j
a(m + i, j) = matrix(i, j)
10 continue
20 continue

Before entry with uplo = 'L' or 'l', the leading (k + 1) by *n* part of the array *a* must contain the lower triangular band part of the symmetric matrix, supplied column-by-column, with the leading diagonal of the matrix in row 1 of the array, the first sub-diagonal starting at position 1 in row 2, and so on. The bottom right *k* by *k* triangle of the array *a* is not referenced.

The following program segment transfers the lower triangular part of a symmetric band matrix from conventional full matrix storage to band storage:

```
do 20, j = 1, n
                   m = 1 - j
                   do 10, i = j, min(n, j + k)
                     a( m + i, j ) = matrix( i, j )
                   10 continue
                  20 continue
lda
                  INTEGER. Specifies the first dimension of a as declared
                  in the calling (sub)program. The value of 1da must be at
                  least (k + 1).
                  REAL for ssbmv
\boldsymbol{X}
                  DOUBLE PRECISION for dsbmv
                  Array, DIMENSION at least (1 + (n - 1) * abs(incx)).
                  Before entry, the incremented array \mathbf{x} must contain the
                  vector x.
                  INTEGER. Specifies the increment for the elements of x.
incx
                  The value of incx must not be zero.
                  REAL for ssbmv
beta
                  DOUBLE PRECISION for dsbmv
                  Specifies the scalar beta.
                  REAL for ssbmv
\boldsymbol{Y}
                  DOUBLE PRECISION for dsbmv
                  Array, DIMENSION at least (1 + (n - 1) * abs(incy)).
                  Before entry, the incremented array y must contain the
                  vector y.
```

incy

INTEGER. Specifies the increment for the elements of *y*. The value of *incy* must not be zero.

Output Parameters

y Overwritten by the updated vector *y*.

?spmv

Computes a matrix-vector product using a symmetric packed matrix.

call sspmv (uplo, n, alpha, ap, x, incx, beta, y, incy)
call dspmv (uplo, n, alpha, ap, x, incx, beta, y, incy)

Discussion

The ?spmv routines perform a matrix-vector operation defined as

 $y := alpha^*a^*x + beta^*y$,

where:

alpha and beta are scalars

x and y are *n*-element vectors

a is an n by n symmetric matrix, supplied in packed form.

Input Parameters

uploCHARACTER*1. Specifies whether the upper or lower
triangular part of the matrix a is supplied in the packed
array ap, as follows:

uplo value	Part of Matrix a Supplied
U or u	The upper triangular part of matrix a is supplied in a p.
L or l	The lower triangular part of matrix <u>a</u> is supplied in <u>ap</u> .

n	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.
alpha	REAL for sspmv DOUBLE PRECISION for dspmv
	Specifies the scalar alpha.
ap	REAL for sspmv DOUBLE PRECISION for dspmv
	Array, DIMENSION at least $((n*(n + 1))/2)$. Before entry with $uplo = 'U'$ or 'u', the array ap must contain the upper triangular part of the symmetric matrix packed sequentially, column-by-column, so that ap(1) contains $a(1, 1)$, $ap(2)$ and $ap(3)$ contain a(1, 2) and $a(2, 2)$ respectively, and so on. Before entry with $uplo = 'L'$ or '1', the array ap must contain the lower triangular part of the symmetric matrix packed sequentially, column-by-column, so that $ap(1)$ contains $a(1, 1)$, $ap(2)$ and $ap(3)$ contain $a(2, 1)$ and $a(3, 1)$ respectively, and so on.
x	REAL for sspmv DOUBLE PRECISION for dspmv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
beta	REAL for sspmv DOUBLE PRECISION for dspmv
	Specifies the scalar $beta$. When $beta$ is supplied as zero, then y need not be set on input.
У	REAL for sspmv DOUBLE PRECISION for dspmv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incy))$. Before entry, the incremented array y must contain the <i>n</i> -element vector y.

incy **INTEGER.** Specifies the increment for the elements of *y*. The value of *incy* must not be zero.

Output Parameters

y Overwritten by the updated vector *y*.

?spr

Performs a rank-1 update of a symmetric packed matrix.

```
call sspr( uplo, n, alpha, x, incx, ap )
call dspr( uplo, n, alpha, x, incx, ap )
```

Discussion

The ?spr routines perform a matrix-vector operation defined as

a:= alpha*x*x' + a,

where:

alpha is a real scalar

- x is an *n*-element vector
- a is an n by n symmetric matrix, supplied in packed form.

Input Parameters

uploCHARACTER*1. Specifies whether the upper or lower
triangular part of the matrix a is supplied in the packed
array ap, as follows:

uplo value	Part of Matrix a Supplied
U or u	The upper triangular part of matrix a is supplied in app.
L or l	The lower triangular part of matrix a is supplied in <i>ap</i> .

n	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.			
alpha	REAL for sspr DOUBLE PRECISION for dspr			
	Specifies the scalar <i>alpha</i> .			
x	REAL for sspr DOUBLE PRECISION for dspr			
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.			
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.			
ap	REAL for sspr DOUBLE PRECISION for dspr			
	Array, DIMENSION at least $((n*(n+1))/2)$. Before entry with $uplo = 'U'$ or 'u', the array ap must contain the upper triangular part of the symmetric matrix packed sequentially, column-by-column, so that ap(1) contains $a(1,1)$, $ap(2)$ and $ap(3)$ contain a(1, 2) and $a(2, 2)$ respectively, and so on.			
	Before entry with $uplo = 'L'$ or 'l', the array ap must contain the lower triangular part of the symmetric matrix packed sequentially, column-by-column, so that $ap(1)$ contains $a(1,1), ap(2)$ and $ap(3)$ contain $a(2,1)$ and $a(3,1)$ respectively, and so on.			
Output Parameters				

ap With uplo = 'U' or 'u', overwritten by the upper triangular part of the updated matrix. With uplo = 'L' or 'l', overwritten by the lower triangular part of the updated matrix.

?spr2

Performs a rank-2 update of a symmetric packed matrix.

call sspr2(uplo, n, alpha, x, incx, y, incy, ap)
call dspr2(uplo, n, alpha, x, incx, y, incy, ap)

Discussion

The ?spr2 routines perform a matrix-vector operation defined as

a:= alpha*x*y' + alpha*y*x' + a,

where:

alpha is a scalar

x and y are *n*-element vectors

a is an *n* by *n* symmetric matrix, supplied in packed form.

Input Parameters

uplo CHARACTER*1. Specifies whether the upper or lower triangular part of the matrix *a* is supplied in the packed array *ap*, as follows:

uplo value	Part of Matrix a Supplied
U or u	The upper triangular part of matrix a is supplied in app.
L or l	The lower triangular part of matrix <u>a</u> is supplied in <u>ap</u> .
n	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.
alpha	REAL for sspr2 DOUBLE PRECISION for dspr2
	Specifies the scalar <i>alpha</i> .

x	REAL for sspr2 DOUBLE PRECISION for dspr2
	Array, DIMENSION at least $(1 + (n - 1) * abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
У	REAL for sspr2 DOUBLE PRECISION for dspr2
	Array, DIMENSION at least $(1 + (n - 1)*abs(incy))$. Before entry, the incremented array y must contain the <i>n</i> -element vector y.
incy	INTEGER. Specifies the increment for the elements of <i>y</i> . The value of <i>incy</i> must not be zero.
ар	REAL for sspr2 DOUBLE PRECISION for dspr2
	Array, DIMENSION at least $((n*(n+1))/2)$. Before entry with $uplo = 'U'$ or 'u', the array ap must contain the upper triangular part of the symmetric matrix packed sequentially, column-by-column, so that ap(1) contains $a(1,1)$, $ap(2)$ and $ap(3)$ contain a(1,2) and $a(2,2)$ respectively, and so on.
	Before entry with $uplo = 'L'$ or 'l', the array ap must contain the lower triangular part of the symmetric matrix packed sequentially, column-by-column, so that $ap(1)$ contains $a(1,1)$, $ap(2)$ and $ap(3)$ contain $a(2,1)$ and $a(3,1)$ respectively, and so on.
Output Parame	ters
ap	With <i>uplo</i> = 'U' or 'u', overwritten by the upper

triangular part of the updated matrix.

With *uplo* = 'L' or 'l', overwritten by the lower triangular part of the updated matrix.

?symv

Computes a matrix-vector product for a symmetric matrix.

call ssymv (uplo, n, alpha, a, lda, x, incx, beta, y, incy) call dsymv (uplo, n, alpha, a, lda, x, incx, beta, y, incy)

Discussion

The ?symv routines perform a matrix-vector operation defined as

```
y := alpha^*a^*x + beta^*y,
```

where:

alpha and beta are scalars

x and y are *n*-element vectors

a is an *n* by *n* symmetric matrix.

Input Parameters

uplo CHARACTER*1. Specifies whether the upper or lower triangular part of the array *a* is to be referenced, as follows:

uplo value	Part of Array a To Be Referenced
U or u	The upper triangular part of array a is to be referenced.
L or l	The lower triangular part of array a is to be referenced.
n	INTEGER. Specifies the order of the matrix <i>a</i> . The value

of *n* must be at least zero.

alpha	REAL for ssymv DOUBLE PRECISION for dsymv
	Specifies the scalar <i>alpha</i> .
a	REAL for ssymv DOUBLE PRECISION for dsymv
	Array, DIMENSION (lda, n) . Before entry with uplo = 'U' or 'u', the leading <i>n</i> by <i>n</i> upper triangular part of the array <i>a</i> must contain the upper triangular part of the symmetric matrix and the strictly lower triangular part of <i>a</i> is not referenced. Before entry with uplo = 'L' or 'l', the leading <i>n</i> by <i>n</i> lower triangular part of the array <i>a</i> must contain the lower triangular part of the symmetric matrix and the strictly upper triangular part of <i>a</i> is not referenced.
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. The value of $1da$ must be at least max(1, n).
x	REAL for ssymv DOUBLE PRECISION for dsymv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
beta	REAL for ssymv DOUBLE PRECISION for dsymv
	Specifies the scalar $beta$. When $beta$ is supplied as zero, then y need not be set on input.
У	REAL for ssymv DOUBLE PRECISION for dsymv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incy))$. Before entry, the incremented array y must contain the <i>n</i> -element vector y.

incy **INTEGER.** Specifies the increment for the elements of *y*. The value of *incy* must not be zero.

Output Parameters

y Overwritten by the updated vector *y*.

?syr

Performs a rank-1 update of a symmetric matrix.

call	ssyr(uplo,	n,	alpha,	x,	incx,	a,	lda)
call	dsyr(uplo,	n,	alpha,	х,	incx,	a,	lda)

Discussion

The ?syr routines perform a matrix-vector operation defined as

 $a := alpha^*x^*x' + a$,

where:

alpha is a real scalar

- x is an *n*-element vector
- a is an *n* by *n* symmetric matrix.

Input Parameters

uplo CHARACTER*1. Specifies whether the upper or lower triangular part of the array **a** is to be referenced, as follows:

uplo value	Part of Array a To Be Referenced The upper triangular part of array a is to be referenced.				
U or u					
L or l	The lower triangular part of array a is to be referenced.				

п	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.			
alpha	REAL for ssyr DOUBLE PRECISION for dsyr			
	Specifies the scalar <i>alpha</i> .			
x	REAL for ssyr DOUBLE PRECISION for dsyr			
	Array, DIMENSION at least $(1 + (n - 1) * abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.			
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.			
a	REAL for ssyr DOUBLE PRECISION for dsyr			
	Array, DIMENSION (lda, n) . Before entry with $uplo = 'U'$ or 'u', the leading <i>n</i> by <i>n</i> upper triangular part of the array <i>a</i> must contain the upper triangular part of the symmetric matrix and the strictly lower triangular part of <i>a</i> is not referenced.			
	Before entry with $uplo = 'L'$ or 'l', the leading <i>n</i> by <i>n</i> lower triangular part of the array <i>a</i> must contain the lower triangular part of the symmetric matrix and the strictly upper triangular part of <i>a</i> is not referenced.			
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. The value of $1 da$ must be at least max(1,n).			
Output Parameters				

а

With uplo = 'U' or 'u', the upper triangular part of the array **a** is overwritten by the upper triangular part of the updated matrix.

With uplo = 'L' or 'l', the lower triangular part of the array *a* is overwritten by the lower triangular part of the updated matrix.

?syr2

Performs a rank-2 update of symmetric matrix.

call ssyr2(uplo, n, alpha, x, incx, y, incy, a, lda)
call dsyr2(uplo, n, alpha, x, incx, y, incy, a, lda)

Discussion

The ?syr2 routines perform a matrix-vector operation defined as

 $a := alpha^*x^*y' + alpha^*y^*x' + a,$

where:

alpha is a scalar

x and y are *n*-element vectors

a is an *n* by *n* symmetric matrix.

Input Parameters

uplo CHARACTER*1. Specifies whether the upper or lower triangular part of the array *a* is to be referenced, as follows:

uplo value	Part of Array a To Be Referenced
U or u	The upper triangular part of array a is to be referenced.
L or l	The lower triangular part of array a is to be referenced.
n	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.
alpha	REAL for ssyr2 DOUBLE PRECISION for dsyr2
	Specifies the scalar <u>alpha</u> .

x	REAL for ssyr2 DOUBLE PRECISION for dsyr2
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
У	REAL for ssyr2 DOUBLE PRECISION for dsyr2
	Array, DIMENSION at least $(1 + (n - 1) * abs(incy))$. Before entry, the incremented array y must contain the <i>n</i> -element vector y.
incy	INTEGER. Specifies the increment for the elements of y . The value of <i>incy</i> must not be zero.
a	REAL for ssyr2 DOUBLE PRECISION for dsyr2
	Array, DIMENSION (lda, n) . Before entry with $uplo = 'U'$ or 'u', the leading <i>n</i> by <i>n</i> upper triangular part of the array <i>a</i> must contain the upper triangular part of the symmetric matrix and the strictly lower triangular part of <i>a</i> is not referenced.
	Before entry with $uplo = 'L'$ or 'l', the leading <i>n</i> by <i>n</i> lower triangular part of the array a must contain the lower triangular part of the symmetric matrix and the strictly upper triangular part of <i>a</i> is not referenced.
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. The value of $1da$ must be at least max $(1, n)$.

а

With uplo = 'U' or 'u', the upper triangular part of the array **a** is overwritten by the upper triangular part of the updated matrix.

With uplo = 'L' or 'l', the lower triangular part of the array **a** is overwritten by the lower triangular part of the updated matrix.

?tbmv

Computes a matrix-vector product using a triangular band matrix.

call stbmv (uplo, trans, diag, n, k, a, lda, x, incx)
call dtbmv (uplo, trans, diag, n, k, a, lda, x, incx)
call ctbmv (uplo, trans, diag, n, k, a, lda, x, incx)
call ztbmv (uplo, trans, diag, n, k, a, lda, x, incx)

Discussion

The ?tbmv routines perform one of the matrix-vector operations defined as

 $x := a^*x, \text{ or } x := a^{*}x, \text{ or } x := \text{ conjg}(a^{*})^*x,$

where:

x is an *n*-element vector

a is an *n* by *n* unit, or non-unit, upper or lower triangular band matrix, with (k + 1) diagonals.

Input Parameters

uplo

CHARACTER*1. Specifies whether the matrix is an upper or lower triangular matrix, as follows:

uplo value	Matrix a
U or u	An upper triangular matrix.
L or l	A lower triangular matrix.
trans	CHARACTER*1. Specifies the operation to be performed, as follows:
trans value	Operation to be Performed
N or n	x := a*x
T or t	$x := a^{\dagger} * x$
C or c	$x := \operatorname{conjg}(a') * x$
diag	CHARACTER*1. Specifies whether or not a is unit triangular, as follows:
diag value	Matrix a
U or u	Matrix a is assumed to be unit triangular.
N or n	Matrix a is not assumed to be unit triangular.
п	INTEGER. Specifies the order of the matrix \mathbf{a} . The value of \mathbf{n} must be at least zero.
k	INTEGER. On entry with $uplo = 'U'$ or 'u', k specifies the number of super-diagonals of the matrix a. On entry with $uplo = 'L'$ or 'l', k specifies the number of sub-diagonals of the matrix a. The value of k must satisfy $0 \leq k$.
a	REAL for stbmv DOUBLE PRECISION for dtbmv COMPLEX for ctbmv DOUBLE COMPLEX for ztbmv
	Array, DIMENSION (<i>lda</i> , <i>n</i>). Before entry with $uplo = 'U'$ or 'u', the leading $(k + 1)$ by <i>n</i> part of the

of the array, the first super-diagonal starting at position 2 in row k, and so on. The top left k by k triangle of the array a is not referenced. The following program segment transfers an upper triangular band matrix from conventional full matrix storage to band storage:

```
do 20, j = 1, n
m = k + 1 - j
do 10, i = max(1, j - k), j
a(m + i, j) = matrix(i, j)
10 continue
20 continue
```

Before entry with uplo = 'L' or 'l', the leading (k + 1) by *n* part of the array **a** must contain the lower triangular band part of the matrix of coefficients, supplied column-by-column, with the leading diagonal of the matrix in row1 of the array, the first sub-diagonal starting at position 1 in row 2, and so on. The bottom right *k* by *k* triangle of the array *a* is not referenced. The following program segment transfers a lower triangular band matrix from conventional full matrix storage to band storage:

```
do 20, j = 1, n
m = 1 - j
do 10, i = j, min(n, j + k)
a(m + i, j) = matrix (i, j)
10 continue
20 continue
```

Note that when diag = 'U' or 'u', the elements of the array a corresponding to the diagonal elements of the matrix are not referenced, but are assumed to be unity.

INTEGER. Specifies the first dimension of *a* as declared in the calling (sub)program. The value of 1da must be at least (k + 1).

lda

x	REAL for stbmv
	DOUBLE PRECISION for dtbmv
	COMPLEX for ctbmv
	DOUBLE COMPLEX for ztbmv
	Array, DIMENSION at least $(1 + (n - 1) * abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	INTEGER. Specifies the increment for the elements of <i>x</i> . The value of <i>incx</i> must not be zero.

?tbsv

Solves a system of linear equations whose coefficients are in a triangular band matrix.

call	stbsv	(uplo,	trans,	diag,	n,	k,	a,	lda,	х,	incx)
call	dtbsv	(uplo,	trans,	diag,	n,	k,	a,	lda,	x,	incx)
call	ctbsv	(uplo,	trans,	diag,	n,	k,	a,	lda,	x,	incx)
call	ztbsv	(uplo,	trans,	diag,	n,	k,	a,	lda,	х,	incx)

Discussion

The ?tbsv routines solve one of the following systems of equations:

 $a^*x = b$, or $a^{*}x = b$, or $conjg(a^{*})^*x = b$,

where:

b and *x* are *n*-element vectors

a is an *n* by *n* unit, or non-unit, upper or lower triangular band matrix, with (k + 1) diagonals.

The routine does not test for singularity or near-singularity. Such tests must be performed before calling this routine.

Input Parameters

uplo	CHARACTER*1. Specifies whether the matrix is an upper or lower triangular matrix, as follows:					
uplo value	Matrix a					
U or u	An upper triangular matrix.					
L or l	A lower triangular matrix.					
trans	CHARACTER*1. Specifies the operation to be performed as follows:					
trans value	Operation to be Performed					
N or n	$a^*x = b$					
T or t	a' * x = b					
C or c	conjg(a')*x = b					
diag	CHARACTER*1. Specifies whether or not a is unit triangular, as follows:					
diag value	Matrix a					
U or u	Matrix a is assumed to be unit triangular.					
N or n	Matrix a is not assumed to be unit triangular.					
п	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.					
k	INTEGER. On entry with $uplo = 'U'$ or 'u', k specifies the number of super-diagonals of the matrix a On entry with $uplo = 'L'$ or 'l', k specifies the number of sub-diagonals of the matrix a. The value of k must satisfy $0 \leq k$.					

REAL for stbsv DOUBLE PRECISION for dtbsv COMPLEX for ctbsv DOUBLE COMPLEX for ztbsv

Array, DIMENSION (1da, n). Before entry with uplo = 'U' or 'u', the leading (k + 1) by n part of the array a must contain the upper triangular band part of the matrix of coefficients, supplied column-by-column, with the leading diagonal of the matrix in row (k + 1) of the array, the first super-diagonal starting at position 2 in row k, and so on. The top left k by k triangle of the array a is not referenced.

The following program segment transfers an upper triangular band matrix from conventional full matrix storage to band storage:

```
do 20, j = 1, n
m = k + 1 - j
do 10, i = max(1, j - k), j
a(m + i, j) = matrix (i, j)
10 continue
20 continue
```

Before entry with uplo = 'L' or 'l', the leading (k + 1) by *n* part of the array **a** must contain the lower triangular band part of the matrix of coefficients, supplied column-by-column, with the leading diagonal of the matrix in row 1 of the array, the first sub-diagonal starting at position 1 in row 2, and so on. The bottom right *k* by *k* triangle of the array **a** is not referenced.

The following program segment transfers a lower triangular band matrix from conventional full matrix storage to band storage:

```
do 20, j = 1, n
m = 1 - j
do 10, i = j, min(n, j + k)
a(m + i, j) = matrix (i, j)
10 continue
20 continue
```

а

	When <i>diag</i> = 'U' or 'u', the elements of the array a corresponding to the diagonal elements of the matrix are not referenced, but are assumed to be unity.
lda	INTEGER. Specifies the first dimension of a as declared in the calling (sub)program. The value of <i>lda</i> must be at least $(k + 1)$.
x	REAL for stbsv DOUBLE PRECISION for dtbsv COMPLEX for ctbsv DOUBLE COMPLEX for ztbsv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element right-hand side vector <i>b</i> .
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.
Output Para	meters

ul Parameters

tor 🗴

?tpmv

Computes a matrix-vector product using a triangular packed matrix.

> call stpmv (uplo, trans, diag, n, ap, x, incx) call dtpmv (uplo, trans, diag, n, ap, x, incx) call ctpmv (uplo, trans, diag, n, ap, x, incx) call ztpmv (uplo, trans, diag, n, ap, x, incx)

Discussion

The ?tpmv routines perform one of the matrix-vector operations defined as

 $x := a^*x, \text{ or } x := a^{*}x, \text{ or } x := \text{ conjg}(a^{*})^*x,$

where:

x is an *n*-element vector

a is an *n* by *n* unit, or non-unit, upper or lower triangular matrix, supplied in packed form.

Input Parameters

uploCHARACTER*1. Specifies whether the matrix a is an
upper or lower triangular matrix, as follows:

uplo value	Matrix a			
<mark>U</mark> or u	An upper triangular matrix.			
L or l	A lower triangular matrix.			
trans	CHARACTER*1. Specifies the operation to be performed, as follows:			
trans value	Operation To Be Performed			
N or n	$x := a^*x$			
T or t	x := a' * x			
C or c	$x := \operatorname{conjg}(a') * x$			
diag	CHARACTER*1. Specifies whether or not a is unit triangular, as follows:			
diag value	Matrix a			
U or u	Matrix a is assumed to be unit triangular.			
N or n	Matrix a is not assumed to be unit triangular.			
n	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.			
ap	REAL for stpmv DOUBLE PRECISION for dtpmv COMPLEX for ctpmv DOUBLE COMPLEX for ztpmv			

Array, DIMENSION at least $((n^{*}(n + 1))/2)$. Before entry with uplo = 'U' or 'u', the array ap must contain the upper triangular matrix packed sequentially, column-by-column, so that ap(1) contains a(1,1), ap(2) and ap(3) contain a(1,2) and a(2,2)respectively, and so on. Before entry with uplo = 'L' or '1', the array ap must contain the lower triangular matrix packed sequentially, column-by-column, so that ap(1) contains a(1,1), ap(2) and ap(3) contain a(2,1) and a(3,1) respectively, and so on. When diag = 'U' or 'u', the diagonal elements of a are not referenced, but are assumed to be unity.

REAL for stpmv DOUBLE PRECISION for dtpmv COMPLEX for ctpmv DOUBLE COMPLEX for ztpmv

Array, DIMENSION at least (1 + (n - 1)*abs(incx)). Before entry, the incremented array x must contain the *n*-element vector x.

INTEGER. Specifies the increment for the elements of **x**. The value of *incx* must not be zero.

Output Parameters

Overwritten with the transformed vector \mathbf{x} .

X

incx

х

?tpsv

Solves a system of linear equations whose coefficients are in a triangular packed matrix.

call stpsv (uplo, trans, diag, n, ap, x, incx)
call dtpsv (uplo, trans, diag, n, ap, x, incx)
call ctpsv (uplo, trans, diag, n, ap, x, incx)
call ztpsv (uplo, trans, diag, n, ap, x, incx)

Discussion

The ?tpsv routines solve one of the following systems of equations

 $a^*x = b$, or $a^{*}x = b$, or $conjg(a^{*})^*x = b$,

where:

b and *x* are *n*-element vectors

a is an n by n unit, or non-unit, upper or lower triangular matrix, supplied in packed form.

This routine does not test for singularity or near-singularity. Such tests must be performed before calling this routine.

Input Parameters

uplo CHARACTER*1. Specifies whether the matrix *a* is an upper or lower triangular matrix, as follows:

uplo value	Matrix a
U or u	An upper triangular matrix.
L or l	A lower triangular matrix.

trans	CHARACTER*1. Specifies the operation to be performed, as follows:
trans value	Operation To Be Performed
N or n	$a^*x = b$
T or t	$a^{+}x = b$
C or c	conjg(a')*x = b
diag	CHARACTER*1. Specifies whether or not a is unit triangular, as follows:
diag value	Matrix a
U or u	Matrix a is assumed to be unit triangular.
N or n	Matrix a is not assumed to be unit triangular.
п	INTEGER. Specifies the order of the matrix a . The value of n must be at least zero.
ap	REAL for stpsv DOUBLE PRECISION for dtpsv COMPLEX for ctpsv DOUBLE COMPLEX for ztpsv
	Array, DIMENSION at least $((n*(n+1))/2)$. Before entry with $uplo = 'U'$ or 'u', the array ap must contain the upper triangular matrix packed sequentially, column-by-column, so that $ap(1)$ contains $a(1, 1)$, ap(2) and $ap(3)$ contain $a(1, 2)$ and $a(2, 2)respectively, and so on. Before entry with uplo = 'L' or'1', the array ap must contain the lower triangularmatrix packed sequentially, column-by-column, so thatap(1)$ contains $a(1, 1)$, $ap(2)$ and $ap(3)$ contain a(2, 1) and $a(3, 1)$ respectively, and so on. When diag = 'U' or 'u', the diagonal elements of a are not referenced, but are assumed to be unity.

x	REAL for stpsv
	DOUBLE PRECISION for dtpsv
	COMPLEX for ctpsv
	DOUBLE COMPLEX for ztpsv
	Array, DIMENSION at least $(1 + (n - 1) * abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element right-hand side vector <i>b</i> .
incx	INTEGER . Specifies the increment for the elements of x .
	The value of <i>incx</i> must not be zero.

Output Parameters

x	Overwritten with the solution vector	x.
X		Χ.

?trmv

Computes a matrix-vector product using a triangular matrix.

call	strmv	(uplo,	trans,	diag,	n,	a,	lda,	x,	incx)
call	dtrmv	(uplo,	trans,	diag,	n,	a,	lda,	x,	incx)
call	ctrmv	(uplo,	trans,	diag,	n,	a,	lda,	x,	incx)
call	ztrmv	(uplo,	trans,	diag,	n,	a,	lda,	x,	incx)

Discussion

The **?trmv** routines perform one of the following matrix-vector operations defined as

 $x := a^*x \text{ or } x := a^{*}x \text{ or } x := \text{conjg}(a^*)^*x,$

where:

x is an *n*-element vector

a is an n by n unit, or non-unit, upper or lower triangular matrix.

Input Parameters

input Parame	ters				
uplo	CHARACTER*1. Specifies whether the matrix a is an upper or lower triangular matrix, as follows:				
uplo value	Matrix a				
U or u	An upper triangular matrix.				
L or l	A lower triangular matrix.				
trans	CHARACTER*1. Specifies the operation to be performed as follows:				
trans value	Operation To Be Performed				
N or n	$x := a^*x$				
T or t	x := a' * x				
C or c	$x := \operatorname{conjg}(a') * x$				
diag	CHARACTER*1. Specifies whether or not a is unit triangular, as follows:				
diag value	Matrix a				
U or u	Matrix a is assumed to be unit triangular.				
N or n	Matrix a is not assumed to be unit triangular.				
п	INTEGER. Specifies the order of the matrix a . The valu of n must be at least zero.				
a	REAL for strmv DOUBLE PRECISION for dtrmv COMPLEX for ctrmv DOUBLE COMPLEX for ztrmv				
	Array, DIMENSION (lda, n) . Before entry with $uplo = 'U'$ or 'u', the leading <i>n</i> by <i>n</i> upper triangular part of the array <i>a</i> must contain the upper triangular matrix and the strictly lower triangular part of <i>a</i> is not referenced. Before entry with $uplo = 'L'$ or 'l', the leading <i>n</i> by <i>n</i> lower triangular part of the array <i>a</i> must				

	contain the lower triangular matrix and the strictly upper triangular part of a is not referenced. When diag = 'U' or 'u', the diagonal elements of a are not referenced either, but are assumed to be unity.	
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. The value of $1 da$ must be at least max(1, n).	
x	REAL for strmv	
	DOUBLE PRECISION for dtrmv COMPLEX for atrmv	
	DOUBLE COMPLEX for ztrmv	
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element vector x.	
incx	INTEGER . Specifies the increment for the elements of \mathbf{x} .	
	The value of <i>incx</i> must not be zero.	
Output Parameters		

x

?trsv

Solves a system of linear equations whose coefficients are in a triangular matrix.

> call strsv (uplo, trans, diag, n, a, lda, x, incx) call dtrsv (uplo, trans, diag, n, a, lda, x, incx) call ctrsv (uplo, trans, diag, n, a, lda, x, incx) call ztrsv (uplo, trans, diag, n, a, lda, x, incx)

Discussion

The?trsv routines solve one of the systems of equations:

 $a^*x = b \text{ or } a^{*}x = b, \text{ or } conjg(a^{*})^*x = b,$

where:

b and *x* are *n*-element vectors

a is an *n* by *n* unit, or non-unit, upper or lower triangular matrix.

The routine does not test for singularity or near-singularity. Such tests must be performed before calling this routine.

Input Parameters

uplo	CHARACTER*1. Specifies whether the matrix is an upper or lower triangular matrix, as follows:	
uplo value	Matrix a	
U or u	An upper triangular matrix.	
L or l	A lower triangular matrix.	

transCHARACTER*1. Specifies the operation to be performed,
as follows:

trans value	Operation To Be Performed	
N or n	$a^*x = b$	
T or t	$a' \star x = b$	
C or c	conjg(a') * x = b	

diag CHARACTER*1. Specifies whether or not *a* is unit triangular, as follows:

diag value	Matrix a
U or u	Matrix a is assumed to be unit triangular.
N or n	Matrix a is not assumed to be unit triangular.
n	INTEGER. Specifies the order of the matrix a . The value

a	REAL for strsv DOUBLE PRECISION for dtrsv COMPLEX for ctrsv DOUBLE COMPLEX for ztrsv
	Array, DIMENSION (lda, n) . Before entry with uplo = 'U' or 'u', the leading <i>n</i> by <i>n</i> upper triangular part of the array <i>a</i> must contain the upper triangular matrix and the strictly lower triangular part of <i>a</i> is not referenced. Before entry with $uplo = 'L'$ or 'l', the leading <i>n</i> by <i>n</i> lower triangular part of the array <i>a</i> must contain the lower triangular matrix and the strictly upper triangular part of <i>a</i> is not referenced. When $diag = 'U'$ or 'u', the diagonal elements of <i>a</i> are not referenced either, but are assumed to be unity.
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. The value of <i>lda</i> must be at least $max(1, n)$.
x	REAL for strsv DOUBLE PRECISION for dtrsv COMPLEX for ctrsv DOUBLE COMPLEX for ztrsv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$. Before entry, the incremented array x must contain the <i>n</i> -element right-hand side vector <i>b</i> .
incx	INTEGER. Specifies the increment for the elements of x . The value of <i>incx</i> must not be zero.

Output Parameters

x Overwritten with the solution vector **x**.

BLAS Level 3 Routines

BLAS Level 3 routines perform matrix-matrix operations. Table 2-3 lists the BLAS Level 3 routine groups and the data types associated with them.

DLAS Leve		oroups and men bala types
Routine Group	Data Types	Description
?gemm	s, d, c, z	Matrix-matrix product of general matrices
?hemm	C, Z	Matrix-matrix product of Hermitian matrices
?herk	C, Z	Rank-k update of Hermitian matrices
?her2k	C, Z	Rank-2k update of Hermitian matrices
?symm	s, d, c, z	Matrix-matrix product of symmetric matrices
?syrk	s, d, c, z	Rank-k update of symmetric matrices
?syr2k	s, d, c, z	Rank-2k update of symmetric matrices
?trmm	s, d, c, z	Matrix-matrix product of triangular matrices
?trsm	s, d, c, z	Linear matrix-matrix solution for triangular matrices

Table 2-3 BLAS Level 3 Routine Groups and Their Data Types

Symmetric Multiprocessing Version of Intel[®] MKL

Many applications spend considerable time for executing BLAS level 3 routines. This time can be scaled by the number of processors available on the system through using the symmetric multiprocessing (SMP) feature built into the Intel MKL Library. The performance enhancements based on the parallel use of the processors are available without any programming effort on your part.

To enhance performance, the library uses the following methods:

• The operation of BLAS level 3 matrix-matrix functions permits to restructure the code in a way which increases the localization of data reference, enhances cache memory use, and reduces the dependency on the memory bus.

 Once the code has been effectively blocked as described above, one of the matrices is distributed across the processors to be multiplied by the second matrix. Such distribution ensures effective cache management which reduces the dependency on the memory bus performance and brings good scaling results.

?gemm

Computes a scalar-matrix-matrix product and adds the result to a scalar-matrix product.

```
call sgemm ( transa, transb, m, n, k, alpha, a, lda,
    b, ldb, beta, c, ldc )
call dgemm ( transa, transb, m, n, k, alpha, a, lda,
    b, ldb, beta, c, ldc )
call cgemm ( transa, transb, m, n, k, alpha, a, lda,
    b, ldb, beta, c, ldc )
call zgemm ( transa, transb, m, n, k, alpha, a, lda,
    b, ldb, beta, c, ldc )
```

Discussion

The **?gemm** routines perform a matrix-matrix operation with general matrices. The operation is defined as

c := alpha*op(a)*op(b) + beta*c,

where:

op(x) is one of op(x) = x or op(x) = x' or op(x) = conjg(x'),

alpha and beta are scalars

a, b and c are matrices:

op(a) is an *m* by *k* matrix

op(b) is a k by n matrix

c is an *m* by *n* matrix.

Input Parameters

CHARACTER*1. Specifies the form of op(a) to be used in the matrix multiplication as follows:

transa value	Form of op(a)
N or n	op(a) = a
T or t	op(a) = a'
C or c	op(a) = conjg(a')

transb

CHARACTER*1. Specifies the form of op(b) to be used in the matrix multiplication as follows:

transb value	Form of op(b)
N or n	op(b) = b
T or t	op(b) = b'
C or c	op(b) = conjg(b')
m	INTEGER. Specifies the number of rows of the matrix $op(a)$ and of the matrix c . The value of m must be at least zero.
n	INTEGER. Specifies the number of columns of the matrix $op(b)$ and the number of columns of the matrix c . The value of n must be at least zero.
k	INTEGER. Specifies the number of columns of the matrix $op(a)$ and the number of rows of the matrix $op(b)$. The value of k must be at least zero.
alpha	REAL for sgemm DOUBLE PRECISION for dgemm COMPLEX for cgemm DOUBLE COMPLEX for zgemm
	Specifies the scalar alpha.

а	REAL for sgemm DOUBLE PRECISION for dgemm COMPLEX for cgemm DOUBLE COMPLEX for zgemm
	Array, DIMENSION (lda , ka), where ka is k when transa = 'N' or 'n', and is m otherwise. Before entry with $transa = 'N'$ or 'n', the leading m by k part of the array a must contain the matrix a , otherwise the leading k by m part of the array a must contain the matrix a .
lda	INTEGER. Specifies the first dimension of a as declared in the calling (sub)program. When $transa = 'N'$ or 'n', then <i>lda</i> must be at least max(1, m), otherwise <i>lda</i> must be at least max(1, k).
b	REAL for sgemm DOUBLE PRECISION for dgemm COMPLEX for cgemm DOUBLE COMPLEX for zgemm
	Array, DIMENSION (ldb, kb) , where kb is n when transb = 'N' or 'n', and is k otherwise. Before entry with $transb = 'N'$ or 'n', the leading k by n part of the array b must contain the matrix b , otherwise the leading n by k part of the array b must contain the matrix b .
ldb	INTEGER. Specifies the first dimension of <i>b</i> as declared in the calling (sub)program. When <i>transb</i> = 'N' or 'n', then <i>ldb</i> must be at least $max(1, k)$, otherwise <i>ldb</i> must be at least $max(1, n)$.
beta	REAL for sgemm DOUBLE PRECISION for dgemm COMPLEX for cgemm DOUBLE COMPLEX for zgemm
	Specifies the scalar beta . When beta is supplied as zero, then <i>c</i> need not be set on input.

C	REAL for sgemm
	DOUBLE PRECISION for dgemm
	COMPLEX for cgemm
	DOUBLE COMPLEX for zgemm
	Array, DIMENSION (ldc, n) . Before entry, the leading m by n part of the array c must contain the matrix c , except when <i>beta</i> is zero, in which case c need not be set on entry.
ldc	INTEGER. Specifies the first dimension of c as declared in the calling (sub)program. The value of <i>ldc</i> must be at least max(1, m).
Output Parame	ters

С

Overwritten by the *m* by *n* matrix (*alpha**op(*a*)*op(*b*) + *beta***c*).

?hemm

Computes a scalar-matrix-matrix product (either one of the matrices is Hermitian) and adds the result to scalar-matrix product.

Discussion

The ?hemm routines perform a matrix-matrix operation using Hermitian matrices. The operation is defined as

c := alpha*a*b + beta*c

or

c := alpha*b*a + beta*c,

where:

alpha and beta are scalars

a is an Hermitian matrix

b and *c* are *m* by *n* matrices.

Input Parameters

sideCHARACTER*1. Specifies whether the Hermitian matrixa appears on the left or right in the operation as follows:

side value	Operation To Be Performed
L or l	c := alpha*a*b + beta*c
Rorr	c := alpha*b*a + beta*c
uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the Hermitian matrix <i>a</i> is to be referenced as follows:
uplo value	Part of Matrix a To Be Referenced
U or u	Only the upper triangular part of the Hermitian matrix is to be referenced.
L or l	Only the lower triangular part of the Hermitian matrix is to be referenced.
m	INTEGER. Specifies the number of rows of the matrix c . The value of m must be at least zero.
n	INTEGER. Specifies the number of columns of the matrix c . The value of n must be at least zero.
alpha	COMPLEX for chemm DOUBLE COMPLEX for zhemm
	Specifies the scalar alpha.

а

lda

b

ldb

COMPLEX for chemm DOUBLE COMPLEX for zhemm

Array, DIMENSION (1da, ka), where ka is m when *side* = L' or 1' and is *n* otherwise. Before entry with *side* = 'L' or 'l', the *m* by *m* part of the array *a* must contain the Hermitian matrix, such that when uplo = 'U' or 'u', the leading m by m upper triangular part of the array a must contain the upper triangular part of the Hermitian matrix and the strictly lower triangular part of a is not referenced, and when uplo = 'L' or 'l', the leading *m* by *m* lower triangular part of the array a must contain the lower triangular part of the Hermitian matrix, and the strictly upper triangular part of *a* is not referenced. Before entry with *side* = 'R' or 'r', the *n* by *n* part of the array *a* must contain the Hermitian matrix, such that when uplo = 'U' or 'u', the leading *n* by *n* upper triangular part of the array *a* must contain the upper triangular part of the Hermitian matrix and the strictly lower triangular part of *a* is not referenced, and when uplo = 'L' or 'l', the leading *n* by *n* lower triangular part of the array a must contain the lower triangular part of the Hermitian matrix, and the strictly upper triangular part of a is not referenced. The imaginary parts of the diagonal elements need not be set, they are assumed to be zero.

INTEGER. Specifies the first dimension of a as declared in the calling (sub) program. When side = 'L' or 'l' then *lda* must be at least max(1, m), otherwise *lda* must be at least max(1, n).

COMPLEX for chemm DOUBLE COMPLEX for zhemm

Array, DIMENSION (1db, n). Before entry, the leading *m* by *n* part of the array *b* must contain the matrix *b*.

INTEGER. Specifies the first dimension of *b* as declared in the calling (sub)program. The value of *ldb* must be at least $\max(1, m)$.

beta	COMPLEX for chemm DOUBLE COMPLEX for zhemm
	Specifies the scalar $beta$. When $beta$ is supplied as zero, then c need not be set on input.
С	COMPLEX for chemm DOUBLE COMPLEX for zhemm
	Array, DIMENSION (c, n) . Before entry, the leading m by n part of the array c must contain the matrix c , except when <i>beta</i> is zero, in which case c need not be set on entry.
ldc	INTEGER. Specifies the first dimension of c as declared in the calling (sub)program. The value of <i>ldc</i> must be at least max(1,m).
Output Parame	ters

С

Overwritten by the m by n updated matrix.

?herk

Performs a rank-n update of a Hermitian matrix.

Discussion

The **?herk** routines perform a matrix-matrix operation using Hermitian matrices. The operation is defined as

c := alpha*a*conjg(a') + beta*c,
or
c := alpha*conjg(a')*a + beta*c,

where:

alpha and beta are real scalars

c is an *n* by *n* Hermitian matrix

a is an *n* by *k* matrix in the first case and a *k* by *n* matrix in the second case.

Input Parameters

uploCHARACTER*1. Specifies whether the upper or lower
triangular part of the array c is to be referenced as
follows:

uplo value	Part of Array <i>c</i> To Be Referenced
U or u	Only the upper triangular part of <i>C</i> is to be referenced.
L or l	Only the lower triangular part of <i>C</i> is to be referenced.
trans	CHARACTER*1. Specifies the operation to be performed as follows:

trans value	Operation to be Performed
N or n	<i>c</i> := <i>alpha</i> *a*conjg(a')+ <i>beta</i> * <i>c</i>
Corc	<i>c</i> := <i>alpha</i> *conjg(<i>a</i> ')* <i>a</i> + <i>beta</i> * <i>c</i>
п	INTEGER. Specifies the order of the matrix c . The value of n must be at least zero.
k	INTEGER. With <i>trans</i> = 'N' or 'n', <i>k</i> specifies the number of columns of the matrix <i>a</i> , and with <i>trans</i> = 'C' or 'c', <i>k</i> specifies the number of rows of the matrix <i>a</i> . The value of <i>k</i> must be at least zero.
alpha	REAL for cherk DOUBLE PRECISION for zherk
	Specifies the scalar alpha.

a	COMPLEX for cherk DOUBLE COMPLEX for zherk
	Array, DIMENSION (<i>lda</i> , <i>ka</i>), where <i>ka</i> is <i>k</i> when trans = 'N' or 'n', and is <i>n</i> otherwise. Before entry with $trans = 'N'$ or 'n', the leading <i>n</i> by <i>k</i> part of the array <i>a</i> must contain the matrix <i>a</i> , otherwise the leading <i>k</i> by <i>n</i> part of the array <i>a</i> must contain the matrix <i>a</i> .
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. When $trans = 'N'$ or 'n', then <i>lda</i> must be at least $max(1, n)$, otherwise <i>lda</i> must be at least $max(1, k)$.
beta	REAL for cherk DOUBLE PRECISION for zherk
	Specifies the scalar beta.
С	COMPLEX for cherk DOUBLE COMPLEX for zherk
	Array, DIMENSION (ldc, n) . Before entry with $uplo = 'U'$ or 'u', the leading <i>n</i> by <i>n</i> upper triangular part of the array <i>c</i> must contain the upper triangular part of the Hermitian matrix and the strictly lower triangular part of <i>c</i> is not referenced.
	Before entry with $uplo = 'L'$ or 'l', the leading <i>n</i> by <i>n</i> lower triangular part of the array <i>c</i> must contain the lower triangular part of the Hermitian matrix and the strictly upper triangular part of <i>c</i> is not referenced.
	The imaginary parts of the diagonal elements need not be set, they are assumed to be zero.
ldc	INTEGER. Specifies the first dimension of c as declared in the calling (sub)program. The value of ldc must be at least max(1, n).

Output Parameters

C

With uplo = 'U' or 'u', the upper triangular part of the array c is overwritten by the upper triangular part of the updated matrix.

With uplo = 'L' or 'l', the lower triangular part of the array c is overwritten by the lower triangular part of the updated matrix.

The imaginary parts of the diagonal elements are set to zero.

?her2k

Performs a rank-2k update of a Hermitian matrix.

call cher2k (uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc) call zher2k (uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc)

Discussion

The ?her2k routines perform a rank-2k matrix-matrix operation using Hermitian matrices. The operation is defined as

```
c := alpha*a*conjg(b') + conjg(alpha)*b*conjg(a') + beta*c,
or
```

```
c := alpha*conjg(b')*a + conjg(alpha)*conjg(a')*b + beta*c,
where:
```

alpha is a scalar and beta is a real scalar

c is an *n* by *n* Hermitian matrix

a and b are n by k matrices in the first case and k by n matrices in the second case.

Input Parameters		
uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the array c is to be referenced as follows:	
uplo value	Part of Array <i>c</i> To Be Referenced	
U or u	Only the upper triangular part of <i>C</i> is to be referenced.	
L or l	Only the lower triangular part of <i>C</i> is to be referenced.	
trans	CHARACTER*1. Specifies the operation to be performed as follows:	
trans value	Operation to be Performed	
trans value N or n	Operation to be Performed c:=alpha*a*conjg(b') +alpha*b*conjg(a') +beta*c	
	c:=alpha*a*conjg(b')	
N or n	<pre>c:=alpha*a*conjg(b') +alpha*b*conjg(a') +beta*c c:=alpha*conjg(a')*b</pre>	
N or n C or c	<pre>c:=alpha*a*conjg(b') +alpha*b*conjg(a') +beta*c c:=alpha*conjg(a')*b +alpha*conjg(b')*a+beta*c INTEGER. Specifies the order of the matrix c. The value</pre>	
N or n C or c n	<pre>c:=alpha*a*conjg(b') +alpha*b*conjg(a') +beta*c c:=alpha*conjg(a')*b +alpha*conjg(b')*a+beta*c INTEGER. Specifies the order of the matrix c. The value of n must be at least zero. INTEGER. With trans = 'N' or 'n', k specifies the number of columns of the matrix a, and with trans = 'C' or 'c', k specifies the number of rows of</pre>	

a	COMPLEX for cher2k DOUBLE COMPLEX for zher2k
	Array, DIMENSION (lda , ka), where ka is k when trans = 'N' or 'n', and is n otherwise. Before entry with $trans = 'N'$ or 'n', the leading n by k part of the array a must contain the matrix a , otherwise the leading k by n part of the array a must contain the matrix a .
lda	INTEGER. Specifies the first dimension of a as declared in the calling (sub)program. When $trans = 'N'$ or 'n', then <i>lda</i> must be at least $max(1, n)$, otherwise <i>lda</i> must be at least $max(1, k)$.
beta	REAL for cher2k DOUBLE PRECISION for zher2k
	Specifies the scalar beta.
b	COMPLEX for cher2k DOUBLE COMPLEX for zher2k
	Array, DIMENSION (ldb , kb), where kb is k when trans = 'N' or 'n', and is n otherwise. Before entry with $trans = 'N'$ or 'n', the leading n by k part of the array b must contain the matrix b , otherwise the leading k by n part of the array b must contain the matrix b .
ldb	INTEGER. Specifies the first dimension of <i>b</i> as declared in the calling (sub)program. When $trans = 'N'$ or 'n', then <i>ldb</i> must be at least $max(1, n)$, otherwise <i>ldb</i> must be at least $max(1, k)$.
С	COMPLEX for cher2k DOUBLE COMPLEX for zher2k
	Array, DIMENSION (ldc, n) . Before entry with $uplo = 'U'$ or 'u', the leading <i>n</i> by <i>n</i> upper triangular part of the array <i>c</i> must contain the upper triangular part of the Hermitian matrix and the strictly lower triangular part of <i>c</i> is not referenced.

Before entry with uplo = 'L' or 'l', the leading *n* by *n* lower triangular part of the array *c* must contain the lower triangular part of the Hermitian matrix and the strictly upper triangular part of *c* is not referenced.

The imaginary parts of the diagonal elements need not be set, they are assumed to be zero.

ldc INTEGER. Specifies the first dimension of *c* as declared in the calling (sub)program. The value of *ldc* must be at least max(1, *n*).

Output Parameters

С

With uplo = 'U' or 'u', the upper triangular part of the array c is overwritten by the upper triangular part of the updated matrix.

With uplo = 'L' or 'l', the lower triangular part of the array c is overwritten by the lower triangular part of the updated matrix.

The imaginary parts of the diagonal elements are set to zero.

?symm

Performs a scalar-matrix-matrix product (one matrix operand is symmetric) and adds the result to a scalar-matrix product.

```
call ssymm ( side, uplo, m, n, alpha, a, lda, b, ldb,
        beta, c, ldc )
call dsymm ( side, uplo, m, n, alpha, a, lda, b, ldb,
        beta, c, ldc )
call csymm ( side, uplo, m, n, alpha, a, lda, b, ldb,
        beta, c, ldc )
call zsymm ( side, uplo, m, n, alpha, a, lda, b, ldb,
        beta, c, ldc )
```

Discussion

The ?symm routines perform a matrix-matrix operation using symmetric matrices. The operation is defined as

c := alpha*a*b + beta*c, or c := alpha*b*a + beta*c, where: alpha and beta are scalars a is a symmetric matrix

b and *c* are *m* by *n* matrices.

Input Parameters

side	CHARACTER*1. Specifies whether the symmetric matrix a appears on the left or right in the operation as follows:
side value	Operation to be Performed
L or l	c := alpha*a*b + beta*c
Rorr	c := alpha*b*a + beta*c
uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the symmetric matrix <i>a</i> is to be referenced as follows:
uplo value	Part of Array a To Be Referenced
U or u	Only the upper triangular part of the symmetric matrix is to be referenced.
L or l	Only the lower triangular part of the symmetric matrix is to be referenced.
m	INTEGER. Specifies the number of rows of the matrix c . The value of <i>m</i> must be at least zero.
п	INTEGER. Specifies the number of columns of the matrix c . The value of n must be at least zero.
alpha	REAL for ssymm DOUBLE PRECISION for dsymm COMPLEX for csymm DOUBLE COMPLEX for zsymm
	Specifies the scalar <u>alpha</u> .
a	REAL for ssymm DOUBLE PRECISION for dsymm COMPLEX for csymm DOUBLE COMPLEX for zsymm
	Array, DIMENSION (lda , ka), where ka is m when side = 'L' or 'l' and is n otherwise. Before entry with $side = 'L'$ or 'l', the m by m part of the array a must contain the symmetric matrix, such that when

uplo = 'U' or 'u', the leading *m* by *m* upper triangular part of the array *a* must contain the upper triangular part of the symmetric matrix and the strictly lower triangular part of *a* is not referenced, and when uplo = 'L' or 'l', the leading *m* by *m* lower triangular part of the array *a* must contain the lower triangular part of the symmetric matrix and the strictly upper triangular part of *a* is not referenced.

Before entry with side = 'R' or 'r', the *n* by *n* part of the array *a* must contain the symmetric matrix, such that when uplo = 'U' or 'u', the leading *n* by *n* upper triangular part of the array *a* must contain the upper triangular part of the symmetric matrix and the strictly lower triangular part of *a* is not referenced, and when uplo = 'L' or 'l', the leading *n* by *n* lower triangular part of the array *a* must contain the lower triangular part of the symmetric matrix and the strictly upper triangular part of the symmetric matrix and the strictly upper triangular part of *a* is not referenced.

INTEGER. Specifies the first dimension of a as declared in the calling (sub)program. When side = 'L' or 'l' then *lda* must be at least max(1, m), otherwise *lda* must be at least max(1, n).

REAL for ssymm DOUBLE PRECISION for dsymm COMPLEX for csymm DOUBLE COMPLEX for zsymm

Array, DIMENSION (1db, n). Before entry, the leading *m* by *n* part of the array b must contain the matrix *b*.

INTEGER. Specifies the first dimension of **b** as declared in the calling (sub)program. The value of *ldb* must be at least max(1, m).

lda

b

ldb

beta	REAL for ssymm
	DOUBLE PRECISION for dsymm
	COMPLEX for csymm
	DOUBLE COMPLEX for zsymm
	Specifies the scalar $beta$. When $beta$ is supplied as zero, then c need not be set on input.
С	REAL for ssymm
	DOUBLE PRECISION for dsymm
	COMPLEX for csymm
	DOUBLE COMPLEX for zsymm
	Array, DIMENSION $(1dc, n)$. Before entry, the leading m by n part of the array c must contain the matrix c , except when beta is zero, in which case c need not be set on entry.
ldc	INTEGER. Specifies the first dimension of c as declared in the calling (sub)program. The value of ldc must be at least max(1, m).
Output Param	eters

c Overwritten by the *m* by *n* updated matrix.

?syrk

Performs a rank-n update of a symmetric matrix.

Discussion

The **?syrk** routines perform a matrix-matrix operation using symmetric matrices. The operation is defined as

c := alpha*a*a' + beta*c, or c := alpha*a'*a + beta*c, where: alpha and beta are scalars

c is an *n* by *n* symmetric matrix

a is an n by k matrix in the first case and a k by n matrix in the second case.

Input Parameters		
uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the array <i>c</i> is to be referenced as follows:	
uplo value	Part of Array <i>c</i> To Be Referenced	
U or u	Only the upper triangular part of <i>c</i> is to be referenced.	
L or l	Only the lower triangular part of c is to be referenced.	
trans	CHARACTER*1. Specifies the operation to be performed as follows:	
trans value	Operation to be Performed	
N or n	c:= alpha*a*a' + beta*c	
T or t	c:= alpha*a'*a + beta*c	
C or c	c:= alpha*a'*a + beta*c	
п	INTEGER. Specifies the order of the matrix c . The value of n must be at least zero.	
k	INTEGER. On entry with $trans = 'N'$ or 'n', k specifies the number of columns of the matrix a , and on entry with $trans = 'T'$ or 't' or 'C' or 'c', k specifies the number of rows of the matrix a . The value of k must be at least zero.	
alpha	REAL for ssyrk DOUBLE PRECISION for dsyrk COMPLEX for csyrk DOUBLE COMPLEX for zsyrk Specifies the scalar <i>alpha</i> .	

a	REAL for ssyrk DOUBLE PRECISION for dsyrk COMPLEX for csyrk DOUBLE COMPLEX for zsyrk
	Array, DIMENSION (lda, ka), where ka is k when trans = 'N' or 'n', and is n otherwise. Before entry with $trans = 'N'$ or 'n', the leading n by k part of the array a must contain the matrix a , otherwise the leading k by n part of the array a must contain the matrix a .
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. When $trans = 'N'$ or 'n', then <i>lda</i> must be at least max(1, <i>n</i>), otherwise <i>lda</i> must be at least max(1, <i>k</i>).
beta	REAL for ssyrk DOUBLE PRECISION for dsyrk COMPLEX for csyrk DOUBLE COMPLEX for zsyrk
	Specifies the scalar <i>beta</i> .
С	REAL for ssyrk DOUBLE PRECISION for dsyrk COMPLEX for csyrk DOUBLE COMPLEX for zsyrk
	Array, DIMENSION (ldc, n) . Before entry with $uplo = 'U'$ or 'u', the leading <i>n</i> by <i>n</i> upper triangular part of the array <i>c</i> must contain the upper triangular part of the symmetric matrix and the strictly lower triangular part of <i>c</i> is not referenced.
	Before entry with $uplo = 'L'$ or 'l', the leading <i>n</i> by <i>n</i> lower triangular part of the array <i>c</i> must contain the lower triangular part of the symmetric matrix and the strictly upper triangular part of <i>c</i> is not referenced.
ldc	INTEGER. Specifies the first dimension of c as declared in the calling (sub)program. The value of <i>ldc</i> must be at least max(1, n).

Output Parameters

cWith uplo = 'U' or 'u', the upper triangular part of the
array c is overwritten by the upper triangular part of the
updated matrix.

With uplo = 'L' or 'l', the lower triangular part of the array c is overwritten by the lower triangular part of the updated matrix.

?syr2k

Performs a rank-2k update of a symmetric matrix.

call ssyr2k (uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc) call dsyr2k (uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc) call csyr2k (uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc) call zsyr2k (uplo, trans, n, k, alpha, a, lda, b, ldb, beta, c, ldc)

Discussion

The ?syr2k routines perform a rank-2k matrix-matrix operation using symmetric matrices. The operation is defined as

```
c := alpha*a*b' + alpha*b*a' + beta*c,
or
c := alpha*a'*b + alpha*b'*a + beta*c,
where:
```

alpha and beta are scalars

c is an *n* by *n* symmetric matrix

a and b are n by k matrices in the first case and k by n matrices in the second case.

Input Parameters

uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the array <i>c</i> is to be referenced as follows:
uplo value	Part of Array <i>c</i> To Be Referenced
U or u	Only the upper triangular part of c is to be referenced.
L or l	Only the lower triangular part of c is to be referenced.
trans	CHARACTER*1. Specifies the operation to be performed as follows:
trans value	Operation to be Performed
N or n	c:= alpha*a*b'+alpha*b*a'+beta*c
T or t	c:= alpha*a'*b+alpha*b'*a+beta*c
C or c	c:= alpha*a'*b+alpha*b'*a+beta*c
п	INTEGER. Specifies the order of the matrix c . The value of n must be at least zero.
k	INTEGER. On entry with $trans = 'N'$ or 'n', k specifies the number of columns of the matrices a and b , and on entry with $trans = 'T'$ or 't' or 'C' or 'c', k specifies the number of rows of the matrices a and b . The value of k must be at least zero.
alpha	REAL for ssyr2k DOUBLE PRECISION for dsyr2k COMPLEX for csyr2k DOUBLE COMPLEX for zsyr2k
	Specifies the scalar <i>alpha</i> .

a	REAL for ssyr2k DOUBLE PRECISION for dsyr2k COMPLEX for csyr2k DOUBLE COMPLEX for zsyr2k
	Array, DIMENSION (lda, ka), where ka is k when trans = 'N' or 'n', and is n otherwise. Before entry with $trans = 'N'$ or 'n', the leading n by k part of the array a must contain the matrix a , otherwise the leading k by n part of the array a must contain the matrix a .
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. When $trans = 'N'$ or 'n', then <i>lda</i> must be at least $max(1,n)$, otherwise <i>lda</i> must be at least $max(1, k)$.
Ь	REAL for ssyr2k DOUBLE PRECISION for dsyr2k COMPLEX for csyr2k DOUBLE COMPLEX for zsyr2k
	Array, DIMENSION (<i>ldb</i> , <i>kb</i>) where <i>kb</i> is <i>k</i> when trans = 'N' or 'n' and is 'n' otherwise. Before entry with $trans = 'N'$ or 'n', the leading <i>n</i> by <i>k</i> part of the array <i>b</i> must contain the matrix <i>b</i> , otherwise the leading <i>k</i> by <i>n</i> part of the array <i>b</i> must contain the matrix <i>b</i> .
ldb	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. When $trans = 'N'$ or 'n', then <i>ldb</i> must be at least $max(1,n)$, otherwise <i>ldb</i> must be at least $max(1, k)$.
beta	REAL for ssyr2k DOUBLE PRECISION for dsyr2k COMPLEX for csyr2k DOUBLE COMPLEX for zsyr2k
	Specifies the scalar beta.

С

REAL for ssyr2k DOUBLE PRECISION for dsyr2k COMPLEX for csyr2k DOUBLE COMPLEX for zsyr2k

Array, DIMENSION (ldc, n). Before entry with uplo = 'U' or 'u', the leading *n* by *n* upper triangular part of the array c must contain the upper triangular part of the symmetric matrix and the strictly lower triangular part of *c* is not referenced.

Before entry with uplo = 'L' or 'l', the leading *n* by *n* lower triangular part of the array *c* must contain the lower triangular part of the symmetric matrix and the strictly upper triangular part of *c* is not referenced.

INTEGER. Specifies the first dimension of c as declared in the calling (sub)program. The value of 1dc must be at least max(1, n).

Output Parameters

С

ldc

With uplo = 'U' or 'u', the upper triangular part of the array c is overwritten by the upper triangular part of the updated matrix.

With uplo = 'L' or 'l', the lower triangular part of the array c is overwritten by the lower triangular part of the updated matrix.

?trmm

Computes a scalar-matrix-matrix product (one matrix operand is triangular).

Discussion

The ?trmm routines perform a matrix-matrix operation using triangular matrices. The operation is defined as

b := alpha*op(a)*b
or
b := alpha*b*op(a)
where:
alpha is a scalar
b is an m by n matrix

a is a unit, or non-unit, upper or lower triangular matrix

op(a) is one of op(a) = a or op(a) = a' or op(a) = conjg(a').

Input Parameters

side	CHARACTER*1. Specifies whether op(a) multiplies b from the left or right in the operation as follows:
side value	Operation To Be Performed
L or l	b := alpha*op(a)*b
Rorr	<pre>b := alpha*b*op(a)</pre>
uplo	CHARACTER*1. Specifies whether the matrix <i>a</i> is an
	upper or lower triangular matrix as follows:
uplo value	Matrix a
U or u	Matrix a is an upper triangular matrix.
L or l	Matrix a is a lower triangular matrix.
transa	CHARACTER*1. Specifies the form of op(a) to be used
	in the matrix multiplication as follows:
transa value	Form of op(a)
N or n	op(a) = a
T or t	op(a) = a'
C or c	op(a) = conjg(a')
diag	CHARACTER*1. Specifies whether or not a is unit triangular as follows:
diag value	Matrix a
U or u	Matrix a is assumed to be unit triangular.
N or n	Matrix a is not assumed to be unit triangular.
m	INTEGER. Specifies the number of rows of <i>b</i> . The value
	of <i>m</i> must be at least zero.
n	INTEGER. Specifies the number of columns of b . The value of n must be at least zero.

Specifies the scalar <i>alpha</i> . When <i>alpha</i> is zero, then a	
is not referenced and <i>b</i> need not be set before entry.	
a REAL for strmm DOUBLE PRECISION for dtrmm COMPLEX for ctrmm DOUBLE COMPLEX for ztrmm	
Array, DIMENSION (lda, k) , where k is m when side = 'L' or 'l' and is n when $side = 'R'$ or 'r'. Before entry with $uplo = 'U'$ or 'u', the leading k by k upper triangular part of the array a must contain the upper triangular matrix and the strictly lower triangular part of a is not referenced.	
Before entry with $uplo = 'L'$ or 'l', the leading k by k lower triangular part of the array a must contain the lower triangular matrix and the strictly upper triangular part of a is not referenced. When $diag = 'U'$ or 'u', the diagonal elements of a are not referenced either, but are assumed to be unity.	
<pre>1da INTEGER. Specifies the first dimension of a as declared in the calling (sub)program. When side = 'L' or 'l', then 1da must be at least max(1, m), when side = 'R' or 'r', then 1da must be at least max(1, n).</pre>	
b REAL for strmm DOUBLE PRECISION for dtrmm COMPLEX for ctrmm DOUBLE COMPLEX for ztrmm	
Array, DIMENSION (ldb, n) . Before entry, the leading m by n part of the array b must contain the matrix b .	
1dbINTEGER. Specifies the first dimension of b as declared in the calling (sub)program. The value of 1db must be at least max(1, m).	

Output Parameters

b Overwritten by the transformed matrix.

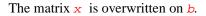
?trsm

Solves a matrix equation (one matrix operand is triangular).

Discussion

The ?trsm routines solve one of the following matrix equations:

```
op(a)*x = alpha*b,
or
x*op(a) = alpha*b,
where:
alpha is a scalar
x and b are m by n matrices
a is a unit, or non-unit, upper or lower triangular matrix
op(a) is one of op(a) = a or op(a) = a' or
op(a) = conjg(a').
```



Input Paramet	ers
side	CHARACTER*1. Specifies whether $op(a)$ appears on the left or right of x for the operation to be performed as follows:
side value	Operation To Be Performed
L or l	op(a)*x = alpha*b
Rorr	x*op(a) = alpha*b
uplo	CHARACTER*1. Specifies whether the matrix <i>a</i> is an upper or lower triangular matrix as follows:
uplo value	Matrix a
U or u	Matrix a is an upper triangular matrix.
L or l	Matrix a is a lower triangular matrix.
transa	CHARACTER*1. Specifies the form of op(a) to be used in the matrix multiplication as follows:
transa value	Form of op(a)
N or n	op(a) = a
T or t	op(a) = a'
C or c	op(a) = conjg(a')
diag	CHARACTER*1. Specifies whether or not a is unit triangular as follows:
diag value	Matrix a
U or u	Matrix a is assumed to be unit triangular.
N or n	Matrix a is not assumed to be unit triangular.
m	INTEGER. Specifies the number of rows of b . The value of m must be at least zero.
п	INTEGER. Specifies the number of columns of b . The value of n must be at least zero.

alpha	REAL for strsm DOUBLE PRECISION for dtrsm COMPLEX for ctrsm DOUBLE COMPLEX for ztrsm
	Specifies the scalar <i>alpha</i> . When <i>alpha</i> is zero, then <i>a</i> is not referenced and <i>b</i> need not be set before entry.
a	REAL for strsm DOUBLE PRECISION for dtrsm COMPLEX for ctrsm DOUBLE COMPLEX for ztrsm
	Array, DIMENSION (<i>lda</i> , <i>k</i>), where <i>k</i> is <i>m</i> when <i>side</i> = 'L' or 'l' and is <i>n</i> when <i>side</i> = 'R' or 'r'. Before entry with <i>uplo</i> = 'U' or 'u', the leading <i>k</i> by <i>k</i> upper triangular part of the array <i>a</i> must contain the upper triangular matrix and the strictly lower triangular part of <i>a</i> is not referenced.
	Before entry with <i>uplo</i> = 'L' or 'l', the leading <i>k</i> by <i>k</i> lower triangular part of the array <i>a</i> must contain the lower triangular matrix and the strictly upper triangular part of <i>a</i> is not referenced. When <i>diag</i> = 'U' or 'u', the diagonal elements of <i>a</i> are not referenced either, but are assumed to be unity.
lda	INTEGER. Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. When <i>side</i> = 'L' or 'l', then <i>lda</i> must be at least max(1, <i>m</i>), when <i>side</i> = 'R' or 'r', then <i>lda</i> must be at least max(1, <i>n</i>).
Ь	REAL for strsm DOUBLE PRECISION for dtrsm COMPLEX for ctrsm DOUBLE COMPLEX for ztrsm
	Array, DIMENSION $(1db, n)$. Before entry, the leading <i>m</i> by <i>n</i> part of the array <i>b</i> must contain the right-hand side matrix <i>b</i> .

b

1dbINTEGER. Specifies the first dimension of b as declaredin the calling (sub)program. The value of 1db must be atleast max(1, m).

Output Parameters

b Overwritten by the solution matrix *x*.

Sparse BLAS Routines and Functions

This section describes Sparse BLAS, an extension of BLAS Level 1 included in Intel[®] Math Kernel Library beginning with Intel MKL release 2.1. Sparse BLAS is a group of routines and functions that perform a number of common vector operations on sparse vectors stored in compressed form.

Sparse vectors are those in which the majority of elements are zeros. Sparse BLAS routines and functions are specially implemented to take advantage of vector sparsity. This allows you to achieve large savings in computer time and memory. If nz is the number of non-zero vector elements, the computer time taken by Sparse BLAS operations will be O(nz).

Vector Arguments in Sparse BLAS

Compressed sparse vectors. Let *a* be a vector stored in an array, and assume that the only non-zero elements of *a* are the following:

 $a(k_1), a(k_2), a(k_3) \dots a(k_{nz}),$

where nz is the total number of non-zero elements in a.

In Sparse BLAS, this vector can be represented in compressed form by two FORTRAN arrays, x (values) and *indx* (indices). Each array has *nz* elements:

```
x(1)=a(k_1), x(2)=a(k_2), \ldots x(nz)=a(k_{nz}),
```

```
indx(1)=k_1, indx(2)=k_2, ... indx(nz)=k_{nz}.
```

Thus, a sparse vector is fully determined by the triple (nz, x, indx). If you pass a negative or zero value of nz to Sparse BLAS, the subroutines do not modify any arrays or variables.

Full-storage vectors. Sparse BLAS routines can also use a vector argument fully stored in a single FORTRAN array (a full-storage vector). If y is a full-storage vector, its elements must be stored contiguously: the first element in y(1), the second in y(2), and so on. This corresponds to an increment *incy* = 1 in BLAS Level 1. No increment value for full-storage vectors is passed as an argument to Sparse BLAS routines or functions.

Naming Conventions in Sparse BLAS

Similar to BLAS, the names of Sparse BLAS subprograms have prefixes that determine the data type involved: **s** and **d** for single- and double-precision real; **c** and **z** for single- and double-precision complex.

If a Sparse BLAS routine is an extension of a "dense" one, the subprogram name is formed by appending the suffix i (standing for *indexed*) to the name of the corresponding "dense" subprogram. For example, the Sparse BLAS routine saxpyi corresponds to the BLAS routine saxpy, and the Sparse BLAS function cdotci corresponds to the BLAS function cdotc.

Routines and Data Types in Sparse BLAS

Routines and data types supported in the Intel MKL implementation of Sparse BLAS are listed in Table 2-4.

Table 2-4 Sparse BLAS Routines and Their Data Types

Routine/ Function	Data Types	Description
?axpyi	s, d, c, z	Scalar-vector product plus vector (routines)
?doti	s, d	Dot product (functions)
<u>?dotci</u>	C, Z	Complex dot product conjugated (functions)
<u>?dotui</u>	C, Z	Complex dot product unconjugated (functions)
?gthr	s, d, c, z	Gathering a full-storage sparse vector into compressed form: <i>nz</i> , <i>x</i> , <i>indx</i> (routines)
<u>?gthrz</u>	s, d, c, z	Gathering a full-storage sparse vector into compressed form and assigning zeros to gathered elements in the full-storage vector (routines)
<u>?roti</u>	s, d	Givens rotation (routines)
?sctr	s, d, c, z	Scattering a vector from compressed form to full-storage form (routines)

BLAS Routines That Can Work With Sparse Vectors

The following BLAS Level 1 routines will give correct results when you pass to them a compressed-form array x (with the increment *incx* = 1):

?asum	sum of absolute values of vector elements
?copy	copying a vector
?nrm2	Euclidean norm of a vector
?scal	scaling a vector
i?amax	index of the element with the largest absolute value or,
	for complex flavors, the largest sum $ \operatorname{Rex}(i) + \operatorname{Imx}(i) $.
i?amin	index of the element with the smallest absolute value or,
	for complex flavors, the smallest sum $ \operatorname{Rex}(i) + \operatorname{Imx}(i) $.

The result *i* returned by *i*?amax and *i*?amin should be interpreted as index in the compressed-form array, so that the largest (smallest) value is x(i); the corresponding index in full-storage array is *indx*(*i*).

You can also call **?rotg** to compute the parameters of Givens rotation and then pass these parameters to the Sparse BLAS routines **?roti**.

?axpyi

Adds a scalar multiple of compressed sparse vector to a full-storage vector.

```
call saxpyi ( nz, a, x, indx, y )
call daxpyi ( nz, a, x, indx, y )
call caxpyi ( nz, a, x, indx, y )
call zaxpyi ( nz, a, x, indx, y )
```

Discussion

The ?axpyi routines perform a vector-vector operation defined as

```
y := a^*x + y
where:
a is a scalar
```

(*nz*, *x*, *indx*) is a sparse vector stored in compressed form

y is a vector in full storage form.

The ?axpyi routines reference or modify only the elements of y whose indices are listed in the array *indx*. The values in *indx* must be distinct.

Input Parameters

nz	INTEGER. The number of elements in x and <i>indx</i> .
a	REAL for saxpyi DOUBLE PRECISION for daxpyi COMPLEX for caxpyi DOUBLE COMPLEX for zaxpyi
	Specifies the scalar a.
x	REAL for saxpyi DOUBLE PRECISION for daxpyi COMPLEX for caxpyi DOUBLE COMPLEX for zaxpyi Array, DIMENSION at least <i>nz</i> .
indx	INTEGER . Specifies the indices for the elements of <i>x</i> .
	Array, DIMENSION at least <i>nz</i> .
У	REAL for saxpyi DOUBLE PRECISION for daxpyi COMPLEX for caxpyi DOUBLE COMPLEX for zaxpyi
	Array, DIMENSION at least max _i (indx(i)).

Output Parameters

y Contains the updated vector *y*.

?doti

Computes the dot product of a compressed sparse real vector by a full-storage real vector.

res = sdoti (nz, x, indx, y)
res = ddoti (nz, x, indx, y)

Discussion

The ?doti functions return the dot product of x and y defined as

x(1)*y(indx(1)) + x(2)*y(indx(2)) + ... + x(nz)*y(indx(nz))

where the triple (*nz*, *x*, *indx*) defines a sparse real vector stored in compressed form, and *y* is a real vector in full storage form. The functions reference only the elements of *y* whose indices are listed in the array *indx*. The values in *indx* must be distinct.

Input Parameters

nz	INTEGER. The number of elements in x and <i>indx</i> .
x	REAL for sdoti DOUBLE PRECISION for ddoti Array, DIMENSION at least <i>nz</i> .
indx	INTEGER. Specifies the indices for the elements of x . Array, DIMENSION at least nz .
У	REAL for sdoti DOUBLE PRECISION for ddoti Array, DIMENSION at least $max_i(indx(i))$.

res	REAL for sdoti
	DOUBLE PRECISION for ddoti
	Contains the dot product of x and y , if nz is positive. Otherwise, <i>res</i> contains 0.

?dotci

Computes the conjugated dot product of a compressed sparse complex vector with a full-storage complex vector.

res = cdotci (nz, x, indx, y)
res = zdotci (nz, x, indx, y)

The values in *indx* must be distinct.

Discussion

The ?dotci functions return the dot product of x and y defined as

 $conjg(x(1))*y(indx(1)) + \ldots + conjg(x(nz))*y(indx(nz))$ where the triple (nz, x, indx) defines a sparse complex vector stored in compressed form, and y is a real vector in full storage form. The functions reference only the elements of y whose indices are listed in the array *indx*.

Input Parameters

nz	INTEGER. The number of elements in x and <i>indx</i> .
x	COMPLEX for cdotci DOUBLE COMPLEX for zdotci Array, DIMENSION at least <i>nz</i> .
indx	INTEGER. Specifies the indices for the elements of x . Array, DIMENSION at least nz .
У	COMPLEX for cdotci DOUBLE COMPLEX for zdotci Array, DIMENSION at least $max_i(indx(i))$.

res	COMPLEX for cdotci
	DOUBLE COMPLEX for zdotci
	Contains the conjugated dot product of \mathbf{x} and \mathbf{y} ,
	if <i>nz</i> is positive. Otherwise, <i>res</i> contains 0.

?dotui

Computes the dot product of a compressed sparse complex vector by a full-storage complex vector.

res = cdotui (nz, x, indx, y)
res = zdotui (nz, x, indx, y)

Discussion

The ?dotui functions return the dot product of x and y defined as

x(1)*y(indx(1)) + x(2)*y(indx(2)) + ... + x(nz)*y(indx(nz))where the triple (nz, x, indx) defines a sparse complex vector stored in compressed form, and y is a real vector in full storage form. The functions reference only the elements of y whose indices are listed in the array indx. The values in indx must be distinct.

Input Parameters

nz	INTEGER. The number of elements in x and <i>indx</i> .
x	COMPLEX for cdotui DOUBLE COMPLEX for zdotui Array, DIMENSION at least nz.
indx	INTEGER. Specifies the indices for the elements of x . Array, DIMENSION at least nz .
У	COMPLEX for cdotui DOUBLE COMPLEX for zdotui Array, DIMENSION at least max _i (<i>indx</i> (<i>i</i>)).

COMPLEX for cdotui
DOUBLE COMPLEX for zdotui
Contains the dot product of x and y , if nz is positive.
Otherwise, <i>res</i> contains 0.

?gthr

Gathers a full-storage sparse vector's elements into compressed form.

call sgthr (nz, y, x, indx)
call dgthr (nz, y, x, indx)
call cgthr (nz, y, x, indx)
call zgthr (nz, y, x, indx)

Discussion

The ?gthr routines gather the specified elements of a full-storage sparse vector y into compressed form (nz, x, indx). The routines reference only the elements of y whose indices are listed in the array *indx*:

x(i) = y(indx(i)), for i=1,2,...nz.

Input Parameters

nz	INTEGER. The number of elements of y to be gathered.
indx	INTEGER. Specifies indices of elements to be gathered. Array, DIMENSION at least nz .
У	REAL for sgthr
	DOUBLE PRECISION for dgthr
	COMPLEX for cgthr
	DOUBLE COMPLEX for zgthr
	Array, DIMENSION at least max _i (indx(i)).

Output Parameters

x	REAL for sgthr
	DOUBLE PRECISION for dgthr
	COMPLEX for cgthr
	DOUBLE COMPLEX for zgthr
	Array, DIMENSION at least <i>nz</i> .
	Contains the vector converted to the commu

Contains the vector converted to the compressed form.

?gthrz

Gathers a sparse vector's elements into compressed form, replacing them by zeros.

```
call sgthrz ( nz, y, x, indx )
call dgthrz ( nz, y, x, indx )
call cgthrz ( nz, y, x, indx )
call zgthrz ( nz, y, x, indx )
```

Discussion

The ?gthrz routines gather the elements with indices specified by the array *indx* from a full-storage vector y into compressed form (*nz*, *x*, *indx*) and overwrite the gathered elements of y by zeros. Other elements of y are not referenced or modified (see also ?gthr).

Input Parameters

nz	INTEGER. The number of elements of y to be gathered.
indx	INTEGER. Specifies indices of elements to be gathered. Array, DIMENSION at least nz .
У	REAL for sgthrz DOUBLE PRECISION for dgthrz COMPLEX for cgthrz
	DOUBLE COMPLEX for zgthrz
	Array, DIMENSION at least max _i (indx(i)).

x	REAL for sgthrz
	DOUBLE PRECISION for dgthrz
	COMPLEX for cgthrz
	DOUBLE COMPLEX for zgthrz
	Array, DIMENSION at least <i>nz</i> .
	Contains the vector converted to the compressed form.
У	The updated vector <i>y</i> .

?roti

Applies Givens rotation to sparse vectors one of which is in compressed form.

```
call sroti ( nz, x, indx, y, c, s ) call droti ( nz, x, indx, y, c, s )
```

Discussion

The **?roti** routines apply the Givens rotation to elements of two real vectors, x (in compressed form nz, x, indx) and y (in full storage form):

x(i) = c*x(i) + s*y(indx(i)) y(indx(i)) = c*y(indx(i)) - s*x(i)

The routines reference only the elements of y whose indices are listed in the array *indx*. The values in *indx* must be distinct.

Input Parameters

nz	INTEGER. The number of elements in x and <i>indx</i> .
x	REAL for sroti DOUBLE PRECISION for droti Array, DIMENSION at least <i>nz</i> .
indx	INTEGER. Specifies the indices for the elements of x . Array, DIMENSION at least nz .
У	REAL for sroti DOUBLE PRECISION for droti Array, DIMENSION at least max _i (indx(i)).
С	A scalar: REAL for sroti DOUBLE PRECISION for droti.
S	A scalar: REAL for sroti DOUBLE PRECISION for droti.

Output Parameters

x and y The updated arrays.

?sctr

Converts compressed sparse vectors into full storage form.

call ssctr (nz, x, indx, y)
call dsctr (nz, x, indx, y)
call csctr (nz, x, indx, y)
call zsctr (nz, x, indx, y)

Discussion

The ?sctr routines scatter the elements of the compressed sparse vector (nz, x, indx) to a full-storage vector y. The routines modify only the elements of y whose indices are listed in the array indx: y(indx(i)) = x(i), for i=1,2,...nz.

Input Parameters

nz	INTEGER. The number of elements of \mathbf{x} to be scattered.
indx	INTEGER. Specifies indices of elements to be scattered. Array, DIMENSION at least nz .
x	REAL for ssctr DOUBLE PRECISION for dsctr COMPLEX for csctr DOUBLE COMPLEX for zsctr
	Array, DIMENSION at least <i>nz</i> .
	Contains the vector to be converted to full-storage form.

У	REAL for ssctr
	DOUBLE PRECISION for dsctr
	COMPLEX for csctr
	DOUBLE COMPLEX for zsctr
	Array, DIMENSION at least $\max_{i} (indx(i))$.
	Contains the vector \mathbf{y} with updated elements.

Fast Fourier Transforms



This chapter describes the fast Fourier transform (FFT) routines implemented in Intel[®] MKL. The FFT routines included consist of two classes: one-dimensional and two-dimensional. Both one-dimensional and two-dimensional routines have been optimized to effectively use cache memory. All routines work with transforms of a power of 2 length.

For a more general set of Discrete Fourier Transform functions in Intel MKL, refer to <u>Advanced DFT Functions</u> in this manual.

Although Intel MKL still supports the FFT interface described later in this chapter, users are encouraged to migrate to the new DFT functions in their application programs. Unlike the FFT routines, the DFT routines support transforms of up to 7D, and transform lengths of other than powers of 2 mixed radix.

This chapter contains these major sections:

- One-dimensional FFTs
- Two-dimensional FFTs

Each of the major sections contains the description of three groups of the FFTs.

One-dimensional FFTs

The one-dimensional FFTs include the following groups:

- Complex-to-Complex Transforms
- Real-to-Complex Transforms
- Complex-to-Real Transforms.

All one-dimensional FFTs are in-place. The transform length must be a power of 2. The complex-to-complex transform routines perform both forward and inverse transforms of a complex vector. The real-to-complex transform routines perform forward transforms of a real vector. The complex-to-real transform routines perform inverse transforms of a complex conjugate-symmetric vector, which is packed in a real array.

Data Storage Types

Each FFT group contains two sets of FFTs having the similar functionality: one set is used for the Fortran-interface and the other for the C-interface. The former set stores the complex data as a Fortran complex data type, while the latter stores the complex data as float arrays of real and imaginary parts separately. These sets are distinguished by naming the FFTs within each set. The names of the FFTs used for the C-interface have the letter "c" added to the end of the FFTs' Fortran names. For example, the names of the cfftld/zfftld FFTs for the corresponding C-interface routines are cfftldc/zfftldc. All names of the C-type data items are lower case.

<u>Table 3-1</u> lists the one-dimensional FFT routine groups and the data types associated with them.

Group	Stored as Fortran Complex Data	Stored as C Real Data	Data	Description
Group	Dala	Redi Dala	Types	8
Complex- to- Complex	<u>cfftld/</u> <u>zfftld</u>	<u>cfftldc/</u> <u>zfftldc</u>	C, Z	Transform complex data to complex data.
Real-to- Complex	<u>scfft1d/</u> dzfft1d	<u>scfftldc/</u> <u>dzfftldc</u>	sc, dz	Transform forward real-to-complex data Complement csfftld/zdfftld and csfftldc/zdfftldc FFTs.
Complex- to-Real	<u>csfft1d/</u> zdfft1d	<u>csfft1dc/</u> zdfft1dc	cs, zd	Transform inverse complex-to-real data Complement scfftld/dzfftld and scfftldc/dzfftldc FFTs.

Table 3-1 One-dimensional FFTs: Names and Data Types

Data Structure Requirements

For C-interface, storage of the complex-to-complex transform routines data requires separate float arrays for the real and imaginary parts. The real-to-complex and complex-to-real pairs require a single float input/output array.

The C-interface requires scalar values to be passed by value.

All transforms require additional memory to store the transform coefficients. When performing multiple FFTs of the same dimension, the

table of coefficients should be created only once and then used on all the FFTs afterwards. Using the same table rather than creating it repeatedly for each FFT produces an obvious performance gain.

Complex-to-Complex One-dimensional FFTs

Each of the complex-to-complex routines computes a forward or inverse FFT of a complex vector.

The forward FFT is computed according to the mathematical equation

$$z_{j} = \sum_{k=0}^{n-1} r_{k} * w^{-j*k}, \quad 0 \le j \le n-1$$

The inverse FFT is computed according to the mathematical equation

$$r_{j} = \frac{1}{n} \sum_{k=0}^{n-1} z_{k} * w^{j*k}, \quad 0 \le j \le n-1$$

where $w = \exp\left[\frac{2\pi i}{n}\right]$, *i* being the imaginary unit.

The operation performed by the complex-to-complex routines is determined by the value of the *isign* parameter used by each of these routines.

If *isign* = -1, perform the forward FFT where input and output are in normal order.

If *isign* = +1, perform the inverse FFT where input and output are in normal order.

If isign = -2, perform the forward FFT where input is in normal order and output is in bit-reversed order.

If *isign* = +2, perform the inverse FFT where input is in bit-reversed order

and output is in normal order.

If *isign* = 0, initialize FFT coefficients for both the forward and inverse FFTs.

The above equations apply to all FFTs with all data types indicated in <u>Table 3-1</u>.

To compute a forward or inverse FFT of a given length, first initialize the coefficients by calling the function with isign = 0. Thereafter, any number of transforms of the same length can be computed by calling the function with isign = +1, -1, +2, -2.

cfft1d/zfft1d

Fortran-interface routines. Compute the forward or inverse FFT of a complex vector (in-place)

```
call cfft1d ( r, n, isign, wsave )
call zfft1d ( r, n, isign, wsave )
```

Discussion

The operation performed by the cfftld/zfftld routines is determined by the value of *isign*. See the equations of the operations for the <u>Complex-to-Complex One-dimensional FFTs</u> above.

Input Parameters

r	COMPLEX for cfftld DOUBLE COMPLEX for zfftld Array, DIMENSION at least (n) . Contains the complex vector on which the transform is to be performed. Not referenced if <i>isign</i> = 0.
n	INTEGER. Transform length; <i>n</i> must be a power of 2.
isign	INTEGER. Flag indicating the type of operation to be performed: if <i>isign</i> = 0, initialize the coefficients <i>wsave</i> ;

	if <i>isign</i> = -1, perform the forward FFT where input and output are in normal order; if <i>isign</i> = +1, perform the inverse FFT where input and output are in normal order;
	if $isign = -2$, perform the forward FFT where input is in normal order and output is in bit-reversed order; if $isign = +2$, perform the inverse FFT where input is in bit-reversed order and output is in normal order.
wsave	COMPLEX for cfftld DOUBLE COMPLEX for zfftld Array, DIMENSION at least $((3*n)/2)$. If <i>isign</i> = 0, then <i>wsave</i> is an output parameter. Otherwise, <i>wsave</i> contains the FFT coefficients initialized on a previous call with <i>isign</i> = 0.
Output Parame	eters
r	Contains the complex result of the transform depending on <i>isign</i> . Does not change if <i>isign</i> = 0.
wsave	If <i>isign</i> = 0, <i>wsave</i> contains the initialized FFT coefficients. Otherwise, <i>wsave</i> does not change.

cfft1dc/zfft1dc

C-interface routines. Compute the forward or inverse FFT of a complex vector (in-place).

```
void cfftldc (float* r, float* i, int n, int isign, float* wsave)
void zfftldc (double* r, double* i, int n, int isign, double* wsave)
```

Discussion

The operation performed by the cfftldc/zfftldc routines is determined by the value of *isign*. See the equations of the operations for the <u>Complex-to-Complex One-dimensional FFTs</u>.

Input Parameters

r	<pre>float* for cfftldc double* for zfftldc Pointer to an array of size at least (n). Contains the real parts of complex vector to be transformed. Not referenced if isign = 0.</pre>
i	float* for cfftldc double* for zfftldc
	Pointer to an array of size at least (<i>n</i>). Contains the imaginary parts of complex vector to be transformed.
	Not referenced if $isign = 0$.
п	int. Transform length; <i>n</i> must be a power of 2.
isign	<pre>int. Flag indicating the type of operation to be performed: if isign = 0, initialize the coefficients wsave; if isign = -1, perform the forward FFT where input and output are in normal order; if isign = +1, perform the inverse FFT where input and output are in normal order; if isign = -2, perform the forward FFT where input is in normal order and output is in bit-reversed order; if isign = +2, perform the inverse FFT where input is in bit-reversed order and output is in normal order.</pre>
wsave	<pre>float* for cfftldc double* for zfftldc Pointer to an array of size at least (3*n). If isign = 0, then wsave is an output parameter. Otherwise, wsave contains the FFT coefficients initialized on a previous call with isign = 0.</pre>

Output Parameters

r

Contains the real part of the transform depending on *isign*. Does not change if *isign* = 0.

i	Contains the imaginary part of the transform depending on <i>isign</i> . Does not change if <i>isign</i> = 0.
wsave	If <i>isign</i> = 0, <i>wsave</i> contains the initialized FFT coefficients. Otherwise, <i>wsave</i> does not change.

Real-to-Complex One-dimensional FFTs

Each of the real-to-complex routines computes forward FFT of a real input vector according to the mathematical equation

$$z_{j} = \sum_{k=0}^{n-1} t_{k} * w^{-j*k}, 0 \le j \le n-1$$

for $t_k = \text{cmplx}(r_k, 0)$, where r_k is the real input vector, $0 \le k \le n-1$. The mathematical result z_j , $0 \le j \le n-1$, is the complex conjugate-symmetric vector, where z(n/2+i) = conjg(z(n/2-i)), $1 \le i \le n/2 - 1$, and moreover z(0) and z(n/2) are real values.

This complex conjugate-symmetric (CCS) vector can be stored in the complex array of size (n/2+1) or in the real array of size (n+2). The data storage of the CCS format is defined later for Fortran-interface and C-interface routines separately.

<u>Table 3-2</u> shows a comparison of the effects of performing the cfftld/ zfftld complex-to-complex FFT on a vector of length n=8 in which all the imaginary elements are zeros, with the real-to-complex scfftld/zdfftld FFT applied to the same vector. The advantage of the latter approach is that only half of the input data storage is required and there is no need to zero the imaginary part. The last two columns are stored in the real array of size (n+2) containing the complex conjugate-symmetric vector in CCS format. To compute a forward FFT of a given length, first initialize the coefficients by calling the routine you are going to use with *isign* = 0. Thereafter, any number of real-to-complex and complex-to-real transforms of the same length can be computed by calling that routine with the *isign* value other than 0.

Table 3-2 Comparison of the Storage Effects of Complex-to-Complex and Real-to-Complex FFTs

	Input Vectors	i	Output Vectors				
cff	t1d	scfft1d	cff	t1d	scfft1d		
Compl	ex Data	Real Data	Comple	ex Data	Rea	l Data	
Real	Imaginary		Real	Imaginary	(Real)	(Imaginary)	
0.841471	0.000000	0.841471	1.543091	0.000000	1.543091	0.000000	
0.909297	0.000000	0.909297	3.875664	0.910042	3.875664	0.910042	
0.141120	0.000000	0.141120	-0.915560	-0.397326	-0.915560	-0.397326	
-0.756802	0.000000	-0.756802	-0.274874	-0.121691	-0.274874	-0.121691	
-0.958924	0.000000	-0.958924	-0.181784	0.000000	-0.181784	0.000000	
-0.279415	0.000000	-0.279415	-0.274874	0.121691			
0.656987	0.000000	0.656987	-0.915560	0.397326			
0.989358	0.000000	0.989358	3.875664	-0.910042			

scfft1d/dzfft1d

Fortran-interface routines. Compute forward FFT of a real vector and represent the complex conjugate-symmetric result in CCS format (in-place).

call scfftld (r, n, isign, wsave)
call dzfftld (r, n, isign, wsave)

Discussion

The operation performed by the scfftld/dzfftld routines is determined by the value of *isign*. See the equations of the operations for <u>Real-to-Complex One-dimensional FFTs</u> above. These routines are complementary to the complex-to-real transform routines csfftld/zdfftld.

Input Parameters

r	REAL for scfftld DOUBLE PRECISION for dzfftld
	Array, DIMENSION at least $(n+2)$. First <i>n</i> elements contain the input vector to be transformed. The elements r(n+1) and $r(n+2)$ are used on output. The array <i>r</i> is not referenced if <i>isign</i> = 0.
п	INTEGER . Transform length; <i>n</i> must be a power of 2.
isign	INTEGER. Flag indicating the type of operation to be performed: if <i>isign</i> is 0, initialize the coefficients <i>wsave</i> ; if <i>isign</i> is not 0, perform the forward FFT.
wsave	REAL for scfftld DOUBLE PRECISION for dzfftld
	Array, DIMENSION at least $(2*n+4)$. If <i>isign</i> = 0, then <i>wsave</i> contains output data. Otherwise, <i>wsave</i> contains coefficients required to perform the FFT that has been initialized on a previous call to this routine or the complementary complex-to-real FFT routine.

r	If <i>isign</i> = 0, <i>r</i> does not change. If <i>isign</i> is not 0, the
	output real-valued array $r(1:n+2)$ contains the
	complex conjugate-symmetric vector $z(1:n)$ packed in
	CCS format for Fortran interface.
	The table below shows the relationship between them.

r(1)	r(2)	r(3)	r(4)	 r(n-1)	r(n)	r(n+1)	r(n+2)	
z(1)	0	REz(2)	IMz(2)	 $\operatorname{RE} z(n/2)$	IMz(n/2)	<i>z</i> (<i>n</i> /2+1)	0	

The full complex vector z(1:n) is defined by $z(i) = \operatorname{cmplx}(r(2*i-1), r(2*i)),$ $1 \le i \le n/2+1,$ $z(n/2+i) = \operatorname{conjg}(z(n/2+2-i)),$ $2 \le i \le n/2.$ Then, z(1:n) is the forward FFT of a real input vector r(1:n).If *isign* = 0, *wsave* contains the coefficients required by the called routine. Otherwise *wsave* does not change.

scfft1dc/dzfft1dc

C-interface routines. Compute forward FFT of a real vector and represent the complex conjugatesymmetric result in CCS format (in-place).

wsave

void scfftldc (float* r, int n, int isign, float* wsave); void dzfftldc (double* r, int n, int isign, double* wsave);

Discussion

The operation performed by the scfftldc/dzfftldc routines is determined by the value of *isign*. See the equations of the operations for the <u>Real-to-Complex One-dimensional FFTs</u> above. These routines are complementary to the complex-to-real transform routines <u>csfftldc/zdfftldc</u>.

Input Parameters

r	float* for scfftldc double* for dzfftldc
	Pointer to an array of size at least $(n+2)$. First <i>n</i> elements contain the input vector to be transformed. The array <i>r</i> is not referenced if <i>isign</i> = 0.
п	int. Transform length; <i>n</i> must be a power of 2.
isign	int . Flag indicating the type of operation to be performed:
	if <i>isign</i> is 0, initialize the coefficients <i>wsave</i> ;
	if <i>isign</i> is not 0, perform the forward FFT.
wsave	float* for scfftldc double* for dzfftldc
	Pointer to an array of size at least $(2*n+4)$. If <i>isign</i> = 0, then <i>wsave</i> contains output data. Otherwise, <i>wsave</i> contains coefficients required to perform the FFT that has been initialized on a previous call to this routine or the complementary complex-to-real FFT routine.

Output Parameters

r	If <i>isign</i> = 0, <i>r</i> does not change. If <i>isign</i> is not 0, the
	output real-valued array $r(0:n+1)$ contains the
	complex conjugate-symmetric vector $z(0:n-1)$
	packed in CCS format for C-interface.
	The table below shows the relationship between them.

r(0)	r(1)	r(2)	 r(n/2)	r(n/2+1)	r(n/2+2)	 r(n)	r(n+1)
z(0)	RE <i>z</i> (1)	RE <i>z</i> (2)	 z(n/2)	0	IMz(1)	 IMz(n/2-1)	0

The full complex vector z(0:n-1) is defined by

 $z(i) = cmplx(r(i), r(n/2+1+i)), 0 \le n/2,$

 $z(n/2+i) = \operatorname{conjg}(z(n/2-i)), 1 \le i \le n/2-1.$ Then, z(0:n-1) is the forward FFT of the real input vector of length *n*.

wsave

If *isign* = 0, *wsave* contains the coefficients required by the called routine. Otherwise *wsave* does not change.

Complex-to-Real One-dimensional FFTs

Each of the complex-to-real routines computes a one-dimensional inverse FFT according to the mathematical equation

 $t_{j} = \frac{1}{n} \sum_{k=0}^{n-1} z_{k} * w^{j * k}, \quad 0 \le j \le n-1$

The mathematical input is the complex conjugate-symmetric vector z_j , $0 \le j \le n-1$, where $z(n/2+i) = \operatorname{conjg}(z(n/2-i)), 1 \le i \le n/2-1$, and moreover z(0) and z(n/2) are real values.

The mathematical result is $t_j = \text{cmplx}(r_j, 0)$, where r_j is a real vector, $0 \le j \le n-1$.

Input to the complex-to-real transform routines is a real array of size (n+2), which contains the complex conjugate-symmetric vector z(0:n-1) in CCS format (see <u>Real-to-Complex One-dimensional FFTs</u> above).

Output of the complex-to-real routines is a real vector of size n.

<u>Table 3-3</u> is identical to <u>Table 3-2</u>, except for reversing the input and output vectors. In the complex-to-real routines the last two columns are stored in the input real array of size (n+2) containing the complex conjugate-symmetric vector in CCS format.

To compute an inverse FFT of a given length, first initialize the coefficients by calling the routine you are going to use with *isign* = 0. Thereafter, any number of real-to-complex and complex-to-real transforms of the same length can be computed by calling the appropriate routine with the *isign* value other than 0.

C	Dutput Vector	s		Input	Vectors		
cff	tld	csfft1d	cff	tld	csfft1d		
Compl	ex Data	Real Data	Compl	ex Data	Rea	I Data	
Real	Imaginary		Real	Imaginary	(Real)	(Imaginary)	
0.841471	0.000000	0.841471	1.543091	0.000000	1.543091	0.000000	
0.909297	0.000000	0.909297	3.875664	0.910042	3.875664	0.910042	
0.141120	0.000000	0.141120	-0.915560	-0.397326	-0.915560	-0.397326	
-0.756802	0.000000	-0.756802	-0.274874	-0.121691	-0.274874	-0.121691	
-0.958924	0.000000	-0.958924	-0.181784	0.000000	-0.181784	0.000000	
-0.279415	0.000000	-0.279415	-0.274874	0.121691			
0.656987	0.000000	0.656987	-0.915560	0.397326			
0.989358	0.000000	0.989358	3.875664	-0.910042			

Table 3-3 Comparison of the Storage Effects of Complex-to-Real and Complex-to-Complex FFTs

csfft1d/zdfft1d

Fortran-interface routines. Compute inverse FFT of a complex conjugate-symmetric vector packed in CCS format (in-place).

```
call csfftld ( r, n, isign, wsave )
call zdfftld ( r, n, isign, wsave )
```

Discussion

The operation performed by the csfftld/zdfftld routines is determined by the value of *isign*. See the equations of the operations for the <u>Complex-to-Real One-dimensional FFTs</u> above.

These routines are complementary to the real-to-complex transform routines scfftld/dzfftld.

Input Parameters

.

r

REAL for csfft1d

DOUBLE PRECISION for zdfftld

Array, DIMENSION at least (n+2). Not referenced if isign = 0.

If *isign* is not 0, then r(1:n+2) contains the complex conjugate-symmetric vector packed in CCS format for Fortran-interface.

The table below shows the relationship between them

r(1)	r(2)	r(3)	r(4)	 r(n-1)	r(n)	<i>r</i> (<i>n</i> +1)	r(n+2)
z(1)	0	RE <i>z</i> (2)	IMz(2)	 RE <i>z(n/2</i>)	IMz(n/2)	z(n/2+1)	0

```
The full complex vector z(1:n) is defined by
```

z(i) = cmplx(r(2*i-1), r(2*i)), $1 \le i \le n/2+1,$ z(n/2+i) = conjg(z(n/2+2-i)), $2 \le i \le n/2.$

After the transform, r(1:n) contains the inverse FFT of the complex conjugate-symmetric vector z(1:n).

п	INTEGER . Transform length; <i>n</i> must be a power of 2.
isign	INTEGER. Flag indicating the type of operation to be performed: if <i>isign</i> is 0, initialize the coefficients wsave; if <i>isign</i> is not 0, perform the inverse FFT.
wsave	REAL for csfftld DOUBLE PRECISION for zdfftld Array, DIMENSION at least $(2*n+4)$. If isign = 0,

then *wsave* contains output data. Otherwise, *wsave*

contains coefficients required to perform the FFT that has been initialized on a previous call to this routine or the complementary real-to-complex FFT routine.

Output Parameters

r	If <i>isign</i> is not 0, then $r(1:n)$ is the real result of the
	inverse FFT of the complex conjugate-symmetric vector
	z(1:n). Does not change if $isign = 0$.
wsave	If <i>isign</i> = 0, <i>wsave</i> contains the coefficients required
	by the called routine. Otherwise <i>wsave</i> does not change.

csfft1dc/zdfft1dc

C-interface routines.Compute inverse FFT of a complex conjugate-symmetric vector packed in CCS format (in-place).

void csfftldc (float* r, int n, int isign, float* wsave)
void zdfftldc (double* r, int n, int isign, double* wsave)

Discussion

The operation performed by the csfftldc/zdfftldc routines is determined by the value of *isign*. See the equations of the operations for the <u>Complex-to-Real One-dimensional FFTs</u> above.

These routines are complementary to the real-to-complex transform routines <u>scfftldc/dzfftldc</u>.

Input Parameters

r float* for csfftldc
double* for zdfftldc

Pointer to an array of size at least (n+2). Not referenced if isign = 0.

If *isign* is not 0, then r(0:n+1) contains the complex conjugate-symmetric vector packed in CCS format for C-interface.

The table below shows the relationship between them.

z(0) RE $z(1)$ RE $z(2)$ $z(n/2)$ 0 IM $z(1)$ IM $z(n/2-1)$ 0	r(0)	r(1)	r(2)	 r(n/2)	r(n/2+1)	r(n/2+2)	 r(n)	r(n+1)
	z(0)	RE <i>z</i> (1)	RE <i>z</i> (2)	 z(n/2)	0	IMz(1)	 IMz(n/2-1)	0

	The full complex vector $z(0:n-1)$ is defined by $z(i) = \operatorname{cmplx}(r(i), r(n/2+1+i)), \ 0 \le i \le n/2,$
	$z(n/2+i) = \operatorname{conjg}(z(n/2-i)), 1 \le i \le n/2-1$. After the transform, $r(0:n-1)$ is the inverse FFT of the complex conjugate-symmetric vector $z(0:n-1)$.
п	int. Transform length; n must be a power of 2.
isign	<pre>int. Flag indicating the type of operation to be performed: if isign = 0, initialize the coefficients wsave; if isign is not 0, perform the inverse FFT.</pre>
wsave	<pre>float* for csfftldc double* for zdfftldc Pointer to an array of size at least (2*n+4). If isign = 0, then wsave contains output data. Otherwise, wsave contains coefficients required to perform the FFT that has been initialized on a previous call to this routine or the complementary real-to-complex FFT routine.</pre>

Γ	If <i>isign</i> is not 0, then $r(0:n-1)$ is the real result of the inverse FFT of the complex conjugate-symmetric vector $z(0:n-1)$. Does not change if <i>isign</i> = 0.
wsave	If <i>isign</i> = 0, <i>wsave</i> contains the coefficients required by the called routine. Otherwise <i>wsave</i> does not change.

Two-dimensional FFTs

The two-dimensional FFTs are functionally the same as one-dimensional FFTs. They contain the following groups:

- Complex-to-Complex Transforms
- Real-to-Complex Transforms
- Complex-to-Real Transforms.

All two-dimensional FFTs are in-place. Transform lengths must be a power of 2. The complex-to-complex transform routines perform both forward and inverse transforms of a complex matrix. The real-to-complex transform routines perform forward transforms of a real matrix. The complex-to-real transform routines perform inverse transforms of a complex conjugate-symmetric matrix, which is packed in a real array.

The naming conventions are also the same as those for one-dimensional FFTs, with "2d" replacing "1d" in all cases. <u>Table 3-4</u> lists the two-dimensional FFT routine groups and the data types associated with them.

Group	Stored as FORTRAN Complex Data	Stored as C Real Data	Data Types	Description
Complex- to- Complex	<u>cfft2d/</u> zfft2d	<u>cfft2dc/</u> zfft2dc	C, Z	Transform complex data to complex data.
Real-to- Complex	<u>scfft2d/</u> dzfft2d	<u>scfft2dc/</u> dzfft2dc	sc, dz	Transform forward real-to-complex data. Complement csfft2d/zdfft2d and csfft2dc/zdfft2dc FFTs.
Complex- to-Real	<u>csfft2d/</u> zdfft2d	<u>csfft2dc/</u> zdfft2dc	cs, zd	Transform inverse complex-to-real data. Complement scfft2d/dzfft2d and scfft2dc/dzfft2dc FFTs.

Table 3-4Two-dimensional FFTs: Names and Data Types

The C-interface requires scalar values to be passed by value. The major difference between the one-dimensional and two-dimensional FFTs is that your application does not need to provide storage for transform coefficients.

The data storage types and data structure requirements are the same as for one-dimensional FFTs. For more information, see the <u>Data Storage Types</u> and <u>Data Structure Requirements</u> sections at the beginning of this chapter.

Complex-to-Complex Two-dimensional FFTs

Each of the complex-to-complex routines computes a forward or inverse FFT of a complex matrix in-place.

The forward FFT is computed according to the mathematical equation

$$z_{i,j} = \sum_{k=0}^{m-1} \sum_{l=0}^{n-1} r_{k,l} * w_m^{-i*k} * w_n^{-j*l}, \quad 0 \le i \le m-1, \quad 0 \le j \le n-1$$

The inverse FFT is computed according to the mathematical equation

$$r_{i,j} = \frac{1}{m*n} \sum_{k=0}^{m-1} \sum_{l=0}^{n-1} z_{k,l} * w_m^{i*k} * w_n^{j*l}, \quad 0 \le i \le m-1, \quad 0 \le j \le n-1$$

where $w_m = \exp\left[\frac{2\pi i}{m}\right]$, $w_n = \exp\left[\frac{2\pi i}{n}\right]$, *i* being the imaginary unit.

The operation performed by the complex-to-complex routines is determined by the value of the *isign* parameter.

If *isign* = -1, perform the forward FFT where input and output are in normal order.

If *isign* = +1, perform the inverse FFT where input and output are in normal order.

If isign = -2, perform the forward FFT where input is in normal order and output is in bit-reversed order.

If isign = +2, perform the inverse FFT where input is in bit-reversed order and output is in normal order.

The above equations apply to all FFTs with all data types indicated in <u>Table 3-4</u>.

cfft2d/zfft2d

Fortran-interface routines. Compute the forward or inverse FFT of a complex matrix (in-place).

call cfft2d (r, m, n, isign)
call zfft2d (r, m, n, isign)

Discussion

The operation performed by the cfft2d/zfft2d routines is determined by the value of *isign*. See the equations of the operations for <u>Complex-to-Complex Two-dimensional FFTs</u>.

r	COMPLEX for cfft2d DOUBLE COMPLEX for zfft2d Array, DIMENSION at least (m, n), with its leading dimension equal to m. This array contains the complex matrix to be transformed.
m	INTEGER . Column transform length (number of rows); <i>m</i> must be a power of 2.
п	INTEGER . Row transform length (number of columns); <i>n</i> must be a power of 2.
isign	<pre>INTEGER. Flag indicating the type of operation to be performed: if isign = -1, perform the forward FFT where input and output are in normal order; if isign = +1, perform the inverse FFT where input and output are in normal order; if isign = -2, perform the forward FFT where input is in normal order and output is in bit-reversed order; if isign = +2, perform the inverse FFT where input is in bit-reversed order and output is in normal order.</pre>

Output Parameters

r

Contains the complex result of the transform depending on *isign*.

cfft2dc/zfft2dc

C-interface routines. Compute the forward or inverse FFT of a complex matrix (in-place).

r

i

т

```
void cfft2dc ( float* r, float* i, int m, int n, int isign )
void zfft2dc ( double* r, double* i, int m, int n, int isign )
```

Discussion

The operation performed by the cfft2dc/zfft2dc routines is determined by the value of *isign*. See the equations of the operations for the <u>Complex-to-Complex Two-dimensional FFTs</u> above.

float* for cfft2dc double* for zfft2dc
Pointer to a two-dimensional array of size at least (m, n) , with its leading dimension equal to n . The array contains the real parts of a complex matrix to be transformed.
float* for cfft2dc double* for zfft2dc
Pointer to a two-dimensional array of size at least (m, n) , with its leading dimension equal to n . The array contains the imaginary parts of a complex matrix to be transformed.
int. Column transform length (number of rows); <i>m</i> must be a power of 2.

n	int. Row transform length (number of columns); <i>n</i> must be a power of 2.
isign	int. Flag indicating the type of operation to be performed:
	 if <i>isign</i> = -1, perform the forward FFT where input and output are in normal order; if <i>isign</i> = +1, perform the inverse FFT where input and output are in normal order; if <i>isign</i> = -2, perform the forward FFT where input is in normal order and output is in bit-reversed order; if <i>isign</i> = +2, perform the inverse FFT where input is in bit-reversed order and output is in normal order.

Output Parameters

r	Contains the real parts of the complex result depending on	isign.

i Contains the imaginary parts of the complex depending on *isign*.

Real-to-Complex Two-dimensional FFTs

Each of the real-to-complex routines computes the forward FFT of a real matrix according to the mathematical equation

$$z_{i,j} = \sum_{k=0}^{m-1} \sum_{l=0}^{n-1} t_{k,l} * w_m^{-i*k} * w_n^{-j*l}, \quad 0 \le i \le m-1, \quad 0 \le j \le n-1$$

 $t_{k,1} = \text{cmplx}(r_{k,1}, 0)$, where $r_{k,1}$ is a real input matrix, $0 \le k \le m-1$, $0 \le l \le n-1$. The mathematical result $z_{i,j}$, $0 \le i \le m-1$, $0 \le j \le n-1$, is the complex matrix of size (m, n). Each column is the complex conjugate-symmetric vector as follows:

for $0 \leq j \leq n-1$,

 $z(m/2+i,j) = \text{conjg}(z(m/2-i,j)), 1 \le i \le m/2-1.$ Moreover, z(0,j) and z(m/2,j) are real values for j=0 and j=n/2.

This mathematical result can be stored in the complex two-dimensional array of size (m/2+1, n/2+1) or in the real two-dimensional array of size (m+2, n+2). The data storage of CCS format is defined later for Fortran-interface and C-interface routines separately.

scfft2d/dzfft2d

Fortran-interface routines. Compute forward FFT of a real matrix and represent the complex conjugate-symmetric result in CCS format (in-place).

```
call scfft2d ( r, m, n )
call dzfft2d ( r, m, n )
```

Discussion

See the equations of the operations for the <u>Real-to-Complex</u> <u>Two-dimensional FFTs</u> above.

These routines are complementary to the complex-to-real transform routines csfft2d/zdfft2d.

r	REAL for scfft2d
	DOUBLE PRECISION for dzfft2d
	Array, DIMENSION at least $(m+2, n+2)$, with its leading
	dimension equal to $(m+2)$. The first <i>m</i> rows and <i>n</i>
	columns of this array contain the real matrix to be
	transformed. <u>Table 3-5</u> presents the input data layout.
m	INTEGER. Column transform length (number of rows); <i>m</i> must be a power of 2.
n	INTEGER. Row transform length (number of columns); <i>n</i> must be a power of 2.

r(1,1)	r(1,2)	•••	r(1,n-1)	r(1,n)	n/u	n/u
r(2,1)	r(2,2)	• • •	r(2,n-1)	r(2,n)	n/u	n/u
r(3,1)	r(3,2)	• • •	r(3,n-1)	r(3,n)	n/u	n/u
r(4,1)	r(4,2)	• • •	r(4,n-1)	r(4,n)	n/u	n/u
•••			•••	•••		
r(m-1,1)	r(m-1,2)		r(m-1,n-1)	r(m-1,n)	n/u	n/u
r(m,1)	r(m,2)		r(m,n-1)	r(m,n)	n/u	n/u
n/u	n/u		n/u	n/u	n/u	n/u
n/u	n/u		n/u	n/u	n/u	n/u

Table 3-5 Fortran-interface Real Data Storage for the Real-to-Complex and Complex-to-Real Two-dimensional FFTs

* n/u - not used

Output Parameters

- *r* The output real array r(1:m+2,1:n+2) contains the complex conjugate-symmetric matrix z(1:m,1:n) packed in CCS format for Fortran-interface as follows:
 - Rows 1 and m+1 contain in n+2 locations the complex conjugate-symmetric vectors z(1, j) and z(m/2+1, j) packed in CCS format (see<u>Real-to-Complex</u>
 <u>One-dimensional FFTs</u> above).

```
The full complex vector z(1, j) is defined by:
```

```
z(1, j) = cmplx(r(1, 2*j-1), r(1, 2*j)), 1 \le j \le n/2+1,
```

```
z(1, n/2+1+j) = conjg(z(1, n/2+1-j)), 1 \le j \le n/2-1.
```

```
The full complex vector z(m/2+1, j) is defined by:
```

z(m/2+1,j) = cmplx(r(m+1,2*j-1),r(m+1,2*j)), $1 \le j \le n/2+1,$

z(m/2+1,n/2+1+j) = conjg(z(m/2+1,n/2+1-j)), 1 ≤j ≤n/2-1;

Rows from 3 to *m* contain in *n* locations complex vectors represented as z(i+1, j) = cmplx(r(2*i+1, j), r(2*i+2, j)), 1 ≤i ≤m/2-1, 1 ≤j ≤n.

• The rest matrix elements can be obtained from

 $z(m/2+1+i, j) = \operatorname{conjg}(z(m/2+1-i, j)),$ $1 \le i \le m/2-1, 1 \le j \le n.$

The storage of the complex conjugate-symmetric matrix z for Fortran-interface is shown in <u>Table 3-6</u>.

Table 3-6Fortran-interface Data Storage of CCS Format for the
Real-to-Complex and Complex-to-Real Two-Dimensional FFTs

z(1,1)	0	RE <i>z</i> (1,2)	IMz(1,2)	 RE <i>z</i> (1, <i>n</i> /2)	IMz(1,n/2)	z(1, n/2+1)	0
0	0	0	0	 0	0	0	0
RE <i>z</i> (2,1)	REz(2,2)	RE <i>z</i> (2,3)	RE <i>z</i> (2,4)	 REz(2,n-1)	RE <i>z</i> (2, <i>n</i>)	n/u	n/u
IMz(2,1)	IMz(2,2)	IMz(2,3)	IMz(2,4)	 IMz(2,n-1)	IMz(2,n)	n/u	n/u
				 		n/u	n/u
RE <i>z</i> (<i>m</i> /2,1)	RE <i>z</i> (<i>m</i> /2,2)	RE <i>z</i> (<i>m</i> /2,3)	RE <i>z(m/</i> 2,4)	 RE <i>z(m/2,</i> <i>n</i> -1)	RE <i>z(m/</i> 2, <i>n</i>)	n/u	n/u
IM <i>z</i> (<i>m</i> /2,1)	IM <i>z</i> (<i>m</i> /2,2)	IM <i>z</i> (<i>m</i> /2,3)	IM <i>z</i> (<i>m</i> /2,4)	 IMz(m/2, n-1)	IMz(m/2, n)	n/u	n/u
<i>z</i> (<i>m</i> /2+1,1)	0	RE <i>z</i> (<i>m</i> /2+1,2)	IM <i>z</i> (<i>m</i> /2+1,2)	 RE <i>z(m/</i> 2+1, <i>n/</i> 2)	IMz(m/2+1, n/2)	z(m/2+1, n/2+1)	0
0	0	0	0	 0	0	n/u	n/u

* n/u - not used

scfft2dc/dzfft2dc

C-interface routine. Compute forward FFT of a real matrix and represent the complex conjugate-symmetric result in CCS format (in-place).

void scfft2dc (float* r, int m, int n)
void dzfft2dc (double* r, int m, int n)

Discussion

See the equations of the operations for the <u>Real-to-Complex</u> <u>Two-dimensional FFTs</u> above.

These routines are complementary to the complex-to-real transform routines csfft2dc/zdfft2dc.

Input Parameters

r	float* for scfft2dc double* for dzfft2dc
	Pointer to an array of size at least $(m+2, n+2)$, with its leading dimension equal to $(n+2)$. The first <i>m</i> rows and <i>n</i> columns of this array contain the real matrix to be transformed.
	Table 3-7 presents the input data layout.
m	<pre>int. Column transform length; m must be a power of 2.</pre>
п	<pre>int. Row transform length; n must be a power of 2.</pre>

Table 3-7C-interface Real Data Storage for a Real-to-Complex
and Complex-to-Real Two-dimensional FFTs

r(0,0)	r(0,1)	 r(0,n-2)	r(0,n-1)	n/u	n/u
r(1,0)	r(1,1)	 r(1,n-2)	r(1,n-1)	n/u	n/u
r(2,0)	r(2,1)	 r(2,n-2)	r(2,n-1)	n/u	n/u
r(3,0)	r(3,1)	 r(3,n-2)	r(3,n-1)	n/u	n/u
r(m-2,0)	r(m-2,1)	 r(m-2,n-2)	r(m-2,n-1)	n/u	n/u
r(m-1,0)	r(m-1,1)	 r(m-1,n-2)	r(m-1,n-1)	n/u	n/u
n/u	n/u	 n/u	n/u	n/u	n/u
n/u	n/u	 n/u	n/u	n/u	n/u

Output Parameters

- *r* The output real array r(0:m+1, 0:n+1) contains the complex conjugate-symmetric matrix z(0:m-1, 0:n-1) packed in CCS format for C-interface as follows:
 - Columns 0 and n/2 contain in m+2 locations the complex conjugate-symmetric vectors z(i, 0) and z(i, n/2) in CCS format (see<u>Real-to-Complex One-dimensional FFTs</u> above). The full complex vector z(i, 0) is defined by:
 z(i, 0) = cmplx(r(i, 0), r(m/2+i+1, 0)), 0 ≤i ≤m/2,

```
z(m/2+i, 0) = \text{conjg}(z(m/2-i, 0)), 1 \le i \le m/2-1.
```

The full complex vector z(i, n/2) is defined by: $z(i, n/2) = cmplx(r(i, n/2), r(m/2+i+1, n/2)), 0 \le \le m/2,$ $z(m/2+i, n/2) = conjg(z(m/2-i, n/2)), 1 \le \le m/2-1.$

Columns from 1 to n/2-1 contain real parts, and columns from n/2+2 to n contain imaginary parts of complex vectors. These values for each vector are stored in m locations represented as follows

z(i, j) = cmplx(r(i, j), r(i, n/2+1+j)), $0 \le i \le m-1, 1 \le j \le n/2-1.$

• The rest matrix elements can be obtained from

z(i, n/2+j) = conjg(z(i, n/2-j)), $0 \le i \le m-1, 1 \le j \le n/2-1.$

The storage of the complex conjugate-symmetric matrix z for C-interface is shown in <u>Table 3-8</u>.

		in pr		wo-unichis				
z(0,0)	REz(0,1)		REz(0, n/2-1)	z(0,n/2)	0	IMz(0,1)	 IMz(0, n/2-1)	0
REz(1,0)	REz(1,1)		REz(1, n/2-1)	REz(1,n/2)	0	IMz(1,1)	 IMz(1, n/2-1)	0
					0		 	0
REz(m/2-1, 0)	REz(m/2-1, 1)		REz(m/2-1, n/2-1)	REz(m/2-1, n/2)	0	IMz(m/2-1, 1)	 IMz(m/2-1, n/2-1)	0
z(m/2,0)	REz(m/2,1)		REz(m/2, n/2-1)	z(m/2,n/2)	0	IMz(m/2,1)	 IMz(m/2, n/2-1)	0
0	REz(m/2+1, 1)		REz(m/2+1, n/2-1)	0	0	IMz(m/2+1, 1)	 IMz(m/2+1, n/2-1)	0
IMz(1,0)	REz(m/2+2, 1)		REz(m/2+2, n/2-1)	IMz(1,n/2)	0	IMz(m/2+2, 1)	 IMz(m/2+2, n/2-1)	0
					0		 	0
IMz(m/2-2, 0)	REz(m-1,1)		REz(m-1, n/2-1)	IMz(m/2-2, n/2)	0	IMz(m-1,1)	 IMz(m-1, n/2-1)	0
IMz(m/2-1, 0)	n/u		n/u	IMz(m/2-1, n/2)	n/u	n/u	 n/u	n/u
0	n/u		n/u	0	n/u	n/u	 n/u	n/u

Table 3-8 C-interface Data Storage of CCS Format for the Real-to-Complex and Complex-to-Real Two-dimensional FFT

Complex-to-Real Two-dimensional FFTs

Each of the complex-to-real routines computes a two-dimensional inverse FFT according to the mathematical equation:

$$t_{i,j} = \frac{1}{m*n} \sum_{k=0}^{m-1} \sum_{l=0}^{n-1} z_{k,l} * w_m^{i*k} * w_n^{j*l}, \quad 0 \le i \le m-1, \quad 0 \le j \le n-1$$

The mathematical input $z_{i,j}$, $0 \le i \le m-1$, $0 \le j \le n-1$, is a complex matrix of size (m, n). Each column is the complex conjugate-symmetric vector as follows:

for $0 \le j \le n-1$, $z(m/2+i,j) = \operatorname{conjg}(z(m/2-i,j)), 1 \le i \le m/2-1$. Moreover, z(0,j) and z(m/2,j) are real values for j=0 and j=n/2.

This mathematical input can be stored in the complex two-dimensional array of size (m/2+1, n/2+1) or in the real two-dimensional array of size (m+2, n+2). For the details of data storage of CCS format see <u>Real-to-Complex One-dimensional FFTs</u> above.

The mathematical result of the transform is $t_{k,1} = \text{cmplx}(r_{k,1},0)$, where $r_{k,1}$ is the real matrix, $0 \le k \le m-1$, $0 \le l \le n-1$.

csfft2d/zdfft2d

Fortran-interface routine. Compute inverse FFT of a complex conjugate-symmetric matrix packed in CCS format (in-place).

```
call csfft2d ( r, m, n )
call zdfft2d ( r, m, n )
```

Discussion

See the equations of the operations for the <u>Complex-to-Real</u> <u>Two-dimensional FFTs</u> above. These routines are complementary to the real-to-complex transform routines <u>scfft2d/dzfft2d</u>.

Input Parameters

```
r
```

SINGLE PRECISION REAL*4 for csfft2d DOUBLE PRECISION REAL*8 for zdfft2d

Array, DIMENSION at least (m+2, n+2), with its leading dimension equal to (m+2). This array contains the complex conjugate-symmetric matrix in CCS format to be transformed. The input data layout is given in <u>Table 3-6</u>.

m	INTEGER. Column transform length (number of rows); <i>m</i> must be a power of 2.
n	INTEGER. Row transform length (number of columns); <i>n</i> must be a power of 2.
Output Parame	ters
r	Contains the real result returned by the transform. For the output data layout, see <u>Table 3-5</u> .

csfft2dc/zdfft2dc

C-interface routines. Compute inverse FFT of a complex conjugate-symmetric matrix packed in CCS format (in-place).

> void csfft2dc (float* r, int m, int n); void zdfft2dc (double* r, int m, int n);

Discussion

r

т

See the equations of the operations for the <u>Complex-to-Real</u> <u>Two-dimensional FFTs</u> above. These routines are complementary to the real-to-complex transform routines scfft2dc/dzfft2dc.

float* for csfft2dc double* for zdfft2dc
Pointer to an array of size at least $(m+2, n+2)$, with its leading dimension equal to $(n+2)$. This array contains the complex conjugate-symmetric matrix in CCS format to be transformed. The input data layout is given in <u>Table 3-8.</u>
int. Column transform length; <i>m</i> must be a power of 2.

п

r

int. Row transform length; *n* must be a power of 2.

Output Parameters

Contains the real result returned by the transform. The output data layout is the same as that for the input data of scfft2dc/dzfft2dc. See Table 3-7 for the details.

LAPACK Routines: Linear Equations



This chapter describes the Intel[®] Math Kernel Library implementation of routines from the LAPACK package that are used for solving systems of linear equations and performing a number of related computational tasks. The library includes LAPACK routines for both real and complex data.

Routines are supported for systems of equations with the following types of matrices:

- general
- banded
- symmetric or Hermitian positive-definite (both full and packed storage)
- symmetric or Hermitian positive-definite banded
- symmetric or Hermitian indefinite (both full and packed storage)
- symmetric or Hermitian indefinite banded
- triangular (both full and packed storage)
- triangular banded
- tridiagonal.

For each of the above matrix types, the library includes routines for performing the following computations: *factoring* the matrix (except for triangular matrices); *equilibrating* the matrix; *solving* a system of linear equations; *estimating the condition number* of a matrix; *refining* the solution of linear equations and computing its error bounds; *inverting* the matrix.

To solve a particular problem, you can either call two or more <u>computational routines</u> or call a corresponding <u>driver routine</u> that combines several tasks in one call, such as ?gesv for factoring and solving. Thus, to solve a system of linear equations with a general matrix, you can first call ?getrf (*LU* factorization) and then ?getrs (computing the solution). Then, you might wish to call ?gerfs to refine the solution and get the error bounds. Alternatively, you can just use the driver routine ?gesvx which performs all these tasks in one call.

Routine Naming Conventions

For each routine introduced in this chapter, you can use the LAPACK name.

LAPACK names are listed in Tables 4-1 and 4-2, and have the structure xyyzzz or xyyzz, which is described below.

The initial letter \mathbf{x} indicates the data type:

- c complex, single precision
- real, double precision z complex, double precision

The second and third letters yy indicate the matrix type and storage scheme:

ge general

S

d

- gb general band
- gt general tridiagonal

real, single precision

- po symmetric or Hermitian positive-definite
- pp symmetric or Hermitian positive-definite (packed storage)
- pb symmetric or Hermitian positive-definite band
- pt symmetric or Hermitian positive-definite tridiagonal
- sy symmetric indefinite
- sp symmetric indefinite (packed storage)
- he Hermitian indefinite
- hp Hermitian indefinite (packed storage)
- tr triangular
- tp triangular (packed storage)
- tb triangular band

For computational routines, the last three letters zzz indicate the computation performed:

- trf form a triangular matrix factorization
- trs solve the linear system with a factored matrix
- con estimate the matrix condition number
- rfs refine the solution and compute error bounds
- tri compute the inverse matrix using the factorization
- equ equilibrate a matrix.

For example, the routine sgetrf performs the triangular factorization of general real matrices in single precision; the corresponding routine for complex matrices is cgetrf.

For driver routines, the names can end either with -sv (meaning a *simple* driver), or with -svx (meaning an *expert* driver).

Matrix Storage Schemes

LAPACK routines use the following matrix storage schemes:

- *Full storage*: a matrix *A* is stored in a two-dimensional array *a*, with the matrix element *a_{ii}* stored in the array element *a*(*i*, *j*).
- *Packed storage* scheme allows you to store symmetric, Hermitian, or triangular matrices more compactly: the upper or lower triangle of the matrix is packed by columns in a one-dimensional array.
- Band storage: an m by n band matrix with kl sub-diagonals and ku super-diagonals is stored compactly in a two-dimensional array ab with kl+ku+l rows and n columns. Columns of the matrix are stored in the corresponding columns of the array, and *diagonals* of the matrix are stored in rows of the array.

In Chapters 4 and 5, arrays that hold matrices in packed storage have names ending in *p*; arrays with matrices in band storage have names ending in *b*.

For more information on matrix storage schemes, see <u>Matrix Arguments</u> in Appendix A.

Mathematical Notation

Descriptions of LAPACK routines use the following notation:

Ax = b	A system of linear equations with an <i>n</i> by <i>n</i> matrix $A = \{a_{ij}\}$, a right-hand side vector $b = \{b_i\}$, and an unknown vector $x = \{x_i\}$.		
AX = B	A set of systems with a common matrix <i>A</i> and multiple right-hand sides. The columns of <i>B</i> are individual right-hand sides, and the columns of <i>X</i> are the corresponding solutions.		
<i>x</i>	the vector with elements $ x_i $ (absolute values of x_i).		
<i>A</i>	the matrix with elements $ a_{ij} $ (absolute values of a_{ij}).		
$ x _{\infty} = \max_{i} x_{i} $	The <i>infinity-norm</i> of the vector <i>x</i> .		
$ A _{\infty} = \max_i \Sigma_j a $	a_{ij} The <i>infinity-norm</i> of the matrix A.		
$ A _{1} = \max_{j} \sum_{i} a_{ij} \text{ The one-norm} \text{ of the matrix} A A _{1} = A^{T} _{\infty} = A^{H} _{\infty}$			
$\kappa(A) = A A^{-1} $	The <i>condition number</i> of the matrix <i>A</i> .		

Error Analysis

In practice, most computations are performed with rounding errors. Besides, you often need to solve a system Ax = b where the data (the elements of *A* and *b*) are not known exactly. Therefore, it's important to understand how the data errors and rounding errors can affect the solution *x*.

Data perturbations. If *x* is the exact solution of Ax = b, and $x + \delta x$ is the exact solution of a perturbed problem $(A + \delta A)x = (b + \delta b)$, then

$$\frac{\|\delta x\|}{\|x\|} \leq \kappa(A) \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|} \right), \text{ where } \kappa(A) = \|A\| \|A^{-1}\|$$

In other words, relative errors in *A* or *b* may be amplified in the solution vector *x* by a factor $\kappa(A) = ||A|| ||A^{-1}||$ called the *condition number* of *A*.

Rounding errors have the same effect as relative perturbations $c(n)\varepsilon$ in the original data. Here ε is the *machine precision*, and c(n) is a modest function of the matrix order *n*. The corresponding solution error is $|| \delta x| |/| |x|| \leq c(n)\kappa(A)\varepsilon$. (The value of c(n) is seldom greater than 10*n*.)

Thus, if your matrix *A* is *ill-conditioned* (that is, its condition number $\kappa(A)$ is very large), then the error in the solution *x* is also large; you may even encounter a complete loss of precision. LAPACK provides routines that allow you to estimate $\kappa(A)$ (see <u>Routines for Estimating the Condition</u> <u>Number</u>) and also give you a more precise estimate for the actual solution error (see <u>Refining the Solution and Estimating Its Error</u>).

Computational Routines

<u>Table 4-1</u> lists the LAPACK computational routines for factorizing, equilibrating, and inverting *real* matrices, estimating their condition numbers, solving systems of equations with real matrices, refining the solution, and estimating its error.

Table 4-2 lists similar routines for *complex* matrices.

Table 4-1 Computational Routines for Systems of Equations with Real Matrices

Matrix type, storage scheme	Factorize matrix	Equilibrate matrix	Solve system	Condition number	Estimate error	Invert matrix
general	?getrf	?geequ	?getrs	?gecon	?gerfs	?getri
general band	?gbtrf	?gbequ	?gbtrs	?gbcon	?gbrfs	
general tridiagonal	<u>?gttrf</u>		<u>?gttrs</u>	?gtcon	?gtrfs	
symmetric positive-definite	?potrf	?poequ	?potrs	?pocon	?porfs	?potri
symmetric positive-definite, packed storage	?pptrf	?ppequ	?pptrs	?ppcon	?pprfs	<u>?pptri</u>
symmetric positive-definite, band	?pbtrf	?pbequ	?pbtrs	?pbcon	?pbrfs	
symmetric positive-definite, tridiagonal	<u>?pttrf</u>		<u>?pttrs</u>	?ptcon	<u>?ptrfs</u>	
symmetric indefinite	?sytrf		?sytrs	?sycon	?syrfs	<u>?sytri</u>
symmetric indefinite, packed storage	<u>?sptrf</u>		?sptrs	?spcon	?sprfs	<u>?sptri</u>
triangular			?trtrs	?trcon	?trrfs	<u>?trtri</u>
triangular, packed storage			?tptrs	?tpcon	?tprfs	<u>?tptri</u>
triangular band			?tbtrs	?tbcon	?tbrfs	

In this table ? denotes **s** (single precision) or **d** (double precision).

Matrix type, storage schemeFactorize matrixEquilibrate matrixSolve systemCondition numberEstimate errorInvert matrixgeneral general deneral tridiagonal?getrf?geequ ?gebrg?getrs?gecon ?getrs?getrs?getrigeneral tridiagonal?gttrf?gbequ ?gbtrg?gbtrs?gbcon ?gtrfs?getrfHermitian positive-definite, packed storage?pbtrf?poequ ?pbtrf?pptrs?ppcon ?pptrs?ppfrs?pptrfHermitian positive-definite, packed storage?pbtrf?pbequ ?pbtrf?pbtrs?pbcon ?pbtrs?pbrfs?pptriHermitian positive-definite, packed storage?ptrf?pbequ ?pbtrf?ptrs?pbcon ?ptrs?pbrfs?pbtriHermitian positive-definite, packed storage?ptrf?pbequ ?pbtrs?ptrs?ptcon ?ptrs?ptrfs?pbtriHermitian indefinite?ptrf?pbequ ?ptrs?ptcon ?ptrs?ptrfs?ptriHermitian indefinite?ptrf?ptrs?ptcon ?sytrs?ptrfs?sytriHermitian indefinite packed storage?ptrf?sytrs?spcon ?sytrs?syrfs?sytriHermitian indefinite, packed storage?ptrf?ptrs?ptrs?spcon ?syrfs?sytriHermitian indefinite, packed storage?sptrf?sptrs?spcon ?spcon?sprfs?sptritriangular packed storage?sptrf?sptrs?spcon ?s							
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packed storage	triangular			<u>?trtrs</u>	?trcon	?trrfs	?trtri
triangular band <u>?tbtrs</u> <u>?tbcon</u> <u>?tbrfs</u>				?tptrs	?tpcon	?tprfs	<u>?tptri</u>
	triangular band			?tbtrs	?tbcon	?tbrfs	

Table 4-2 Computational Routines for Systems of Equations with Complex Matrices

In this table ? stands for c (single precision complex) or z (double precision complex).

Routines for Matrix Factorization

This section describes the LAPACK routines for matrix factorization. The following factorizations are supported:

- *LU* factorization
- Cholesky factorization of real symmetric positive-definite matrices
- Cholesky factorization of Hermitian positive-definite matrices
- Bunch-Kaufman factorization of real and complex symmetric matrices
- Bunch-Kaufman factorization of Hermitian matrices.

You can compute the LU factorization using full and band storage of matrices; the Cholesky factorization using full, packed, and band storage; and the Bunch-Kaufman factorization using full and packed storage.

?getrf

Computes the LU factorization of a general m by n matrix.

call	sgetrf	(т,	n,	a,	lda,	ipiv,	info)
call	dgetrf	(m,	n,	a,	lda,	ipiv,	info)
call	cgetrf	(m,	n,	a,	lda,	ipiv,	info)
call	zgetrf	(m,	n,	a,	lda,	ipiv,	info)

Discussion

The routine forms the *LU* factorization of a general *m* by *n* matrix *A* as A = PLU

where *P* is a permutation matrix, *L* is lower triangular with unit diagonal elements (lower trapezoidal if m > n) and *U* is upper triangular (upper trapezoidal if m < n). Usually *A* is square (m = n), and both *L* and *U* are triangular. The routine uses partial pivoting, with row interchanges.

Input Parameters

m	INTEGER. The number of rows in the matrix $A (m \ge 0)$.
n	INTEGER. The number of columns in A $(n \ge 0)$.
а	REAL for sgetrf
	DOUBLE PRECISION for dgetrf
	COMPLEX for cgetrf
	DOUBLE COMPLEX for zgetrf.
	Array, DIMENSION (<i>lda</i> , *). Contains the matrix A.
	The second dimension of a must be at least max(1, n).
lda	INTEGER . The first dimension of <i>a</i> .

Output Parameters

a	Overwritten by L and U . The unit diagonal elements of L are not stored.
ipiv	INTEGER. Array, DIMENSION at least max(1,min(<i>m</i> , <i>n</i>)). The pivot indices: row <i>i</i> was interchanged with row <i>ipiv(i)</i> .
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$, the <i>i</i> th parameter had an illegal value. If <i>info</i> = <i>i</i> , u_{ii} is 0. The factorization has been completed, but <i>U</i> is exactly singular. Division by 0 will occur if you use the factor <i>U</i> for solving a system of linear equations.

Application Notes

The computed L and U are the exact factors of a perturbed matrix A + E, where

 $|E| \le c(\min(m, n))\varepsilon P|L||U|$

c(n) is a modest linear function of *n*, and ε is the machine precision.

The approximate number of floating-point operations for real flavors is

 $(2/3)n^3$ if m = n, $(1/3)n^2(3m-n)$ if m > n,

$(1/3)m^2(3n-m)$ if m < n.

The number of operations for complex flavors is 4 times greater.

After calling this routine with m = n, you can call the following:

?getrs	to solve $AX = B$ or $A^T X = B$ or $A^H X = B$;
<u>?gecon</u>	to estimate the condition number of <i>A</i> ;
<u>?getri</u>	to compute the inverse of <i>A</i> .

?gbtrf

Computes the LU factorization of a general m by n band matrix.

call sgbtrf (m, n, kl, ku, ab, ldab, ipiv, info)
call dgbtrf (m, n, kl, ku, ab, ldab, ipiv, info)
call cgbtrf (m, n, kl, ku, ab, ldab, ipiv, info)
call zgbtrf (m, n, kl, ku, ab, ldab, ipiv, info)

Discussion

The routine forms the LU factorization of a general *m* by *n* band matrix A with *kl* non-zero sub-diagonals and *ku* non-zero super-diagonals. Usually A is square (m = n), and then

A = PLU

where *P* is a permutation matrix; *L* is lower triangular with unit diagonal elements and at most kl non-zero elements in each column; *U* is an upper triangular band matrix with kl + ku super-diagonals. The routine uses partial pivoting, with row interchanges (which creates the additional kl super-diagonals in *U*).

m	INTEGER. The number of rows in the matrix $A \ (m \ge 0)$.
n	INTEGER. The number of columns in $A (n \ge 0)$.
kl	INTEGER. The number of sub-diagonals within the
	band of $A(kl \ge 0)$.
ku	INTEGER . The number of super-diagonals within the
	band of A ($ku \ge 0$).
ab	REAL for sgbtrf
	DOUBLE PRECISION for dgbtrf
	COMPLEX for cgbtrf
	DOUBLE COMPLEX for zgbtrf.
	Array, DIMENSION (1dab, *).

	The array <i>ab</i> contains the matrix A in band storage
	(see Matrix Storage Schemes).
	The second dimension of ab must be at least max(1, n).
)	INTEGER . The first dimension of the array <i>ab</i> .
	$(1dab \ge 2k1 + ku + 1)$

Output Parameters

ldab

ab	Overwritten by L and U. The diagonal and $kl + ku$ super-diagonals of U are stored in the first $1 + kl + ku$ rows of <i>ab</i> . The multipliers used to form L are stored in the next kl rows.
ipiv	INTEGER. Array, DIMENSION at least max(1,min(m,n)). The pivot indices: row <i>i</i> was interchanged with row <i>ipiv(i)</i> .
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th parameter had an illegal value. If <i>info</i> = <i>i</i> , u_{ii} is 0. The factorization has been completed, but <i>U</i> is exactly singular. Division by 0 will occur if you use the factor <i>U</i> for solving a system of linear equations.

Application Notes

The computed L and U are the exact factors of a perturbed matrix A + E, where

 $|E| \le c(kl + ku + 1)\mathcal{E} P|L||U|$

c(k) is a modest linear function of k, and ε is the machine precision.

The total number of floating-point operations for real flavors varies between approximately 2n(ku+1)kl and 2n(kl+ku+1)kl. The number of operations for complex flavors is 4 times greater. All these estimates assume that kl and ku are much less than $\min(m, n)$.

After calling this routine with m = n, you can call the following:

<u>?gbtrs</u>	to solve $AX = B$ or $A^T X = B$ or $A^H X = B$;
<u>?gbcon</u>	to estimate the condition number of A.

?gttrf

Computes the LU factorization of a tridiagonal matrix.

call sgttrf (n, dl, d, du, du2, ipiv, info)
call dgttrf (n, dl, d, du, du2, ipiv, info)
call cgttrf (n, dl, d, du, du2, ipiv, info)
call zgttrf (n, dl, d, du, du2, ipiv, info)

Discussion

The routine computes the LU factorization of a real or complex tridiagonal matrix A in the form

$$A = PLU$$

where P is a permutation matrix; L is lower bidiagonal with unit diagonal elements; and U is an upper triangular matrix with nonzeroes in only the main diagonal and first two superdiagonals. The routine uses elimination with partial pivoting and row interchanges .

n	INTEGER. The order of the matrix $A (n \ge 0)$.
dl, d, du	REAL for sgttrf
	DOUBLE PRECISION for dgttrf
	COMPLEX for cgttrf
	DOUBLE COMPLEX for zgttrf.
	Arrays containing elements of A.
	The array $d1$ of dimension $(n - 1)$ contains the
	sub-diagonal elements of A.
	The array d of dimension n contains the diagonal
	elements of A.
	The array du of dimension $(n - 1)$ contains the
	super-diagonal elements of A.

Output Parameters

dl	Overwritten by the $(n-1)$ multipliers that define the matrix <i>L</i> from the <i>LU</i> factorization of A.
d	Overwritten by the n diagonal elements of the upper triangular matrix U from the LU factorization of A.
du	Overwritten by the $(n-1)$ elements of the first super-diagonal of <i>U</i> .
du2	REAL for sgttrf DOUBLE PRECISION for dgttrf COMPLEX for cgttrf DOUBLE COMPLEX for zgttrf. Array, dimension (n-2). On exit, <i>du2</i> contains (n-2) elements of the second super-diagonal of <i>U</i> .
ipiv	INTEGER. Array, dimension (n). The pivot indices: row <i>i</i> was interchanged with row <i>ipiv(i)</i> .
info	INTEGER. If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, u_{ii} is 0. The factorization has been completed, but <i>U</i> is exactly singular. Division by zero will occur if you use the factor <i>U</i> for solving a system of linear equations.

Application Notes

<u>?gbtrs</u>	to solve $AX = B$ or $A^T X = B$ or $A^H X = B$;
<u>?gbcon</u>	to estimate the condition number of A.

?potrf

Computes the Cholesky factorization of a symmetric (Hermitian) positive-definite matrix.

> call spotrf (uplo, n, a, lda, info) call dpotrf (uplo, n, a, lda, info) call cpotrf (uplo, n, a, lda, info) call zpotrf (uplo, n, a, lda, info)

Discussion

This routine forms the Cholesky factorization of a symmetric positivedefinite or, for complex data, Hermitian positive-definite matrix A:

$A = U^H U$	if uplo='U'
$A = LL^H$	if uplo='L'

where L is a lower triangular matrix and U is upper triangular.

Input Parameters

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether the upper or lower triangular part of A
	is stored and how A is factored:
	If $uplo = 'U'$, the array <i>a</i> stores the upper triangular
	part of the matrix A, and A is factored as $U^H U$.
	If $uplo = 'L'$, the array <i>a</i> stores the lower triangular
	part of the matrix A; A is factored as LL^H .
п	INTEGER. The order of matrix $A (n \ge 0)$.
a	REAL for spotrf
	DOUBLE PRECISION for dpotrf
	COMPLEX for cpotrf
	DOUBLE COMPLEX for zpotrf.
	Array, DIMENSION (1da, *).

The array *a* contains either the upper or the lower triangular part of the matrix A (see *uplo*). The second dimension of *a* must be at least max(1, n). **INTEGER**. The first dimension of *a*.

Output Parameters

lda

a	The upper or lower triangular part of a is overwritten by the Cholesky factor U or L , as specified by $uplo$.
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$, the <i>i</i> th parameter had an illegal value. If <i>info</i> = <i>i</i> , the leading minor of order <i>i</i> (and hence the matrix <i>A</i> itself) is not positive-definite, and the factorization could not be completed. This may indicate an error in forming the matrix <i>A</i> .

Application Notes

If uplo = 'U', the computed factor U is the exact factor of a perturbed matrix A + E, where

 $|E| \le c(\mathbf{n}) \varepsilon |U^{H}| |U|, |e_{ij}| \le c(\mathbf{n}) \varepsilon \sqrt{a_{ii} a_{jj}}$

c(n) is a modest linear function of *n*, and ε is the machine precision.

A similar estimate holds for uplo = 'L'.

The total number of floating-point operations is approximately $(1/3)n^3$ for real flavors or $(4/3)n^3$ for complex flavors.

After calling this routine, you can call the following:

<u>?potrs</u>	to solve $AX = B$;
<u>?pocon</u>	to estimate the condition number of <i>A</i> ;
<u>?potri</u>	to compute the inverse of <i>A</i> .

?pptrf

Computes the Cholesky factorization of a symmetric (Hermitian) positive-definite matrix using packed storage.

call	spptrf	(uplo,	n,	ap,	info)
call	dpptrf	(uplo,	n,	ap,	info)
call	cpptrf	(uplo,	n,	ap,	info)
call	zpptrf	(uplo,	n,	ap,	info)

Discussion

This routine forms the Cholesky factorization of a symmetric positivedefinite or, for complex data, Hermitian positive-definite packed matrix A:

$A = U^H U$	if uplo='U'
$A = LL^H$	if uplo='L'

where L is a lower triangular matrix and U is upper triangular.

Input Parameters

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether the upper or lower triangular part of A
	is packed in the array <i>ap</i> , and how A is factored:
	If $uplo = U'$, the array <i>ap</i> stores the upper triangular part of the matrix A, and A is factored as $U^H U$.
	If $uplo = 'L'$, the array ap stores the lower triangular
	part of the matrix A; A is factored as LL^H .
n	INTEGER . The order of matrix $A (n \ge 0)$.
ар	REAL for spptrf
	DOUBLE PRECISION for dpptrf
	COMPLEX for cpptrf
	DOUBLE COMPLEX for zpptrf.
	Array, DIMENSION at least $max(1,n(n+1)/2)$.

The array ap contains either the upper or the lower triangular part of the matrix A (as specified by uplo) in packed storage (see <u>Matrix Storage Schemes</u>).

Output Parameters

ap	The upper or lower triangular part of <i>A</i> in packed storage is overwritten by the Cholesky factor <i>U</i> or <i>L</i> , as specified by <i>uplo</i> .
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$, the <i>i</i> th parameter had an illegal value. If <i>info</i> = i , the leading minor of order i (and hence the matrix A itself) is not positive-definite, and the factorization could not be completed. This may indicate an error in forming the matrix A .

Application Notes

If uplo = 'U', the computed factor *U* is the exact factor of a perturbed matrix A + E, where

$$|E| \le c(\mathbf{n}) \varepsilon |U^{H}| |U|, |e_{ij}| \le c(\mathbf{n}) \varepsilon \sqrt{a_{ii} a_{jj}}$$

c(n) is a modest linear function of *n*, and ε is the machine precision.

A similar estimate holds for uplo = 'L'.

The total number of floating-point operations is approximately $(1/3)n^3$ for real flavors and $(4/3)n^3$ for complex flavors.

After calling this routine, you can call the following:

<u>?pptrs</u>	to solve $AX = B$;
<u>?ppcon</u>	to estimate the condition number of <i>A</i> ;
<u>?pptri</u>	to compute the inverse of A .

?pbtrf

Computes the Cholesky factorization of a symmetric (Hermitian) positive-definite band matrix.

call spbtrf (uplo, n, kd, ab, ldab, info)
call dpbtrf (uplo, n, kd, ab, ldab, info)
call cpbtrf (uplo, n, kd, ab, ldab, info)
call zpbtrf (uplo, n, kd, ab, ldab, info)

Discussion

This routine forms the Cholesky factorization of a symmetric positivedefinite or, for complex data, Hermitian positive-definite band matrix *A*:

$A = U^H U$	if uplo='U'
$A = LL^H$	if uplo='L'

where L is a lower triangular matrix and U is upper triangular.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether the upper or lower triangular part of A
	is stored in the array <i>ab</i> , and how A is factored:
	If $uplo = 'U'$, the array <i>ab</i> stores the upper triangular
	part of the matrix A, and A is factored as $U^H U$.
	If $uplo = 'L'$, the array <i>ab</i> stores the lower triangular
	part of the matrix A; A is factored as LL^H .
n	INTEGER. The order of matrix $A (n \ge 0)$.
kd	INTEGER. The number of super-diagonals or
	sub-diagonals in the matrix A $(kd \ge 0)$.
ab	REAL for spbtrf
	DOUBLE PRECISION for dpbtrf
	COMPLEX for cpbtrf
	DOUBLE COMPLEX for zpbtrf.
	Array, DIMENSION (1dab,*).
kd	part of the matrix A; A is factored as LL^{H} . INTEGER. The order of matrix A $(n \ge 0)$. INTEGER. The number of super-diagonals or sub-diagonals in the matrix A $(kd \ge 0)$. REAL for spbtrf DOUBLE PRECISION for dpbtrf COMPLEX for cpbtrf DOUBLE COMPLEX for zpbtrf.

	The array ap contains either the upper or the lower triangular part of the matrix A (as specified by $uplo$) in <i>band storage</i> (see <u>Matrix Storage Schemes</u>). The second dimension of ab must be at least max $(1, n)$.
ldab	INTEGER. The first dimension of the array <i>ab</i> . ($1dab \ge kd + 1$)
Output Parame	ters
ap	The upper or lower triangular part of A (in band storage) is overwritten by the Cholesky factor U or L , as specified by $uplo$.
info	INTEGER. If $info=0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, the leading minor of order <i>i</i> (and hence the matrix <i>A</i> itself) is not positive-definite, and the

matrix A itself) is not positive-definite, and the factorization could not be completed. This may indicate

an error in forming the matrix A.

Application Notes

If uplo = 'U', the computed factor U is the exact factor of a perturbed matrix A + E, where

 $|E| \le c(\mathbf{kd} + 1)\varepsilon |U^{H}||U|, |e_{ij}| \le c(\mathbf{kd} + 1)\varepsilon \sqrt{a_{ii}a_{jj}}$

c(n) is a modest linear function of *n*, and ε is the machine precision.

A similar estimate holds for uplo = 'L'.

The total number of floating-point operations for real flavors is approximately $n(kd+1)^2$. The number of operations for complex flavors is 4 times greater. All these estimates assume that kd is much less than n.

After calling this routine, you can call the following:

?pbtrs to solve AX = B; ?pbcon to estimate the condition number of A;

?pttrf

Computes the factorization of a symmetric (Hermitian) positive-definite tridiagonal matrix.

```
call spttrf ( n, d, e, info )
call dpttrf ( n, d, e, info )
call cpttrf ( n, d, e, info )
call zpttrf ( n, d, e, info )
```

Discussion

This routine forms the factorization of a symmetric positive-definite or, for complex data, Hermitian positive-definite tridiagonal matrix *A*:

 $A = LDL^H$, where *D* is diagonal and *L* is unit lower bidiagonal. The factorization may also be regarded as having the form $A = U^H DU$, where *D* is unit upper bidiagonal.

Input Parameters

п	INTEGER. The order of the matrix $A (n \ge 0)$.
d	REAL for spttrf, cpttrf
	DOUBLE PRECISION for dpttrf, zpttrf.
	Array, dimension (n). Contains the diagonal elements
	of A.
е	REAL for spttrf
	DOUBLE PRECISION for dpttrf
	COMPLEX for cpttrf
	DOUBLE COMPLEX for zpttrf.
	Array, dimension $(n - 1)$. Contains the sub-diagonal
	elements of A.

Output Parameters

d

Overwritten by the *n* diagonal elements of the diagonal matrix *D* from the LDL^H factorization of A.

е	Overwritten by the $(n - 1)$ off-diagonal elements of the unit bidiagonal factor <i>L</i> or <i>U</i> from the factorization of A.
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$, the <i>i</i> th parameter had an illegal value. If <i>info</i> = i , the leading minor of order i (and hence the matrix A itself) is not positive-definite; if $i < n$, the factorization could not be completed, while if $i = n$, the factorization was completed, but $d(n) = 0$.

?sytrf

Computes the Bunch-Kaufman factorization of a symmetric matrix.

```
call ssytrf ( uplo, n, a, lda, ipiv, work, lwork, info )
call dsytrf ( uplo, n, a, lda, ipiv, work, lwork, info )
call csytrf ( uplo, n, a, lda, ipiv, work, lwork, info )
call zsytrf ( uplo, n, a, lda, ipiv, work, lwork, info )
```

Discussion

This routine forms the Bunch-Kaufman factorization of a symmetric matrix:

if uplo='U',	$A = PUDU^T P^T$
if uplo='L',	$A = PLDL^T P^T$

where *A* is the input matrix, *P* is a permutation matrix, *U* and *L* are upper and lower triangular matrices with unit diagonal, and *D* is a symmetric block-diagonal matrix with 1-by-1 and 2-by-2 diagonal blocks. *U* and *L* have 2-by-2 unit diagonal blocks corresponding to the 2-by-2 blocks of *D*.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether the upper or lower triangular part of A
	is stored and how A is factored:
	If $uplo = 'U'$, the array <i>a</i> stores the upper triangular
	part of the matrix A, and A is factored as $PUDU^T P^T$.
	If $uplo = 'L'$, the array <i>a</i> stores the lower triangular
	part of the matrix A; A is factored as $PLDL^TP^T$.
n	INTEGER. The order of matrix A $(n \ge 0)$.
а	REAL for ssytrf
	DOUBLE PRECISION for dsytrf
	COMPLEX for csytrf
	DOUBLE COMPLEX for zsytrf.
	Array, DIMENSION (1da, *).

	The array a contains either the upper or the lower
	triangular part of the matrix A (see uplo).
	The second dimension of a must be at least max(1, n).
lda	INTEGER. The first dimension of a ; at least max $(1, n)$.
work	Same type as a. Workspace array of dimension <i>lwork</i>
lwork	INTEGER. The size of the <i>work</i> array $(lwork \ge n)$
	See <u>Application notes</u> for the suggested value of <i>lwork</i> .

Output Parameters

a	The upper or lower triangular part of a is overwritten by details of the block-diagonal matrix D and the multipliers used to obtain the factor U (or L).
work(1)	If <i>info</i> =0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
ipiv	INTEGER.
	Array, DIMENSION at least max(1, <i>n</i>).
	Contains details of the interchanges and the block
	structure of <i>D</i> .
	If $ipiv(i) = k > 0$, then d_{ii} is a 1-by-1 block, and the
	ith row and column of A was interchanged with the kth
	row and column.
	If $uplo = 'U'$ and $ipiv(i) = ipiv(i-1) = -m < 0$,
	then D has a 2-by-2 block in rows/columns i and $i-1$,
	and $(i-1)$ th row and column of A was interchanged
	with the <i>m</i> th row and column.
	If $uplo = 'L'$ and $ipiv(i) = ipiv(i+1) = -m < 0$,
	then D has a 2-by-2 block in rows/columns i and $i+1$,
	and $(i+1)$ th row and column of A was interchanged
	with the <i>m</i> th row and column.
info	INTEGER. If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.
	If $info = i$, d_{ii} is 0. The factorization has been
	completed, but D is exactly singular. Division by 0 will
	occur if you use D for solving a system of linear
	equations.

Application Notes

For better performance, try using *lwork* =n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work(1)* and use this value for subsequent runs.

The 2-by-2 unit diagonal blocks and the unit diagonal elements of U and L are not stored. The remaining elements of U and L are stored in the corresponding columns of the array a, but additional row interchanges are required to recover U or L explicitly (which is seldom necessary).

If ipiv(i) = i for all $i = 1 \dots n$, then all off-diagonal elements of U(L) are stored explicitly in the corresponding elements of the array **a**.

If uplo = 'U', the computed factors *U* and *D* are the exact factors of a perturbed matrix A + E, where

 $|E| \le c(\mathbf{n})\varepsilon P|U||D||U^{\mathsf{T}}|P^{\mathsf{T}}$

c(n) is a modest linear function of *n*, and ε is the machine precision. A similar estimate holds for the computed *L* and *D* when uplo = 'L'.

The total number of floating-point operations is approximately $(1/3)n^3$ for real flavors or $(4/3)n^3$ for complex flavors.

After calling this routine, you can call the following:

<u>?sytrs</u>	to solve $AX = B$;
<u>?sycon</u>	to estimate the condition number of <i>A</i> ;
<u>?sytri</u>	to compute the inverse of <i>A</i> .

?hetrf

Computes the Bunch-Kaufman factorization of a complex Hermitian matrix.

> call chetrf (uplo, n, a, lda, ipiv, work, lwork, info) call zhetrf (uplo, n, a, lda, ipiv, work, lwork, info)

Discussion

This routine forms the Bunch-Kaufman factorization of a Hermitian matrix:

if uplo='U',	$A = PUDU^{H}P^{T}$
if uplo='L',	$A = PLDL^{H}P^{T}$

where A is the input matrix, P is a permutation matrix, U and L are upper and lower triangular matrices with unit diagonal, and D is a Hermitian block-diagonal matrix with 1-by-1 and 2-by-2 diagonal blocks. U and L have 2-by-2 unit diagonal blocks corresponding to the 2-by-2 blocks of D.

Input Parameters

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether the upper or lower triangular part of A
	is stored and how A is factored:
	If $uplo = 'U'$, the array <i>a</i> stores the upper triangular part of the matrix A, and A is factored as $PUDU^{H}P^{T}$.
	If $uplo = 'L'$, the array a stores the lower triangular part of the matrix A; A is factored as $PLDL^{H}P^{T}$.
n	INTEGER. The order of matrix A $(n \ge 0)$.
a	COMPLEX for chetrf
	DOUBLE COMPLEX for zhetrf.
	Array, DIMENSION (1da,*).
	The array a contains either the upper or the lower
	triangular part of the matrix A (see uplo).
	The second dimension of a must be at least $max(1, n)$.

lda	INTEGER . The first dimension of a ; at least max $(1, n)$.
work	Same type as a. Workspace array of dimension <i>lwork</i>
lwork	INTEGER. The size of the work array $(lwork \ge n)$
	See <u>Application notes</u> for the suggested value of <i>lwork</i> .

a	The upper or lower triangular part of a is overwritten by details of the block-diagonal matrix D and the multipliers used to obtain the factor U (or L).
work(1)	If <i>info</i> =0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
ipiv	INTEGER. Array, DIMENSION at least $\max(1,n)$. Contains details of the interchanges and the block structure of <i>D</i> . If $ipiv(i) = k > 0$, then d_{ii} is a 1-by-1 block, and the <i>i</i> th row and column of <i>A</i> was interchanged with the <i>k</i> th row and column.
	If $uplo = 'U'$ and $ipiv(i) = ipiv(i-1) = -m < 0$, then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> -1, and (<i>i</i> -1) th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column.
	If $uplo = 'L'$ and $ipiv(i) = ipiv(i+1) = -m < 0$, then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> +1, and (<i>i</i> +1) th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column.
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$, the <i>i</i> th parameter had an illegal value. If <i>info</i> = i , d_{ii} is 0. The factorization has been completed, but <i>D</i> is exactly singular. Division by 0 will occur if you use <i>D</i> for solving a system of linear equations.

Application Notes

This routine is suitable for Hermitian matrices that are not known to be positive-definite. If A is in fact positive-definite, the routine does not perform interchanges, and no 2-by-2 diagonal blocks occur in D.

For better performance, try using *lwork* =n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The 2-by-2 unit diagonal blocks and the unit diagonal elements of U and L are not stored. The remaining elements of U and L are stored in the corresponding columns of the array a, but additional row interchanges are required to recover U or L explicitly (which is seldom necessary).

If ipiv(i) = i for all $i = 1 \dots n$, then all off-diagonal elements of U(L) are stored explicitly in the corresponding elements of the array a.

If uplo = 'U', the computed factors *U* and *D* are the exact factors of a perturbed matrix A + E, where

$$|E| \leq c(\mathbf{n}) \varepsilon P |U| |D| |U^{\mathsf{T}}| P^{\mathsf{T}}$$

c(n) is a modest linear function of *n*, and ε is the machine precision. A similar estimate holds for the computed *L* and *D* when uplo = 'L'.

The total number of floating-point operations is approximately $(4/3)n^3$.

After calling this routine, you can call the following:

<u>?hetrs</u>	to solve $AX = B$;
<u>?hecon</u>	to estimate the condition number of <i>A</i> ;
<u>?hetri</u>	to compute the inverse of <i>A</i> .

?sptrf

Computes the Bunch-Kaufman factorization of a symmetric matrix using packed storage.

call	ssptrf	(uplo,	n,	ap,	ipiv,	info)
call	dsptrf	(uplo,	n,	ap,	ipiv,	info)
call	csptrf	(uplo,	n,	ap,	ipiv,	info)
call	zsptrf	(uplo,	n,	ap,	ipiv,	info)

Discussion

This routine forms the Bunch-Kaufman factorization of a symmetric matrix *A* using packed storage:

if uplo='U',	$A = PUDU^T P^T$
if uplo='L',	$A = PLDL^T P^T$

where *P* is a permutation matrix, *U* and *L* are upper and lower triangular matrices with unit diagonal, and *D* is a symmetric block-diagonal matrix with 1-by-1 and 2-by-2 diagonal blocks. *U* and *L* have 2-by-2 unit diagonal blocks corresponding to the 2-by-2 blocks of *D*.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether the upper or lower triangular part of A is packed in the array ap and how A is factored:
	If $uplo = 'U'$, the array <i>ap</i> stores the upper triangular part of the matrix <i>A</i> , and <i>A</i> is factored as $PUDU^TP^T$.
	If $uplo = 'L'$, the array ap stores the lower triangular part of the matrix A; A is factored as $PLDL^TP^T$.
n	INTEGER. The order of matrix $A (n \ge 0)$.

ар	REAL for ssptrf
	DOUBLE PRECISION for dsptrf
	COMPLEX for csptrf
	DOUBLE COMPLEX for zsptrf.
	Array, DIMENSION at least $\max(1, n(n+1)/2)$.
	The array <i>ap</i> contains either the upper or the lower
	triangular part of the matrix A (as specified by uplo) in
	packed storage (see Matrix Storage Schemes).

ap	The upper or lower triangle of A (as specified by <i>uplo</i>) is overwritten by details of the block-diagonal matrix D and the multipliers used to obtain the factor U (or L).
ipiv	INTEGER. Array, DIMENSION at least max(1, <i>n</i>). Contains details of the interchanges and the block structure of <i>D</i> . If $ipiv(i) = k > 0$, then d_{ii} is a 1-by-1 block, and the <i>i</i> th row and column of <i>A</i> was interchanged with the <i>k</i> th row and column.
	If $uplo = 'U'$ and $ipiv(i) = ipiv(i-1) = -m < 0$, then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> -1, and (<i>i</i> -1) th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column.
	If $uplo = 'L'$ and $ipiv(i) = ipiv(i+1) = -m < 0$, then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> +1, and (<i>i</i> +1) th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column.
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$, the <i>i</i> th parameter had an illegal value. If <i>info</i> = <i>i</i> , d_{ii} is 0. The factorization has been completed, but <i>D</i> is exactly singular. Division by 0 will occur if you use <i>D</i> for solving a system of linear equations.

Application Notes

The 2-by-2 unit diagonal blocks and the unit diagonal elements of U and L are not stored. The remaining elements of U and L overwrite elements of the corresponding columns of the matrix A, but additional row interchanges are required to recover U or L explicitly (which is seldom necessary).

If ipiv(i) = i for all $i = 1 \dots n$, then all off-diagonal elements of U(L) are stored explicitly in packed form.

If uplo = 'U', the computed factors *U* and *D* are the exact factors of a perturbed matrix A + E, where

$$|E| \leq c(\mathbf{n}) \varepsilon P|U||D||U^{T}|P^{T}$$

c(n) is a modest linear function of *n*, and ε is the machine precision. A similar estimate holds for the computed *L* and *D* when uplo = 'L'.

The total number of floating-point operations is approximately $(1/3)n^3$ for real flavors or $(4/3)n^3$ for complex flavors.

After calling this routine, you can call the following:

<u>?sptrs</u>	to solve $AX = B$;
<u>?spcon</u>	to estimate the condition number of <i>A</i> ;
<u>?sptri</u>	to compute the inverse of A .

?hptrf

Computes the Bunch-Kaufman factorization of a complex Hermitian matrix using packed storage.

call	chptrf	(uplo,	n,	ap,	ipiv,	info)
call	zhptrf	(uplo,	n,	ap,	ipiv,	info)

Discussion

This routine forms the Bunch-Kaufman factorization of a Hermitian matrix using packed storage:

if uplo='U',	$A = PUDU^{H}P^{T}$
if uplo='L',	$A = PLDL^H P^T$

where *A* is the input matrix, *P* is a permutation matrix, *U* and *L* are upper and lower triangular matrices with unit diagonal, and *D* is a Hermitian block-diagonal matrix with 1-by-1 and 2-by-2 diagonal blocks. *U* and *L* have 2-by-2 unit diagonal blocks corresponding to the 2-by-2 blocks of *D*.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether the upper or lower triangular part of A is packed and how A is factored:
	If $uplo = 'U'$, the array ap stores the upper triangular part of the matrix A, and A is factored as $PUDU^{H}P^{T}$. If $uplo = 'L'$, the array ap stores the lower triangular part of the matrix A; A is factored as $PLDL^{H}P^{T}$.
n	INTEGER. The order of matrix $A (n \ge 0)$.
ap	COMPLEX for chptrf DOUBLE COMPLEX for zhptrf. Array, DIMENSION at least $max(1,n(n+1)/2)$.

The array *ap* contains either the upper or the lower triangular part of the matrix *A* (as specified by *uplo*) in *packed storage* (see <u>Matrix Storage Schemes</u>).

Output Parameters

ap	The upper or lower triangle of A (as specified by $uplo$) is overwritten by details of the block-diagonal matrix D and the multipliers used to obtain the factor U (or L).
ipiv	INTEGER. Array, DIMENSION at least max $(1,n)$. Contains details of the interchanges and the block structure of D . If $ipiv(i) = k > 0$, then d_{ii} is a 1-by-1 block, and the <i>i</i> th row and column of A was interchanged with the <i>k</i> th row and column.
	If $uplo = 'U'$ and $ipiv(i) = ipiv(i-1) = -m < 0$, then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> -1, and (<i>i</i> -1) th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column.
	If $uplo = 'L'$ and $ipiv(i) = ipiv(i+1) = -m < 0$, then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> +1, and (<i>i</i> +1) th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column.
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th parameter had an illegal value. If <i>info</i> = <i>i</i> , d_{ii} is 0. The factorization has been completed, but <i>D</i> is exactly singular. Division by 0 will occur if you use <i>D</i> for solving a system of linear equations.

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Application Notes

The 2-by-2 unit diagonal blocks and the unit diagonal elements of U and L are not stored. The remaining elements of U and L are stored in the corresponding columns of the array a, but additional row interchanges are required to recover U or L explicitly (which is seldom necessary).

If ipiv(i) = i for all $i = 1 \dots n$, then all off-diagonal elements of U(L) are stored explicitly in the corresponding elements of the array a.

If uplo = 'U', the computed factors *U* and *D* are the exact factors of a perturbed matrix A + E, where

 $|E| \le c(\mathbf{n}) \varepsilon P|U||D||U^T|P^T$

c(n) is a modest linear function of *n*, and ε is the machine precision. A similar estimate holds for the computed *L* and *D* when uplo = 'L'. The total number of floating-point operations is approximately $(4/3)n^3$. After calling this routine, you can call the following:

<u>?hptrs</u>	to solve $AX = B$;
<u>?hpcon</u>	to estimate the condition number of <i>A</i> ;
<u>?hptri</u>	to compute the inverse of A.

Routines for Solving Systems of Linear Equations

This section describes the LAPACK routines for solving systems of linear equations. Before calling most of these routines, you need to factorize the matrix of your system of equations (see <u>Routines for Matrix Factorization</u>in this chapter). However, the factorization is not necessary if your system of equations has a triangular matrix.

?getrs

Solves a system of linear equations with an LU-factored square matrix, with multiple right-hand sides.

call	sgetrs	(trans,	n,	nrhs,	a,	lda,	ipiv,	b,	ldb,	info)
call	dgetrs	(trans,	n,	nrhs,	a,	lda,	ipiv,	b,	ldb,	info)
call	cgetrs	(trans,	n,	nrhs,	a,	lda,	ipiv,	b,	ldb,	info)
call	zgetrs	(trans,	n,	nrhs,	a,	lda,	ipiv,	b,	ldb,	info)

Discussion

This routine solves for *X* the following systems of linear equations:

AX = B	if trans='N',
$A^T X = B$	if trans='T',
$A^H X = B$	if <i>trans</i> ='C' (for complex matrices only).

Before calling this routine, you must call $\underline{?getrf}$ to compute the *LU* factorization of *A*.

trans	CHARACTER*1. Must be 'N' or 'T' or 'C'. Indicates the form of the equations: If $trans = 'N'$, then $AX = B$ is solved for X. If $trans = 'T'$, then $A^TX = B$ is solved for X. If $trans = 'C'$, then $A^HX = B$ is solved for X.
n nrhs	INTEGER. The order of <i>A</i> ; the number of rows in $B (n \ge 0)$. INTEGER. The number of right-hand sides $(nrhs \ge 0)$.
a, b	REAL for sgetrs DOUBLE PRECISION for dgetrs COMPLEX for cgetrs DOUBLE COMPLEX for zgetrs. Arrays: a(lda,*), b(ldb,*).

	The array <i>a</i> contains the matrix <i>A</i> . The array <i>b</i> contains the matrix <i>B</i> whose columns are the right-hand sides for the systems of equations.
	The second dimension of a must be at least $\max(1,n)$, the second dimension of b at least $\max(1,nrhs)$.
lda	INTEGER . The first dimension of a ; $1da \ge max(1, n)$.
ldb	INTEGER. The first dimension of <i>b</i> ; $ldb \ge max(1, n)$.
ipiv	INTEGER. Array, DIMENSION at least $max(1,n)$. The <i>ipiv</i> array, as returned by <u>?getrf</u> .

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER. If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

For each right-hand side *b*, the computed solution is the exact solution of a perturbed system of equations (A + E)x = b where $|E| \le c(n) \mathcal{E} P|L||U|$

c(n) is a modest linear function of *n*, and ε is the machine precision.

If x_0 is the true solution, the computed solution *x* satisfies this error bound:

$$\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(n) \operatorname{cond}(A, x)\varepsilon$$

where $\operatorname{cond}(A, x) = || || A^{-1} || A || x|| || \infty || || \infty || A^{-1} || \infty || A || \infty = \kappa_{\infty}(A).$

Note that $\operatorname{cond}(A,x)$ can be much smaller than $\kappa_{\infty}(A)$; the condition number of A^T and A^H might or might not be equal to $\kappa_{\infty}(A)$.

The approximate number of floating-point operations for one right-hand side vector *b* is $2n^2$ for real flavors and $8n^2$ for complex flavors.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?gecon</u>. To refine the solution and estimate the error, call <u>?gerfs</u>.

?gbtrs

Solves a system of linear equations with an LU-factored band matrix, with multiple right-hand sides.

call sgbtrs (trans, n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info) call dgbtrs (trans, n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info) call cgbtrs (trans, n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info) call zgbtrs (trans, n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)

Discussion

This routine solves for *X* the following systems of linear equations:

AX = B	if trans='N',
$A^T X = B$	if trans='T',
$A^H X = B$	if <i>trans</i> ='C' (for complex matrices only).

Here *A* is an *LU*-factored general band matrix of order *n* with kl non-zero sub-diagonals and *ku* non-zero super-diagonals. Before calling this routine, you must call <u>?gbtrf</u> to compute the *LU* factorization of *A*.

trans	CHARACTER*1. Must be 'N' or 'T' or 'C'.
n	INTEGER . The order of <i>A</i> ; the number of rows in B ($n \ge 0$).
kl	INTEGER . The number of sub-diagonals within the band
	of A ($k \perp \geq 0$).
ku	INTEGER . The number of super-diagonals within the band
	of A ($ku \ge 0$).
nrhs	INTEGER . The number of right-hand sides $(nrhs \ge 0)$.
ab, b	REAL for sgbtrs
	DOUBLE PRECISION for dgbtrs
	COMPLEX for cgbtrs
	DOUBLE COMPLEX for zgbtrs.
	Arrays: ab(ldab,*), b(ldb,*).

	The array <i>ab</i> contains the matrix <i>A</i> in <i>band storage</i>
	(see Matrix Storage Schemes).
	The array <i>b</i> contains the matrix <i>B</i> whose columns are the
	right-hand sides for the systems of equations.
	The second dimension of <i>ab</i> must be at least $max(1, n)$,
	the second dimension of b at least max(1, <i>nrhs</i>).
ldab	INTEGER . The first dimension of the array <i>ab</i> .
	$(1dab \ge 2k1 + ku + 1).$
ldb	INTEGER . The first dimension of <i>b</i> ; $1db \ge max(1, n)$.
ipiv	INTEGER. Array, DIMENSION at least max(1, <i>n</i>).
	The <i>ipiv</i> array, as returned by <u>?gbtrf</u> .
Output Paramet	ers
h	Overwritten by the solution matrix X

Ø	Overwritten by the solution matrix A.
info	INTEGER . If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

For each right-hand side *b*, the computed solution is the exact solution of a perturbed system of equations (A + E)x = b, where

 $|E| \le c(kl + ku + 1)\mathcal{E} P|L||U|$

c(k) is a modest linear function of k, and ε is the machine precision.

If x_0 is the true solution, the computed solution x satisfies this error bound:

$$\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(kl + ku + 1) \operatorname{cond}(A, x)\varepsilon$$

where $\operatorname{cond}(A, x) = || || A^{-1} || A|| || x|| ||_{\infty} / || x||_{\infty} \leq ||A^{-1}||_{\infty} ||A||_{\infty} = \kappa_{\infty}(A).$

Note that $\operatorname{cond}(A,x)$ can be much smaller than $\kappa_{\infty}(A)$; the condition number of A^T and A^H might or might not be equal to $\kappa_{\infty}(A)$.

The approximate number of floating-point operations for one right-hand side vector is 2n(ku + 2k1) for real flavors. The number of operations for complex flavors is 4 times greater. All these estimates assume that k1 and ku are much less than min(m, n).

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?gbcon</u>. To refine the solution and estimate the error, call <u>?gbrfs</u>.

?gttrs

Solves a system of linear equations with a tridiagonal matrix using the LU factorization computed by ?gttrf.

call sgttrs (trans, n, nrhs, dl, d, du, du2, ipiv, b, ldb, info) call dgttrs (trans, n, nrhs, dl, d, du, du2, ipiv, b, ldb, info) call cgttrs (trans, n, nrhs, dl, d, du, du2, ipiv, b, ldb, info) call zgttrs (trans, n, nrhs, dl, d, du, du2, ipiv, b, ldb, info)

Discussion

This routine solves for *X* the following systems of linear equations with multiple right hand sides:

AX = B	if trans='N',
$A^T X = B$	if trans='T',
$A^H X = B$	if <i>trans</i> ='C' (for complex matrices only).

Before calling this routine, you must call $\underline{?gttrf}$ to compute the *LU* factorization of *A*.

trans	CHARACTER*1. Must be 'N' or 'T' or 'C'. Indicates the form of the equations: If $trans = 'N'$, then $AX = B$ is solved for X. If $trans = 'T'$, then $A^TX = B$ is solved for X. If $trans = 'C'$, then $A^HX = B$ is solved for X.
n	INTEGER. The order of $A \ (n \ge 0)$.
nrhs	INTEGER. The number of right-hand sides, i.e., the number of columns in B (<i>nrhs</i> \ge 0).
dl,d,du,du2,b	REAL for sgttrs
	DOUBLE PRECISION for dgttrs
	COMPLEX for cgttrs
	DOUBLE COMPLEX for zgttrf.

	Arrays: $dl(n-1)$, $d(n)$, $du(n-1)$, $du2(n-2)$,
	b(ldb,nrhs).
	The array $d1$ contains the $(n - 1)$ multipliers that define
	the matrix L from the LU factorization of A .
	The array <i>d</i> contains the <i>n</i> diagonal elements of the upper
	triangular matrix U from the LU factorization of A .
	The array du contains the $(n - 1)$ elements of the first
	super-diagonal of U.
	The array du_2 contains the $(n - 2)$ elements of the
	second super-diagonal of U.
	The array b contains the matrix B whose columns are the
	right-hand sides for the systems of equations.
ldb	INTEGER. The leading dimension of <i>b</i> ; $1db \ge max(1, n)$.
ipiv	INTEGER.
	Array, DIMENSION (n).
	The <i>ipiv</i> array, as returned by <u>?gttrf</u> .

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER . If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

For each right-hand side *b*, the computed solution is the exact solution of a perturbed system of equations (A + E)x = b where $|E| \le c(n) \varepsilon P|L||U|$

c(n) is a modest linear function of *n*, and ε is the machine precision.

If x_0 is the true solution, the computed solution *x* satisfies this error bound:

$$\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(n) \operatorname{cond}(A, x)\varepsilon$$

where $\operatorname{cond}(A, x) = || || A^{-1} || A|| || x|| ||_{\infty} / || x||_{\infty} \le || A^{-1} ||_{\infty} || A||_{\infty} = \kappa_{\infty}(A).$

Note that $\operatorname{cond}(A, x)$ can be much smaller than $\kappa_{\infty}(A)$; the condition number of A^T and A^H might or might not be equal to $\kappa_{\infty}(A)$.

The approximate number of floating-point operations for one right-hand side vector *b* is $2n^2$ for real flavors and $8n^2$ for complex flavors.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?gecon</u>. To refine the solution and estimate the error, call <u>?gerfs</u>.

?potrs

Solves a system of linear equations with a Cholesky-factored symmetric (Hermitian) positive-definite matrix.

call spotrs (uplo, n, nrhs, a, lda, b, ldb, info)
call dpotrs (uplo, n, nrhs, a, lda, b, ldb, info)
call cpotrs (uplo, n, nrhs, a, lda, b, ldb, info)
call zpotrs (uplo, n, nrhs, a, lda, b, ldb, info)

Discussion

This routine solves for *X* the system of linear equations AX = B with a symmetric positive-definite or, for complex data, Hermitian positive-definite matrix *A*, given the Cholesky factorization of *A*:

$A = U^H U$	if <i>uplo</i> = 'U'
$A = LL^H$	if $uplo = 'L'$

where L is a lower triangular matrix and U is upper triangular. The system is solved with multiple right-hand sides stored in the columns of the matrix B.

Before calling this routine, you must call $\underline{?potrf}$ to compute the Cholesky factorization of *A*.

a, b	REAL for spotrs
	DOUBLE PRECISION for dpotrs
	COMPLEX for cpotrs
	DOUBLE COMPLEX for zpotrs.
	Arrays: a(lda,*), b(ldb,*).
	The array a contains the factor U or L (see uplo).
	The array b contains the matrix B whose columns are
	the right-hand sides for the systems of equations.
	The second dimension of a must be at least $max(1,n)$,
	the second dimension of b at least max(1, <i>nrhs</i>).
lda	INTEGER. The first dimension of a ; $1da \ge max(1, n)$.
ldb	INTEGER. The first dimension of b; $1db \ge max(1, n)$.

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER. If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

If uplo = 'U', the computed solution for each right-hand side b is the exact solution of a perturbed system of equations (A + E)x = b, where $|E| \le c(n)\varepsilon |U^{H}||U|$

c(n) is a modest linear function of *n*, and ε is the machine precision. A similar estimate holds for *uplo* = 'L'.

If x_0 is the true solution, the computed solution *x* satisfies this error bound:

$$\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(n) \operatorname{cond}(A, x)\varepsilon$$

where $\operatorname{cond}(A,x) = || || A^{-1} || A|| |x|| || \infty || || \infty || A^{-1} || \infty || A|| \infty = \kappa_{\infty}(A).$

Note that cond(A,x) can be much smaller than $\kappa_{\infty}(A)$.

The approximate number of floating-point operations for one right-hand side vector *b* is $2n^2$ for real flavors and $8n^2$ for complex flavors.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?pocon</u>. To refine the solution and estimate the error, call <u>?porfs</u>.

?pptrs

Solves a system of linear equations with a packed Cholesky-factored symmetric (Hermitian) positive-definite matrix.

call spptrs (uplo, n, nrhs, ap, b, ldb, info)
call dpptrs (uplo, n, nrhs, ap, b, ldb, info)
call cpptrs (uplo, n, nrhs, ap, b, ldb, info)
call zpptrs (uplo, n, nrhs, ap, b, ldb, info)

Discussion

This routine solves for *X* the system of linear equations AX = B with a packed symmetric positive-definite or, for complex data, Hermitian positive-definite matrix *A*, given the Cholesky factorization of *A*:

$A = U^H U$	if <i>uplo</i> = 'U'
$A = LL^H$	if <i>uplo</i> = 'L'

where L is a lower triangular matrix and U is upper triangular. The system is solved with multiple right-hand sides stored in the columns of the matrix B.

Before calling this routine, you must call <u>?pptrf</u> to compute the Cholesky factorization of *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates how the input matrix A has been factored:
	If $uplo = U'$, the array a stores the packed factor U of
	the Cholesky factorization $A = U^H U$.
	If $uplo = 'L'$, the array a stores the packed factor <i>L</i> of
	the Cholesky factorization $A = LL^H$.
п	INTEGER. The order of matrix $A (n \ge 0)$.
nrhs	INTEGER . The number of right-hand sides $(nrhs \ge 0)$.

REAL for spptrs
DOUBLE PRECISION for dpptrs
COMPLEX for cpptrs
DOUBLE COMPLEX for zpptrs.
Arrays: $ap(*), b(ldb, *)$
The dimension of ap must be at least $\max(1, n(n+1)/2)$.
The array ap contains the factor U or L, as specified by
uplo, in packed storage (see <u>Matrix Storage Schemes</u>).
The array <i>b</i> contains the matrix <i>B</i> whose columns are
the right-hand sides for the systems of equations. The
second dimension of b must be at least max(1, <i>nrhs</i>).
INTEGER. The first dimension of b ; $ldb \ge max(1, n)$.

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER. If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

If uplo = 'U', the computed solution for each right-hand side b is the exact solution of a perturbed system of equations (A + E)x = b, where $|E| \le c(n)\varepsilon |U^{H}||U|$

c(n) is a modest linear function of *n*, and ε is the machine precision.

A similar estimate holds for uplo = 'L'.

If x_0 is the true solution, the computed solution x satisfies this error bound:

$$\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(n) \operatorname{cond}(A, x)\varepsilon$$

where $\operatorname{cond}(A, x) = || || A^{-1} || A|| || x|| ||_{\infty} / || x||_{\infty} \le ||A^{-1}||_{\infty} ||A||_{\infty} = \kappa_{\infty}(A).$

Note that cond(A,x) can be much smaller than $\kappa_{\infty}(A)$.

The approximate number of floating-point operations for one right-hand side vector *b* is $2n^2$ for real flavors and $8n^2$ for complex flavors.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?ppcon</u>. To refine the solution and estimate the error, call <u>?pprfs</u>.

?pbtrs

Solves a system of linear equations with a Cholesky-factored symmetric (Hermitian) positive-definite band matrix.

> call spbtrs (uplo, n, kd, nrhs, ab, ldab, b, ldb, info) call dpbtrs (uplo, n, kd, nrhs, ab, ldab, b, ldb, info) call cpbtrs (uplo, n, kd, nrhs, ab, ldab, b, ldb, info) call zpbtrs (uplo, n, kd, nrhs, ab, ldab, b, ldb, info)

Discussion

This routine solves for *X* the system of linear equations AX = B with a symmetric positive-definite or, for complex data, Hermitian positive-definite *band* matrix *A*, given the Cholesky factorization of *A*:

 $A = U^{H}U \qquad \text{if } uplo='U'$ $A = LL^{H} \qquad \text{if } uplo='L'$

where L is a lower triangular matrix and U is upper triangular. The system is solved with multiple right-hand sides stored in the columns of the matrix B.

Before calling this routine, you must call <u>?pbtrf</u> to compute the Cholesky factorization of *A* in the band storage form.

uplo	CHARACTER*1. Must be 'U' or 'L'.	
	Indicates how the input matrix A has been factored:	
	If $uplo = U'$, the array a stores the factor U of the	
	factorization $A = U^H U$ in the band storage form.	
	If $uplo = 'L'$, the array <i>a</i> stores the factor <i>L</i> of the	
	factorization $A = LL^H$ in the band storage form.	
п	INTEGER . The order of matrix $A (n \ge 0)$.	
kd	INTEGER . The number of super-diagonals or	
	sub-diagonals in the matrix A ($kd \ge 0$).	
nrhs	INTEGER. The number of right-hand sides $(nrhs \ge 0)$.	

ab, b	REAL for spbtrs
	DOUBLE PRECISION for dpbtrs
	COMPLEX for cpbtrs
	DOUBLE COMPLEX for zpbtrs.
	Arrays: ab(ldab,*), b(ldb,*).
	The array <i>ab</i> contains the Cholesky factor, as returned by
	the factorization routine, in band storage form.
The array b contains the matrix B whose columns	
	right-hand sides for the systems of equations.
	The second dimension of <i>ab</i> must be at least $max(1, n)$,
	the second dimension of b at least max $(1,nrhs)$.
ldab	INTEGER. The first dimension of the array <i>ab</i> .
	$(1dab \ge kd + 1).$
ldb	INTEGER. The first dimension of b ; $1db \ge max(1, n)$.

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER. If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

For each right-hand side *b*, the computed solution is the exact solution of a perturbed system of equations (A + E)x = b, where

$$|E| \le c(\mathbf{kd}+1)\varepsilon P|U^{H}||U|$$
 or $|E| \le c(\mathbf{kd}+1)\varepsilon P|L^{H}||L|$

c(k) is a modest linear function of k, and ε is the machine precision.

If x_0 is the true solution, the computed solution x satisfies this error bound:

$$\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(kd + 1) \operatorname{cond}(A, x)\mathcal{E}$$

where $\operatorname{cond}(A, x) = || || A^{-1} || A| || x| || ||_{\infty} / || x| ||_{\infty} \leq || A^{-1} ||_{\infty} || A| ||_{\infty} = \kappa_{\infty}(A)$. Note that $\operatorname{cond}(A, x)$ can be much smaller than $\kappa_{\infty}(A)$.

The approximate number of floating-point operations for one right-hand side vector is $4n^*kd$ for real flavors and $16n^*kd$ for complex flavors.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?pbcon</u>. To refine the solution and estimate the error, call <u>?pbrfs</u>.

?pttrs

Solves a system of linear equations with a symmetric (Hermitian) positive-definite tridiagonal matrix using the factorization computed by ?pttrf.

call spttrs (n, nrhs, d, e, b, ldb, info)
call dpttrs (n, nrhs, d, e, b, ldb, info)
call cpttrs (uplo, n, nrhs, d, e, b, ldb, info)
call zpttrs (uplo, n, nrhs, d, e, b, ldb, info)

Discussion

This routine solves for X a system of linear equations AX = B with a symmetric (Hermitian) positive-definite tridiagonal matrix A. Before calling this routine, you must call <u>?pttrf</u> to compute the LDL^H or U^HDU factorization of A.

uplo	CHARACTER*1. Used for cpttrs/zpttrs only. Must be 'U' or 'L'.
	Specifies whether the superdiagonal or the subdiagonal of the tridiagonal matrix <i>A</i> is stored and how <i>A</i> is factored:
	If $uplo = 'U'$, the array <i>e</i> stores the superdiagonal of <i>A</i> , and <i>A</i> is factored as $U^H DU$; If $uplo = 'L'$, the array <i>e</i> stores the subdiagonal of <i>A</i> , and <i>A</i> is factored as LDL^H .
n	INTEGER. The order of $A \ (n \ge 0)$.
nrhs	INTEGER. The number of right-hand sides, i.e., the number of columns of the matrix B (<i>nrhs</i> \geq 0).

d	REAL for spttrs, cpttrs
	DOUBLE PRECISION for dpttrs, zpttrs.
	Array, dimension (n). Contains the diagonal elements
	of the diagonal matrix D from the factorization
	computed by <u>?pttrf</u> .
e, b	REAL for spttrs
	DOUBLE PRECISION for dpttrs
	COMPLEX for cpttrs
	DOUBLE COMPLEX for zpttrs.
	Arrays: $e(n-1)$, $b(1db, nrhs)$.
	The array e contains the $(n - 1)$ off-diagonal elements
of the unit bidiagonal factor U or L from the	
	factorization computed by <u>?pttrf</u> (see uplo).
	The array b contains the matrix B whose columns are
	the right-hand sides for the systems of equations.
ldb	INTEGER. The leading dimension of b; $1db \ge max(1, n)$.
Output Param	eters

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER . If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

?sytrs

Solves a system of linear equations with a UDU- or LDL-factored symmetric matrix.

call ssytrs (uplo, n, nrhs, a, lda, ipiv, b, ldb, info) call dsytrs (uplo, n, nrhs, a, lda, ipiv, b, ldb, info) call csytrs (uplo, n, nrhs, a, lda, ipiv, b, ldb, info) call zsytrs (uplo, n, nrhs, a, lda, ipiv, b, ldb, info)

Discussion

This routine solves for *X* the system of linear equations AX = B with a symmetric matrix *A*, given the Bunch-Kaufman factorization of *A*:

if uplo='U',	$A = PUDU^T P^T$
if uplo='L',	$A = PLDL^T P^T$

where *P* is a permutation matrix, *U* and *L* are upper and lower triangular matrices with unit diagonal, and *D* is a symmetric block-diagonal matrix. The system is solved with multiple right-hand sides stored in the columns of the matrix *B*. You must supply to this routine the factor *U* (or *L*) and the array *ipiv* returned by the factorization routine $\frac{2\text{sytrf}}{2}$.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix A has been factored:	
	If $uplo = 'U'$, the array <i>a</i> stores the upper triangular factor <i>U</i> of the factorization $A = PUDU^T P^T$. If $uplo = 'L'$, the array <i>a</i> stores the lower triangular	
	factor L of the factorization $A = PLDL^T P^T$.	
n	INTEGER. The order of matrix $A (n \ge 0)$.	
nrhs	INTEGER. The number of right-hand sides $(nrhs \ge 0)$.	
ipiv	INTEGER. Array, DIMENSION at least max(1, <i>n</i>). The <i>ipiv</i> array, as returned by <u>?sytrf</u> .	

a, b	REAL for ssytrs	
	DOUBLE PRECISION for dsytrs	
	COMPLEX for csytrs	
	DOUBLE COMPLEX for zsytrs.	
Arrays: $a(lda,*), b(ldb,*)$.		
	The array a contains the factor U or L (see uplo).	
	The array b contains the matrix B whose columns are the	
right-hand sides for the system of equations.		
	The second dimension of a must be at least $\max(1, n)$,	
the	the second dimension of b at least max(1, <i>nrhs</i>).	
lda	INTEGER. The first dimension of a ; $1da \ge max(1, n)$.	
ldb	INTEGER. The first dimension of <i>b</i> ; $1db \ge max(1, n)$.	

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER . If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

For each right-hand side *b*, the computed solution is the exact solution of a perturbed system of equations (A + E)x = b, where

$$|E| \le c(\mathbf{n})\varepsilon P|U||D||U^{\mathsf{T}}|P^{\mathsf{T}} \text{ or } |E| \le c(\mathbf{n})\varepsilon P|L||D||L^{\mathsf{T}}|P^{\mathsf{T}}$$

c(n) is a modest linear function of *n*, and ε is the machine precision.

If x_0 is the true solution, the computed solution *x* satisfies this error bound:

$$\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(n) \operatorname{cond}(A, x) \varepsilon$$

Note that cond(A,x) can be much smaller than $\kappa_{\infty}(A)$.

The total number of floating-point operations for one right-hand side vector is approximately $2n^2$ for real flavors or $8n^2$ for complex flavors.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?sycon</u>. To refine the solution and estimate the error, call <u>?syrfs</u>.

?hetrs

Solves a system of linear equations with a UDU- or LDL-factored Hermitian matrix.

call chetrs (uplo, n, nrhs, a, lda, ipiv, b, ldb, info) call zhetrs (uplo, n, nrhs, a, lda, ipiv, b, ldb, info)

Discussion

This routine solves for *X* the system of linear equations AX = B with a Hermitian matrix *A*, given the Bunch-Kaufman factorization of *A*:

if uplo = 'U',	$A = PUDU^{H}P^{T}$
if uplo='L',	$A = PLDL^H P^T$

where P is a permutation matrix, U and L are upper and lower triangular matrices with unit diagonal, and D is a symmetric block-diagonal matrix. The system is solved with multiple right-hand sides stored in the columns of the matrix B. You must supply to this routine the factor U (or L) and the array *ipiv* returned by the factorization routine <u>?hetrf</u>.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix A has been factored:
	If $uplo = 'U'$, the array a stores the upper triangular factor U of the factorization $A = PUDU^{H}P^{T}$.
	If $uplo = 'L'$, the array a stores the lower triangular factor <i>L</i> of the factorization $A = PLDL^H P^T$.
n	INTEGER . The order of matrix $A (n \ge 0)$.
nrhs	INTEGER . The number of right-hand sides $(nrhs \ge 0)$.
ipiv	INTEGER . Array, DIMENSION at least max(1, <i>n</i>). The <i>ipiv</i> array, as returned by <u>?hetrf</u> .

a, b	COMPLEX for chetrs.
	DOUBLE COMPLEX for zhetrs.
	Arrays: $a(lda,*), b(ldb,*).$
	The array a contains the factor U or L (see uplo).
	The array b contains the matrix B whose columns are the
	right-hand sides for the system of equations.
	The second dimension of a must be at least max(1, n),
	the second dimension of b at least max $(1, nrhs)$.
lda	INTEGER. The first dimension of a ; $1da \ge max(1, n)$.
ldb	INTEGER. The first dimension of b ; $ldb \ge max(1, n)$.

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER . If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

For each right-hand side *b*, the computed solution is the exact solution of a perturbed system of equations (A + E)x = b, where

$$|E| \le c(\mathbf{n})\varepsilon P|U||D||U^{H}|P^{T} \text{ or } |E| \le c(\mathbf{n})\varepsilon P|L||D||L^{H}|P^{T}$$

c(n) is a modest linear function of *n*, and ε is the machine precision.

If x_0 is the true solution, the computed solution *x* satisfies this error bound:

$$\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(n) \operatorname{cond}(A, x)\varepsilon$$

where $\operatorname{cond}(A, x) = || || A^{-1} || A || x|| || \infty || || \infty || A^{-1} || \infty || A || \infty = \kappa_{\infty}(A).$

Note that cond(A,x) can be much smaller than $\kappa_{\infty}(A)$.

The total number of floating-point operations for one right-hand side vector is approximately $8n^2$.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?hecon</u>. To refine the solution and estimate the error, call <u>?herfs</u>.

?sptrs

Solves a system of linear equations with a UDU- or LDL-factored symmetric matrix using packed storage.

call ssptrs (uplo, n, nrhs, ap, ipiv, b, ldb, info)
call dsptrs (uplo, n, nrhs, ap, ipiv, b, ldb, info)
call csptrs (uplo, n, nrhs, ap, ipiv, b, ldb, info)
call zsptrs (uplo, n, nrhs, ap, ipiv, b, ldb, info)

Discussion

This routine solves for *X* the system of linear equations AX = B with a symmetric matrix *A*, given the Bunch-Kaufman factorization of *A*:

if uplo='U',	$A = PUDU^T P^T$
if uplo='L',	$A = PLDL^T P^T$

where *P* is a permutation matrix, *U* and *L* are upper and lower *packed* triangular matrices with unit diagonal, and *D* is a symmetric block-diagonal matrix. The system is solved with multiple right-hand sides stored in the columns of the matrix *B*. You must supply the factor *U* (or *L*) and the array *ipiv* returned by the factorization routine <u>?sptrf</u>.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates how the input matrix A has been factored:
	If $uplo = 'U'$, the array <i>ap</i> stores the packed factor <i>U</i> of the factorization $A = PUDU^T P^T$.
	If $uplo = 'L'$, the array <i>ap</i> stores the packed factor <i>L</i> of
	the factorization $A = PLDL^T P^T$.
п	INTEGER. The order of matrix $A (n \ge 0)$.
nrhs	INTEGER. The number of right-hand sides $(nrhs \ge 0)$.
ipiv	INTEGER. Array, DIMENSION at least max(1,n).
	The <i>ipiv</i> array, as returned by <u>?sptrf</u> .

ap, b	REAL for ssptrs
	DOUBLE PRECISION for dsptrs
	COMPLEX for csptrs
	DOUBLE COMPLEX for zsptrs.
	Arrays: ap(*), b(ldb, *)
	The dimension of <i>ap</i> must be at least $\max(1, n(n+1)/2)$.
	The array ap contains the factor U or L, as specified by
	uplo, in packed storage (see Matrix Storage Schemes).
	The array b contains the matrix B whose columns are
	the right-hand sides for the system of equations. The
	second dimension of b must be at least max $(1,nrhs)$.
ldb	INTEGER . The first dimension of b; $1db \ge max(1, n)$.

b	Overwritten by the solution matrix X.
info	INTEGER . If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

For each right-hand side *b*, the computed solution is the exact solution of a perturbed system of equations (A + E)x = b, where

 $|E| \leq c(n)\varepsilon P|U||D||U^{T}|P^{T}$ or $|E| \leq c(n)\varepsilon P|L||D||L^{T}|P^{T}$

c(n) is a modest linear function of *n*, and ε is the machine precision.

If x_0 is the true solution, the computed solution *x* satisfies this error bound:

$$\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(n) \operatorname{cond}(A, x)\varepsilon$$

where $cond(A,x) = || || A^{-1} || A| || x| || ||_{\infty} / || x| ||_{\infty} \le || A^{-1} ||_{\infty} || A| ||_{\infty} = \kappa_{\infty}(A).$

Note that cond(A,x) can be much smaller than $\kappa_{\infty}(A)$.

The total number of floating-point operations for one right-hand side vector is approximately $2n^2$ for real flavors or $8n^2$ for complex flavors.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?spcon</u>. To refine the solution and estimate the error, call <u>?sprfs</u>.

?hptrs

Solves a system of linear equations with a UDU- or LDL-factored Hermitian matrix using packed storage.

call chptrs (uplo, n, nrhs, ap, ipiv, b, ldb, info)
call zhptrs (uplo, n, nrhs, ap, ipiv, b, ldb, info)

Discussion

This routine solves for *X* the system of linear equations AX = B with a Hermitian matrix *A*, given the Bunch-Kaufman factorization of *A*:

if uplo='U',	$A = PUDU^{H}P^{T}$
if uplo='L',	$A = PLDL^H P^T$

where *P* is a permutation matrix, *U* and *L* are upper and lower *packed* triangular matrices with unit diagonal, and *D* is a symmetric block-diagonal matrix. The system is solved with multiple right-hand sides stored in the columns of the matrix *B*.

You must supply to this routine the arrays ap (containing *U* or *L*) and *ipiv* in the form returned by the factorization routine <u>?hptrf</u>.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix A has been factored:
	If $uplo = 'U'$, the array <i>ap</i> stores the packed factor <i>U</i> of the factorization $A = PUDU^H P^T$.
	If $uplo = 'L'$, the array ap stores the packed factor L of the factorization $A = PLDL^H P^T$.
n	INTEGER. The order of matrix A ($n \ge 0$).
nrhs	INTEGER. The number of right-hand sides $(nrhs \ge 0)$.
ipiv	INTEGER. Array, DIMENSION at least max $(1,n)$. The <i>ipiv</i> array, as returned by <u>?hptrf</u> .

ap, b	COMPLEX for chptrs.
	DOUBLE COMPLEX for zhptrs.
	Arrays: ap(*), b(1db,*)
	The dimension of a_p must be at least max $(1, n(n+1)/2)$.
	The array ap contains the factor U or L, as specified by
	uplo, in packed storage (see <u>Matrix Storage Schemes</u>).
	The array <i>b</i> contains the matrix <i>B</i> whose columns are
	the right-hand sides for the system of equations. The
	second dimension of b must be at least max $(1,nrhs)$.
ldb	INTEGER . The first dimension of b ; $1db \ge max(1, n)$.

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER. If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

For each right-hand side *b*, the computed solution is the exact solution of a perturbed system of equations (A + E)x = b, where

$$|E| \le c(\mathbf{n}) \mathcal{E} P|U||D||U^{H}|P^{T}$$
 or $|E| \le c(\mathbf{n}) \mathcal{E} P|L||D||L^{H}|P^{T}$

c(n) is a modest linear function of *n*, and ε is the machine precision.

If x_0 is the true solution, the computed solution *x* satisfies this error bound:

$$\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(n) \operatorname{cond}(A, x)\varepsilon$$

where $\operatorname{cond}(A, x) = || || A^{-1} || A| || x| || |_{\infty} / || x| ||_{\infty} \le || A^{-1} ||_{\infty} || A| ||_{\infty} = \kappa_{\infty}(A).$

Note that cond(A,x) can be much smaller than $\kappa_{\infty}(A)$.

The total number of floating-point operations for one right-hand side vector is approximately $8n^2$ for complex flavors.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?hpcon</u>. To refine the solution and estimate the error, call <u>?hprfs</u>.

?trtrs

Solves a system of linear equations with a triangular matrix, with multiple right-hand sides.

> call strtrs (uplo,trans,diag,n,nrhs,a,lda,b,ldb,info) call dtrtrs (uplo,trans,diag,n,nrhs,a,lda,b,ldb,info) call ctrtrs (uplo,trans,diag,n,nrhs,a,lda,b,ldb,info) call ztrtrs (uplo,trans,diag,n,nrhs,a,lda,b,ldb,info)

Discussion

This routine solves for *X* the following systems of linear equations with a triangular matrix *A*, with multiple right-hand sides stored in *B*:

AX = B	if trans='N',
$A^T X = B$	if trans='T',
$A^H X = B$	if <i>trans</i> ='C' (for complex matrices only).

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether A is upper or lower triangular:
	If $uplo = 'U'$, then A is upper triangular.
	If $uplo = 'L'$, then A is lower triangular.
trans	CHARACTER*1. Must be 'N' or 'T' or 'C'.
	If $trans = 'N'$, then $AX = B$ is solved for X.
	If $trans = 'T'$, then $A^T X = B$ is solved for X.
	If $trans = 'C'$, then $A^H X = B$ is solved for X.
diag	CHARACTER*1. Must be 'N' or 'U'.
	If $diag = 'N'$, then A is not a unit triangular matrix.
	If $diag = 'U'$, then A is unit triangular: diagonal elements
	of <i>A</i> are assumed to be 1 and not referenced in the array a .
n	INTEGER. The order of <i>A</i> ; the number of rows in B ($n \ge 0$).
nrhs	INTEGER. The number of right-hand sides $(nrhs \ge 0)$.

a, b	REAL for strtrs
	DOUBLE PRECISION for dtrtrs
	COMPLEX for ctrtrs
	DOUBLE COMPLEX for ztrtrs.
	Arrays: a(lda,*), b(ldb,*).
	The array <i>a</i> contains the matrix <i>A</i> .
	The array b contains the matrix B whose columns are the
	right-hand sides for the systems of equations.
	The second dimension of a must be at least $max(1,n)$, the second dimension of b at least $max(1,nrhs)$.
lda	INTEGER. The first dimension of <i>a</i> ; $1da \ge max(1, n)$.
ldb	INTEGER. The first dimension of <i>b</i> ; $ldb \ge max(1, n)$.

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER . If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

For each right-hand side *b*, the computed solution is the exact solution of a perturbed system of equations (A + E)x = b where

 $|E| \le c(\mathbf{n}) \mathcal{E} |A|$

c(n) is a modest linear function of *n*, and ε is the machine precision. If x_0 is the true solution, the computed solution *x* satisfies this error bound: $\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(n) \operatorname{cond}(A, x)\varepsilon$, provided $c(n) \operatorname{cond}(A, x)\varepsilon < 1$

where cond(A, x) = $|| |A^{-1}| |A| |x| ||_{\infty} / ||x||_{\infty} \le |A^{-1}||_{\infty} ||A||_{\infty} = \kappa_{\infty}(A)$.

Note that $\operatorname{cond}(A,x)$ can be much smaller than $\kappa_{\infty}(A)$; the condition number of A^T and A^H might or might not be equal to $\kappa_{\infty}(A)$.

The approximate number of floating-point operations for one right-hand side vector *b* is n^2 for real flavors and $4n^2$ for complex flavors.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?trcon</u>. To estimate the error in the solution, call <u>?trrfs</u>.

?tptrs

Solves a system of linear equations with a packed triangular matrix, with multiple right-hand sides.

```
call stptrs (uplo,trans,diag,n,nrhs,ap,b,ldb,info)
call dtptrs (uplo,trans,diag,n,nrhs,ap,b,ldb,info)
call ctptrs (uplo,trans,diag,n,nrhs,ap,b,ldb,info)
call ztptrs (uplo,trans,diag,n,nrhs,ap,b,ldb,info)
```

Discussion

This routine solves for *X* the following systems of linear equations with a packed triangular matrix *A*, with multiple right-hand sides stored in *B*:

AX = B	if trans='N',
$A^T X = B$	if trans='T',
$A^H X = B$	if <i>trans=</i> 'C' (for complex matrices only).

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether A is upper or lower triangular:
	If $uplo = 'U'$, then A is upper triangular.
	If $uplo = 'L'$, then A is lower triangular.
trans	CHARACTER*1. Must be 'N' or 'T' or 'C'.
	If $trans = 'N'$, then $AX = B$ is solved for X.
	If <i>trans</i> = T' , then $A^T X = B$ is solved for X.
	If <i>trans</i> = C' , then $A^H X = B$ is solved for X.
diag	CHARACTER*1. Must be 'N' or 'U'.
	If $diag = 'N'$, then A is not a unit triangular matrix. If $diag = 'U'$, then A is unit triangular: diagonal elements
	are assumed to be 1 and not referenced in the array ap.
n	INTEGER . The order of <i>A</i> ; the number of rows in $B (n \ge 0)$.
nrhs	INTEGER . The number of right-hand sides $(nrhs \ge 0)$.

ap, b	REAL for stptrs
	DOUBLE PRECISION for dtptrs
	COMPLEX for ctptrs
	DOUBLE COMPLEX for ztptrs.
	Arrays: $ap(*), b(ldb, *)$
	The dimension of ap must be at least $\max(1, n(n+1)/2)$.
	The array ap contains the matrix A in packed storage
	(see Matrix Storage Schemes).
	The array b contains the matrix B whose columns are the
	right-hand sides for the system of equations. The second
	dimension of b must be at least $max(1,nrhs)$.
ldb	INTEGER . The first dimension of b; $1db \ge max(1, n)$.

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER . If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

For each right-hand side *b*, the computed solution is the exact solution of a perturbed system of equations (A + E)x = b where

 $|E| \le c(\mathbf{n}) \mathcal{E} |A|$

c(n) is a modest linear function of *n*, and ε is the machine precision.

If x_0 is the true solution, the computed solution *x* satisfies this error bound: $\|x - x_0\|_{\infty}$

$$\frac{\| \| \| \|_{\infty}}{\| \|_{\infty}} \leq c(n) \operatorname{cond}(A, x)\varepsilon, \text{ provided } c(n) \operatorname{cond}(A, x)\varepsilon < 1$$

where $\operatorname{cond}(A,x) = || || A^{-1} || A|| |x|| ||_{\infty} / || x||_{\infty} \le ||A^{-1}||_{\infty} ||A||_{\infty} = \kappa_{\infty}(A).$

Note that $\operatorname{cond}(A,x)$ can be much smaller than $\kappa_{\infty}(A)$; the condition number of A^T and A^H might or might not be equal to $\kappa_{\infty}(A)$.

The approximate number of floating-point operations for one right-hand side vector *b* is n^2 for real flavors and $4n^2$ for complex flavors.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?tpcon</u>. To estimate the error in the solution, call <u>?tprfs</u>.

?tbtrs

Solves a system of linear equations with a band triangular matrix, with multiple right-hand sides.

call stbtrs (uplo, trans, diag, n, kd, nrhs, ab, ldab, b, ldb, info) call dtbtrs (uplo, trans, diag, n, kd, nrhs, ab, ldab, b, ldb, info) call ctbtrs (uplo, trans, diag, n, kd, nrhs, ab, ldab, b, ldb, info) call ztbtrs (uplo, trans, diag, n, kd, nrhs, ab, ldab, b, ldb, info)

Discussion

This routine solves for *X* the following systems of linear equations with a band triangular matrix *A*, with multiple right-hand sides stored in *B*:

AX = B	if trans='N',
$A^T X = B$	if trans='T',
$A^H X = B$	if <i>trans</i> ='C' (for complex matrices only).

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether A is upper or lower triangular:
	If $uplo = 'U'$, then A is upper triangular.
	If $uplo = 'L'$, then A is lower triangular.
trans	CHARACTER*1. Must be 'N' or 'T' or 'C'.
	If $trans = 'N'$, then $AX = B$ is solved for X.
	If <i>trans</i> = 'T', then $A^T X = B$ is solved for X.
	If $trans = 'C'$, then $A^H X = B$ is solved for X.
diag	CHARACTER*1. Must be 'N' or 'U'.
	If $diag = 'N'$, then A is not a unit triangular matrix.
	If $diag = 'U'$, then A is unit triangular: diagonal elements
	are assumed to be 1 and not referenced in the array ab.
п	INTEGER . The order of <i>A</i> ; the number of rows in $B (n \ge 0)$.
kd	INTEGER . The number of super-diagonals or
	sub-diagonals in the matrix A $(kd \ge 0)$.
nrhs	INTEGER . The number of right-hand sides $(nrhs \ge 0)$.

ab, b	REAL for stbtrs
	DOUBLE PRECISION for dtbtrs
	COMPLEX for ctbtrs
	DOUBLE COMPLEX for ztbtrs.
	Arrays: $ab(ldab, *), b(ldb, *).$
	The array <i>ab</i> contains the matrix A in <i>band storage</i> form.
	The array b contains the matrix B whose columns are the
	right-hand sides for the systems of equations.
	The second dimension of <i>ab</i> must be at least $max(1, n)$,
	the second dimension of b at least max $(1,nrhs)$.
ldab	INTEGER. The first dimension of <i>ab</i> ; $1 dab \ge kd + 1$.
ldb	INTEGER. The first dimension of b; $ldb \ge max(1, n)$.

b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER . If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

For each right-hand side *b*, the computed solution is the exact solution of a perturbed system of equations (A + E)x = b where

 $|E| \le c(\mathbf{n}) \mathcal{E} |A|$

c(n) is a modest linear function of n, and ε is the machine precision. If x_0 is the true solution, the computed solution x satisfies this error bound:

$$\frac{\|x - x_0\|_{\infty}}{\|x\|_{\infty}} \le c(n) \operatorname{cond}(A, x)\varepsilon, \text{ provided } c(n) \operatorname{cond}(A, x)\varepsilon < 1$$

where $\operatorname{cond}(A, x) = || || A^{-1} || A|| || x|| ||_{\infty} / || x||_{\infty} \le ||A^{-1}||_{\infty} ||A||_{\infty} = \kappa_{\infty}(A).$

Note that $\operatorname{cond}(A, x)$ can be much smaller than $\kappa_{\infty}(A)$; the condition number of A^T and A^H might or might not be equal to $\kappa_{\infty}(A)$.

The approximate number of floating-point operations for one right-hand side vector *b* is $2n^{*}kd$ for real flavors and $8n^{*}kd$ for complex flavors.

To estimate the condition number $\kappa_{\infty}(A)$, call <u>?tbcon</u>. To estimate the error in the solution, call <u>?tbrfs</u>.

Routines for Estimating the Condition Number

This section describes the LAPACK routines for estimating the *condition number* of a matrix. The condition number is used for analyzing the errors in the solution of a system of linear equations (see <u>Error Analysis</u>). Since the condition number may be arbitrarily large when the matrix is nearly singular, the routines actually compute the *reciprocal* condition number.

?gecon

Estimates the reciprocal of the condition number of a general matrix in either the 1-norm or the infinity-norm.

```
call sgecon ( norm,n,a,lda,anorm,rcond,work,iwork,info )
call dgecon ( norm,n,a,lda,anorm,rcond,work,iwork,info )
call cgecon ( norm,n,a,lda,anorm,rcond,work,rwork,info )
call zgecon ( norm,n,a,lda,anorm,rcond,work,rwork,info )
```

Discussion

This routine estimates the reciprocal of the condition number of a general matrix *A* in either the 1-norm or infinity-norm:

$$\kappa_{1}(A) = ||A||_{1} ||A^{-1}||_{1} = \kappa_{\infty}(A^{T}) = \kappa_{\infty}(A^{H})$$

$$\kappa_{\infty}(A) = ||A||_{\infty} ||A^{-1}||_{\infty} = \kappa_{1}(A^{T}) = \kappa_{1}(A^{H})$$

Before calling this routine:

- compute anorm (either $||A||_1 = \max_j \sum_i |a_{ij}|$ or $||A||_{\infty} = \max_i \sum_j |a_{ij}|$)
- call <u>?getrf</u> to compute the *LU* factorization of *A*.

```
normCHARACTER*1. Must be '1' or '0' or 'I'.If norm = '1' or '0', then the routine estimates \kappa_1(A).If norm = 'I', then the routine estimates \kappa_{\infty}(A).nINTEGER. The order of the matrix A (n \ge 0).
```

a, work	REAL for sgecon
	DOUBLE PRECISION for dgecon
	COMPLEX for cgecon
	DOUBLE COMPLEX for zgecon.
	Arrays: a(lda,*), work(*).
	The array a contains the LU-factored matrix A, as
	returned by <u>?getrf</u> .
	The second dimension of a must be at least $\max(1, n)$.
	The array work is a workspace for the routine.
	The dimension of <i>work</i> must be at least $max(1, 4*n)$ for
	real flavors and $max(1, 2*n)$ for complex flavors.
anorm	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	The norm of the <i>original</i> matrix A (see <u>Discussion</u>).
lda	INTEGER. The first dimension of <i>a</i> ; $1 da \ge max(1, n)$.
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, n)$.
rwork	REAL for cgecon
	DOUBLE PRECISION for zgecon
	Workspace array, DIMENSION at least $max(1, 2*n)$.

rcond	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal of the condition number.
	The routine sets <i>rcond</i> =0 if the estimate underflows; in
	this case the matrix is singular (to working precision).
	However, anytime <i>rcond</i> is small compared to 1.0,
	for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER. If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b or $A^{H}x = b$; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors and $8n^2$ for complex flavors.

?gbcon

Estimates the reciprocal of the condition number of a band matrix in either the 1-norm or the infinity-norm.

```
call sgbcon (norm,n,kl,ku,ab,ldab,ipiv,anorm,rcond,work,iwork,info)
call dgbcon (norm,n,kl,ku,ab,ldab,ipiv,anorm,rcond,work,iwork,info)
call cgbcon (norm,n,kl,ku,ab,ldab,ipiv,anorm,rcond,work,rwork,info)
call zgbcon (norm,n,kl,ku,ab,ldab,ipiv,anorm,rcond,work,rwork,info)
```

Discussion

This routine estimates the reciprocal of the condition number of a general band matrix *A* in either the 1-norm or infinity-norm:

$$\begin{split} \kappa_1(A) &= ||A||_1 ||A^{-1}||_1 = \kappa_{\infty}(A^T) = \kappa_{\infty}(A^H) \\ \kappa_{\infty}(A) &= ||A||_{\infty} ||A^{-1}||_{\infty} = \kappa_1(A^T) = \kappa_1(A^H) \,. \end{split}$$

Before calling this routine:

- compute anorm (either $||A||_1 = \max_i \sum_i |a_{ij}|$ or $||A||_{\infty} = \max_i \sum_j |a_{ij}|$)
- call <u>?gbtrf</u> to compute the *LU* factorization of *A*.

norm	CHARACTER*1. Must be '1' or '0' or 'I'.
	If <i>norm</i> = '1' or '0', then the routine estimates $\kappa_1(A)$.
	If $norm = 'I'$, then the routine estimates $\kappa_{\infty}(A)$.
n	INTEGER . The order of the matrix $A (n \ge 0)$.
kl	INTEGER . The number of sub-diagonals within the band
	of A ($kl \ge 0$).
ku	INTEGER . The number of super-diagonals within the
	band of A ($ku \ge 0$).
ldab	INTEGER. The first dimension of the array <i>ab</i> .
	$(1dab \ge 2k1 + ku + 1).$
ipiv	INTEGER. Array, DIMENSION at least max(1, <i>n</i>).
-	The <i>ipiv</i> array, as returned by <u>?gbtrf</u> .

ab, work	REAL for sgbcon
	DOUBLE PRECISION for dgbcon
	COMPLEX for cgbcon
	DOUBLE COMPLEX for zgbcon.
	Arrays: ab(ldab,*), work(*).
	The array <i>ab</i> contains the factored band matrix A , as returned by <u>?gbtrf</u> .
	The second dimension of ab must be at least max $(1,n)$. The array <i>work</i> is a workspace for the routine.
	The dimension of <i>work</i> must be at least $max(1, 3*n)$ for real flavors and $max(1, 2*n)$ for complex flavors.
anorm	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. The norm of the <i>original</i> matrix <i>A</i> (see <u>Discussion</u>).
iwork	INTEGER. Workspace array, DIMENSION at least $max(1, n)$.
rwork	REAL for cgbcon DOUBLE PRECISION for zgbcon Workspace array, DIMENSION at least max(1, 2*n).

rcond	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal of the condition number.
	The routine sets <i>rcond</i> =0 if the estimate underflows; in
	this case the matrix is singular (to working precision).
	However, anytime <i>rcond</i> is small compared to 1.0,
	for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER . If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b or $A^{H}x = b$; the number is usually 4 or 5 and never more than 11. Each solution requires approximately 2n(ku + 2k1) floating-point operations for real flavors and 8n(ku + 2k1) for complex flavors.

?gtcon

Estimates the reciprocal of the condition number of a tridiagonal matrix using the factorization computed by <code>?gttrf</code>.

```
call sgtcon ( norm,n,dl,d,du,du2,ipiv,anorm,rcond,work,iwork,info )
call dgtcon ( norm,n,dl,d,du,du2,ipiv,anorm,rcond,work,iwork,info )
call cgtcon ( norm,n,dl,d,du,du2,ipiv,anorm,rcond,work,info )
call zgtcon ( norm,n,dl,d,du,du2,ipiv,anorm,rcond,work,info )
```

Discussion

This routine estimates the reciprocal of the condition number of a real or complex tridiagonal matrix *A* in either the 1-norm or infinity-norm:

$$\begin{split} \kappa_{1}(A) &= ||A||_{1} ||A^{-1}||_{1} \\ \kappa_{\infty}(A) &= ||A||_{\infty} ||A^{-1}||_{\infty} \end{split}$$

An estimate is obtained for $||A^{-1}||$, and the reciprocal of the condition number is computed as *rcond* = 1 / ($||A|| ||A^{-1}||$).

Before calling this routine:

- compute anorm (either $||A||_1 = \max_i \sum_i |a_{ij}|$ or $||A||_{\infty} = \max_i \sum_j |a_{ij}|$)
- call $\underline{?gttrf}$ to compute the *LU* factorization of *A*.

-	
norm	CHARACTER*1. Must be '1' or '0' or 'I'. If $norm = '1'$ or '0', then the routine estimates $\kappa_1(A)$.
	If <i>norm</i> = 'I', then the routine estimates $\kappa_{\infty}(A)$.
n	INTEGER. The order of the matrix $A (n \ge 0)$.
dl,d,du,du2	REAL for sgtcon
	DOUBLE PRECISION for dgtcon
	COMPLEX for cgtcon
	DOUBLE COMPLEX for zgtcon.
	Arrays: $dl(n-1)$, $d(n)$, $du(n-1)$, $du2(n-2)$.
	The array $d1$ contains the $(n - 1)$ multipliers that define
	the matrix L from the LU factorization of A as computed by $\frac{?gttrf}{}$.
	The array d contains the <i>n</i> diagonal elements of the
	upper triangular matrix U from the LU factorization of A .
	The array du contains the $(n - 1)$ elements of the first super-diagonal of U .
	The array du_2 contains the $(n - 2)$ elements of the
	second super-diagonal of U.
ipiv	INTEGER.
	Array, DIMENSION (n).
	The array of pivot indices, as returned by <u>?gttrf</u> .
anorm	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	The norm of the <i>original</i> matrix A (see <i>Discussion</i>).
work	REAL for sgtcon
	DOUBLE PRECISION for dgtcon
	COMPLEX for cgtcon
	DOUBLE COMPLEX for zgtcon.
	Workspace array, DIMENSION (2*n).
iwork	INTEGER.
	Workspace array, DIMENSION (n).
	Used for real flavors only.

rcond	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. An estimate of the reciprocal of the condition number.
	The routine sets <i>rcond</i> =0 if the estimate underflows; in this case the matrix is singular (to working precision). However, anytime <i>rcond</i> is small compared to 1.0, for the working precision, the matrix may be poorly conditioned or even singular.
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors and $8n^2$ for complex flavors.

?pocon

Estimates the reciprocal of the condition number of a symmetric (Hermitian) positive-definite matrix.

```
call spocon ( uplo,n,a,lda,anorm,rcond,work,iwork,info )
call dpocon ( uplo,n,a,lda,anorm,rcond,work,iwork,info )
call cpocon ( uplo,n,a,lda,anorm,rcond,work,rwork,info )
call zpocon ( uplo,n,a,lda,anorm,rcond,work,rwork,info )
```

Discussion

This routine estimates the reciprocal of the condition number of a symmetric (Hermitian) positive-definite matrix *A*:

 $\kappa_1(A) = ||A||_1 ||A^{-1}||_1$ (since *A* is symmetric or Hermitian, $\kappa_{\infty}(A) = \kappa_1(A)$). Before calling this routine:

- compute *anorm* (either $||A||_1 = \max_i \sum_i |a_{ij}|$ or $||A||_{\infty} = \max_i \sum_j |a_{ij}|$)
- call <u>?potrf</u> to compute the Cholesky factorization of *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix <i>A</i> has been factored:
	If $uplo = U'$, the array a stores the upper triangular factor <i>U</i> of the factorization $A = U^H U$.
	If $uplo = 'L'$, the array a stores the lower triangular factor <i>L</i> of the factorization $A = LL^{H}$.
п	INTEGER . The order of the matrix $A (n \ge 0)$.
a, work	REAL for spocon
	DOUBLE PRECISION for dpocon
	COMPLEX for cpocon
	DOUBLE COMPLEX for zpocon.
	Arrays: a(lda,*), work(*).

	The array a contains the factored matrix A, as returned
	by <u>?potrf</u> .
	The second dimension of a must be at least $max(1,n)$.
	The array <i>work</i> is a workspace for the routine.
	The dimension of <i>work</i> must be at least $max(1, 3*n)$ for
	real flavors and $max(1, 2*n)$ for complex flavors.
lda	INTEGER . The first dimension of <i>a</i> ; $1da \ge max(1, n)$.
anorm	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	The norm of the <i>original</i> matrix A (see Discussion).
iwork	INTEGER.
	Workspace array, DIMENSION at least max(1, n).
rwork	REAL for cpocon
	DOUBLE PRECISION for zpocon
	Workspace array, DIMENSION at least max(1, n).

rcond	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal of the condition number.
	The routine sets <i>rcond</i> =0 if the estimate underflows; in
	this case the matrix is singular (to working precision).
	However, anytime <i>rcond</i> is small compared to 1.0,
	for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors and $8n^2$ for complex flavors.

?ppcon

Estimates the reciprocal of the condition number of a packed symmetric (Hermitian) positive-definite matrix.

```
call sppcon ( uplo,n,ap,anorm,rcond,work,iwork,info )
call dppcon ( uplo,n,ap,anorm,rcond,work,iwork,info )
call cppcon ( uplo,n,ap,anorm,rcond,work,rwork,info )
call zppcon ( uplo,n,ap,anorm,rcond,work,rwork,info )
```

Discussion

This routine estimates the reciprocal of the condition number of a packed symmetric (Hermitian) positive-definite matrix *A*:

 $\kappa_1(A) = ||A||_1 ||A^{-1}||_1$ (since *A* is symmetric or Hermitian, $\kappa_{\infty}(A) = \kappa_1(A)$). Before calling this routine:

- compute *anorm* (either $||A||_1 = \max_i \sum_i |a_{ij}|$ or $||A||_{\infty} = \max_i \sum_j |a_{ij}|$)
- call <u>?pptrf</u> to compute the Cholesky factorization of *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix A has been factored:
	If $uplo = 'U'$, the array <i>ap</i> stores the upper triangular factor <i>U</i> of the factorization $A = U^H U$.
	If $uplo = 'L'$, the array <i>ap</i> stores the lower triangular factor <i>L</i> of the factorization $A = LL^{H}$.
n	INTEGER . The order of the matrix $A (n \ge 0)$.
ap, work	REAL for sppcon
	DOUBLE PRECISION for dppcon
	COMPLEX for cppcon
	DOUBLE COMPLEX for zppcon.
	Arrays: ap(*), work(*).

	The array <i>ap</i> contains the packed factored matrix <i>A</i> , as
	returned by <u>?pptrf</u> .
	The dimension of ap must be at least $\max(1, n(n+1)/2)$.
	The array <i>work</i> is a workspace for the routine.
	The dimension of <i>work</i> must be at least $max(1, 3*n)$ for
	real flavors and $max(1, 2*n)$ for complex flavors.
anorm	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	The norm of the <i>original</i> matrix A (see <i>Discussion</i>).
iwork	INTEGER.
	Workspace array, DIMENSION at least max(1, n).
rwork	REAL for cppcon
	DOUBLE PRECISION for zppcon
	Workspace array, DIMENSION at least $max(1, n)$.

rcond	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal of the condition number.
	The routine sets <i>rcond</i> =0 if the estimate underflows; in
	this case the matrix is singular (to working precision).
	However, anytime <i>rcond</i> is small compared to 1.0,
	for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors and $8n^2$ for complex flavors.

?pbcon

Estimates the reciprocal of the condition number of a symmetric (Hermitian) positive-definite band matrix.

call spbcon (uplo, n, kd, ab, ldab, anorm, rcond, work, iwork, info) call dpbcon (uplo, n, kd, ab, ldab, anorm, rcond, work, iwork, info) call cpbcon (uplo, n, kd, ab, ldab, anorm, rcond, work, rwork, info) call zpbcon (uplo, n, kd, ab, ldab, anorm, rcond, work, rwork, info)

Discussion

This routine estimates the reciprocal of the condition number of a symmetric (Hermitian) positive-definite band matrix *A*:

 $\kappa_1(A) = ||A||_1 ||A^{-1}||_1$ (since *A* is symmetric or Hermitian, $\kappa_{\infty}(A) = \kappa_1(A)$). Before calling this routine:

- compute anorm (either $||A||_1 = \max_i \sum_i |a_{ij}|$ or $||A||_{\infty} = \max_i \sum_i |a_{ij}|$)
- call <u>?pbtrf</u> to compute the Cholesky factorization of *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates how the input matrix A has been factored:
	If $uplo = 'U'$, the array <i>ab</i> stores the upper triangular
	factor U of the Cholesky factorization $A = U^H U$.
	If $uplo = 'L'$, the array <i>ab</i> stores the lower triangular
	factor L of the factorization $A = LL^{H}$.
n	INTEGER . The order of the matrix $A (n \ge 0)$.
kd	INTEGER. The number of super-diagonals or
	sub-diagonals in the matrix A (kd ≥ 0).
ldab	INTEGER. The first dimension of the array <i>ab</i> .
	$(1dab \ge kd + 1).$
ab, work	REAL for spbcon
	DOUBLE PRECISION for dpbcon
	COMPLEX for cpbcon
	DOUBLE COMPLEX for zpbcon.

	Arrays: ab(ldab,*), work(*).
	The array <i>ab</i> contains the factored matrix <i>A</i> in band form, as returned by <u>?pbtrf</u> .
	The second dimension of ab must be at least max $(1, n)$, The array <i>work</i> is a workspace for the routine.
	The dimension of <i>work</i> must be at least $max(1, 3*n)$ for real flavors and $max(1, 2*n)$ for complex flavors.
anorm	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. The norm of the <i>original</i> matrix A (see <i>Discussion</i>).
iwork	INTEGER. Workspace array, DIMENSION at least max(1, <i>n</i>).
rwork	REAL for cpbcon DOUBLE PRECISION for zpbcon. Workspace array, DIMENSION at least max(1, <i>n</i>).

rcond	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal of the condition number.
	The routine sets <u>rcond</u> =0 if the estimate underflows; in
	this case the matrix is singular (to working precision).
	However, anytime <i>rcond</i> is small compared to 1.0,
	for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER. If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately 4n(kd + 1) floating-point operations for real flavors and 16n(kd + 1) for complex flavors.

?ptcon

Estimates the reciprocal of the condition number of a symmetric (Hermitian) positive-definite tridiagonal matrix.

```
call sptcon (n, d, e, anorm, rcond, work, info)
call dptcon (n, d, e, anorm, rcond, work, info)
call cptcon (n, d, e, anorm, rcond, work, info)
call zptcon (n, d, e, anorm, rcond, work, info)
```

Discussion

This routine computes the reciprocal of the condition number (in the 1-norm) of a real symmetric or complex Hermitian positive-definite tridiagonal matrix using the factorization $A = LDL^H$ or $A = U^HDU$ computed by <u>?pttrf</u>:

 $\kappa_1(A) = ||A||_1 ||A^{-1}||_1$ (since A is symmetric or Hermitian, $\kappa_{\infty}(A) = \kappa_1(A)$).

The norm $||A^{-1}||$ is computed by a direct method, and the reciprocal of the condition number is computed as $rcond = 1/(||A|| ||A^{-1}||)$.

Before calling this routine:

- compute *anorm* as $||A||_1 = \max_i \sum_i |a_{ij}|$
- call <u>?pttrf</u> to compute the factorization of A.

п	INTEGER . The order of the matrix $A \ (n \ge 0)$.
d, work	REAL for single precision flavors
	DOUBLE PRECISION for double precision flavors.
	Arrays, dimension (n).
	The array d contains the n diagonal elements of the
	diagonal matrix D from the factorization of A, as
	computed by <u>?pttrf</u> ;
	work is a workspace array.

е	REAL for sptcon
	DOUBLE PRECISION for dptcon
	COMPLEX for cptcon
	DOUBLE COMPLEX for zptcon.
	Array, DIMENSION (n - 1).
	Contains off-diagonal elements of the unit bidiagonal
	factor U or L from the factorization computed by <u>?pttrf</u>
anorm	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	The 1- norm of the <i>original</i> matrix A (see <i>Discussion</i>).

rcond	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal of the condition number.
	The routine sets <i>rcond</i> =0 if the estimate underflows; in
	this case the matrix is singular (to working precision).
	However, anytime <i>rcond</i> is small compared to 1.0,
	for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately 4n(kd + 1) floating-point operations for real flavors and 16n(kd + 1) for complex flavors.

?sycon

Estimates the reciprocal of the condition number of a symmetric matrix.

call ssycon (uplo, n, a, lda, ipiv, anorm, rcond, work, iwork, info) call dsycon (uplo, n, a, lda, ipiv, anorm, rcond, work, iwork, info) call csycon (uplo, n, a, lda, ipiv, anorm, rcond, work, rwork, info) call zsycon (uplo, n, a, lda, ipiv, anorm, rcond, work, rwork, info)

Discussion

This routine estimates the reciprocal of the condition number of a symmetric matrix *A*:

 $\kappa_1(A) = ||A||_1 ||A^{-1}||_1$ (since A is symmetric, $\kappa_{\infty}(A) = \kappa_1(A)$).

Before calling this routine:

- compute anorm (either $||A||_1 = \max_i \sum_i |a_{ij}|$ or $||A||_{\infty} = \max_i \sum_j |a_{ij}|$)
- call <u>?sytrf</u> to compute the factorization of A.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates how the input matrix A has been factored:
	If $uplo = 'U'$, the array <i>a</i> stores the upper triangular factor <i>U</i> of the factorization $A = PUDU^TP^T$.
	If $uplo = 'L'$, the array <i>a</i> stores the lower triangular factor <i>L</i> of the factorization $A = PLDL^TP^T$.
n	INTEGER. The order of matrix A ($n \ge 0$).
a, work	REAL for ssycon
	DOUBLE PRECISION for dsycon
	COMPLEX for csycon
	DOUBLE COMPLEX for zsycon.
	Arrays: a(lda,*), work(*).
	The array a contains the factored matrix A , as returned
	by <u>?sytrf</u> .
	The second dimension of a must be at least $max(1,n)$.

	The array <i>work</i> is a workspace for the routine. The dimension of <i>work</i> must be at least $max(1, 2*n)$.
lda	INTEGER. The first dimension of <i>a</i> ; $lda \ge max(1, n)$.
ipiv	INTEGER. Array, DIMENSION at least max $(1,n)$. The array <i>ipiv</i> , as returned by <u>?sytrf</u> .
anorm	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. The norm of the <i>original</i> matrix <i>A</i> (see <i>Discussion</i>).
iwork	INTEGER. Workspace array, DIMENSION at least max(1, <i>n</i>).
rwork	REAL for csycon DOUBLE PRECISION for zsycon. Workspace array, DIMENSION at least max(1, <i>n</i>).

rcond	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal of the condition number.
	The routine sets <i>rcond</i> =0 if the estimate underflows; in
	this case the matrix is singular (to working precision).
	However, anytime r cond is small compared to 1.0,
	for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors and $8n^2$ for complex flavors.

?hecon

Estimates the reciprocal of the condition number of a Hermitian matrix.

```
call checon (uplo, n, a, lda, ipiv, anorm, rcond, work, rwork, info) call zhecon (uplo, n, a, lda, ipiv, anorm, rcond, work, rwork, info)
```

Discussion

This routine estimates the reciprocal of the condition number of a Hermitian matrix *A*:

 $\kappa_1(A) = ||A||_1 ||A^{-1}||_1$ (since A is Hermitian, $\kappa_{\infty}(A) = \kappa_1(A)$).

Before calling this routine:

- compute anorm (either $||A||_1 = \max_i \sum_i |a_{ij}|$ or $||A||_{\infty} = \max_i \sum_i |a_{ij}|$)
- call <u>?hetrf</u> to compute the factorization of *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix A has been factored:
	If $uplo = U'$, the array a stores the upper triangular factor U of the factorization $A = PUDU^H P^T$.
	If $uplo = 'L'$, the array a stores the lower triangular factor <i>L</i> of the factorization $A = PLDL^H P^T$.
п	INTEGER. The order of matrix $A (n \ge 0)$.
a, work	COMPLEX for checon DOUBLE COMPLEX for zhecon. Arrays: a (1da, *), work(*). The array a contains the factored matrix A, as returned by <u>?hetrf</u> . The second dimension of a must be at least max(1,n).
	The array <i>work</i> is a workspace for the routine. The dimension of <i>work</i> must be at least $max(1, 2*n)$.

lda	INTEGER. The first dimension of <i>a</i> ; $1da \ge max(1, n)$.
ipiv	INTEGER. Array, DIMENSION at least $max(1,n)$. The array <i>ipiv</i> , as returned by <u>?hetrf</u> .
anorm	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. The norm of the <i>original</i> matrix <i>A</i> (see <i>Discussion</i>).
rwork	REAL for checon DOUBLE PRECISION for zhecon Workspace array, DIMENSION at least max(1, <i>n</i>).

rcond	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. An estimate of the reciprocal of the condition number. The routine sets <i>rcond</i> =0 if the estimate underflows; in this case the matrix is singular (to working precision). However, anytime <i>rcond</i> is small compared to 1.0, for the working precision, the matrix may be poorly conditioned or even singular.
info	INTEGER. If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 5 and never more than 11. Each solution requires approximately $8n^2$ floating-point operations.

?spcon

Estimates the reciprocal of the condition number of a packed symmetric matrix.

```
call sspcon ( uplo, n, ap, ipiv, anorm, rcond, work, iwork, info )
call dspcon ( uplo, n, ap, ipiv, anorm, rcond, work, iwork, info )
call cspcon ( uplo, n, ap, ipiv, anorm, rcond, work, rwork, info )
call zspcon ( uplo, n, ap, ipiv, anorm, rcond, work, rwork, info )
```

Discussion

This routine estimates the reciprocal of the condition number of a packed symmetric matrix *A*:

 $\kappa_1(A) = ||A||_1 ||A^{-1}||_1$ (since A is symmetric, $\kappa_{\infty}(A) = \kappa_1(A)$).

Before calling this routine:

- compute anorm (either $||A||_1 = \max_i \sum_i |a_{ij}|$ or $||A||_{\infty} = \max_i \sum_i |a_{ij}|$)
- call <u>?sptrf</u> to compute the factorization of A.

Input Parameters

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates how the input matrix A has been factored:
	If $uplo = 'U'$, the array ap stores the packed upper triangular factor U of the factorization $A = PUDU^TP^T$. If $uplo = 'L'$, the array ap stores the packed lower triangular factor L of the factorization $A = PLDL^TP^T$.
n	INTEGER. The order of matrix $A (n \ge 0)$.
ap, work	REAL for sspcon
	DOUBLE PRECISION for dspcon
	COMPLEX for cspcon
	DOUBLE COMPLEX for zspcon.
	Arrays: $ap(*)$, $work(*)$.
	The array ap contains the packed factored matrix A, as returned by <u>?sptrf</u> .

The dimension of *ap* must be at least $\max(1, n(n+1)/2)$.

	The array <i>work</i> is a workspace for the routine. The dimension of <i>work</i> must be at least $max(1, 2*n)$.
ipiv	INTEGER. Array, DIMENSION at least max $(1,n)$. The array <i>ipiv</i> , as returned by <u>?sptrf</u> .
anorm	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. The norm of the <i>original</i> matrix <i>A</i> (see <i>Discussion</i>).
iwork	INTEGER. Workspace array, DIMENSION at least max(1, <i>n</i>).
rwork	REAL for cspcon DOUBLE PRECISION for zspcon Workspace array, DIMENSION at least max(1, <i>n</i>).

rcond	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. An estimate of the reciprocal of the condition number. The routine sets <i>rcond</i> =0 if the estimate underflows; in this case the matrix is singular (to working precision).
	However, anytime <i>rcond</i> is small compared to 1.0, for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors and $8n^2$ for complex flavors.

?hpcon

Estimates the reciprocal of the condition number of a packed Hermitian matrix.

```
call chpcon ( uplo, n, ap, ipiv, anorm, rcond, work, rwork, info )
call zhpcon ( uplo, n, ap, ipiv, anorm, rcond, work, rwork, info )
```

Discussion

This routine estimates the reciprocal of the condition number of a Hermitian matrix *A*:

 $\kappa_1(A) = ||A||_1 ||A^{-1}||_1$ (since A is Hermitian, $\kappa_{\infty}(A) = \kappa_1(A)$).

Before calling this routine:

- compute *anorm* (either $||A||_1 = \max_i \sum_i |a_{ij}|$ or $||A||_{\infty} = \max_i \sum_j |a_{ij}|$)
- call <u>?hptrf</u> to compute the factorization of *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix A has been factored:
	If $uplo = 'U'$, the array ap stores the packed upper triangular factor U of the factorization $A = PUDU^TP^T$.
	If $uplo = 'L'$, the array ap stores the packed lower triangular factor <i>L</i> of the factorization $A = PLDL^TP^T$.
n	INTEGER. The order of matrix $A (n \ge 0)$.
ap, work	COMPLEX for chpcon DOUBLE COMPLEX for zhpcon. Arrays: ap(*), work(*).
	The array <i>ap</i> contains the packed factored matrix <i>A</i> , as returned by <u>?hptrf</u> . The dimension of <i>ap</i> must be at least $max(1,n(n+1)/2)$.
	The array <i>work</i> is a workspace for the routine. The dimension of <i>work</i> must be at least $max(1, 2*n)$.

ipiv	INTEGER. Array, DIMENSION at least max(1, <i>n</i>). The array <i>ipiv</i> , as returned by <u>?hptrf</u> .
anorm	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. The norm of the <i>original</i> matrix A (see Discussion).
rwork	REAL for chpcon DOUBLE PRECISION for zhpcon. Workspace array, DIMENSION at least $max(1, n)$.

rcond	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal of the condition number.
	The routine sets <i>rcond</i> =0 if the estimate underflows; in
	this case the matrix is singular (to working precision).
	However, anytime <i>rcond</i> is small compared to 1.0,
	for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 5 and never more than 11. Each solution requires approximately $8n^2$ floating-point operations.

?trcon

Estimates the reciprocal of the condition number of a triangular matrix.

call strcon (norm, uplo, diag, n, a, lda, rcond, work, iwork, info) call dtrcon (norm, uplo, diag, n, a, lda, rcond, work, iwork, info) call ctrcon (norm, uplo, diag, n, a, lda, rcond, work, rwork, info) call ztrcon (norm, uplo, diag, n, a, lda, rcond, work, rwork, info)

Discussion

This routine estimates the reciprocal of the condition number of a triangular matrix *A* in either the 1-norm or infinity-norm:

$$\begin{split} \kappa_{1}(A) &= ||A||_{1} ||A^{-1}||_{1} = \kappa_{\infty}(A^{T}) = \kappa_{\infty}(A^{H}) \\ \kappa_{\infty}(A) &= ||A||_{\infty} ||A^{-1}||_{\infty} = \kappa_{1}(A^{T}) = \kappa_{1}(A^{H}) . \end{split}$$

norm	CHARACTER*1. Must be '1' or '0' or 'I'. If <i>norm</i> = '1' or '0', then the routine estimates $\kappa_1(A)$. If <i>norm</i> = 'I', then the routine estimates $\kappa_{\infty}(A)$.
uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether A is upper or lower triangular: If $uplo = 'U'$, the array a stores the upper triangle of A, other array elements are not referenced. If $uplo = 'L'$, the array a stores the lower triangle of A, other array elements are not referenced.
diag	CHARACTER*1. Must be 'N' or 'U'. If $diag = 'N'$, then A is not a unit triangular matrix. If $diag = 'U'$, then A is unit triangular: diagonal elements are assumed to be 1 and not referenced in the array a.
n	INTEGER. The order of the matrix $A \ (n \ge 0)$.

a, work	REAL for strcon
	DOUBLE PRECISION for dtrcon
	COMPLEX for ctrcon
	DOUBLE COMPLEX for ztrcon.
	Arrays: a(lda,*), work(*).
	The array a contains the matrix A .
	The second dimension of a must be at least $\max(1, n)$.
	The array <i>work</i> is a workspace for the routine.
	The dimension of work must be at least max $(1, 3*n)$ for
	real flavors and $max(1, 2*n)$ for complex flavors.
lda	INTEGER. The first dimension of a; $1 da \ge max(1, n)$.
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, n)$.
rwork	REAL for ctrcon
	DOUBLE PRECISION for ztrcon.
	Workspace array, DIMENSION at least $max(1, n)$.

rcond	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal of the condition number.
	The routine sets <i>rcond</i> =0 if the estimate underflows; in
	this case the matrix is singular (to working precision).
	However, anytime <i>rcond</i> is small compared to 1.0,
	for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately n^2 floating-point operations for real flavors and $4n^2$ operations for complex flavors.

?tpcon

Estimates the reciprocal of the condition number of a packed triangular matrix.

call stpcon	<pre>(norm,uplo,diag,n,ap,rcond,work,iwork,info)</pre>
call dtpcon	(norm,uplo,diag,n,ap,rcond,work,iwork,info)
call ctpcon	(norm,uplo,diag,n,ap,rcond,work,rwork,info)
call ztpcon	(norm,uplo,diag,n,ap,rcond,work,rwork,info)

Discussion

This routine estimates the reciprocal of the condition number of a packed triangular matrix *A* in either the 1-norm or infinity-norm:

$$\begin{split} \kappa_1(A) &= ||A||_1 ||A^{-1}||_1 = \kappa_{\infty}(A^T) = \kappa_{\infty}(A^H) \\ \kappa_{\infty}(A) &= ||A||_{\infty} ||A^{-1}||_{\infty} = \kappa_1(A^T) = \kappa_1(A^H) \;. \end{split}$$

norm	CHARACTER*1. Must be '1' or '0' or 'I'. If <i>norm</i> = '1' or '0', then the routine estimates $\kappa_1(A)$. If <i>norm</i> = 'I', then the routine estimates $\kappa_{\infty}(A)$.
uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether A is upper or lower triangular: If $uplo = 'U'$, the array ap stores the upper triangle of A in packed form. If $uplo = 'L'$, the array ap stores the lower triangle of A in packed form.
diag	CHARACTER*1. Must be 'N' or 'U'. If $diag = 'N'$, then A is not a unit triangular matrix. If $diag = 'U'$, then A is unit triangular: diagonal elements are assumed to be 1 and not referenced in the array <i>ap</i> .
п	INTEGER . The order of the matrix $A (n \ge 0)$.

REAL for stpcon
DOUBLE PRECISION for dtpcon
COMPLEX for ctpcon
DOUBLE COMPLEX for ztpcon.
Arrays: ap(*), work(*).
The array <i>ap</i> contains the packed matrix <i>A</i> .
The dimension of ap must be at least $\max(1, n(n+1)/2)$.
The array <i>work</i> is a workspace for the routine.
The dimension of <i>work</i> must be at least $max(1, 3*n)$ for real flavors and $max(1, 2*n)$ for complex flavors.
INTEGER.
Workspace array, DIMENSION at least $max(1, n)$.
REAL for ctpcon
DOUBLE PRECISION for ztpcon
Workspace array, DIMENSION at least $max(1, n)$.

rcond	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal of the condition number.
	I I
	The routine sets $rcond = 0$ if the estimate underflows; in
	this case the matrix is singular (to working precision).
	However, anytime <i>rcond</i> is small compared to 1.0,
	for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.
	ii <u>fiilo</u> – – f, me fui parameter nad an megar value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately n^2 floating-point operations for real flavors and $4n^2$ operations for complex flavors.

?tbcon

Estimates the reciprocal of the condition number of a triangular band matrix.

```
call stbcon ( norm,uplo,diag,n,kd,ab,ldab,rcond,work,iwork,info )
call dtbcon ( norm,uplo,diag,n,kd,ab,ldab,rcond,work,iwork,info )
call ctbcon ( norm,uplo,diag,n,kd,ab,ldab,rcond,work,rwork,info )
call ztbcon ( norm,uplo,diag,n,kd,ab,ldab,rcond,work,rwork,info )
```

Discussion

This routine estimates the reciprocal of the condition number of a triangular band matrix *A* in either the 1-norm or infinity-norm:

$$\begin{split} \kappa_1(A) &= ||A||_1 ||A^{-1}||_1 = \kappa_{\infty}(A^T) = \kappa_{\infty}(A^H) \\ \kappa_{\infty}(A) &= ||A||_{\infty} ||A^{-1}||_{\infty} = \kappa_1 (A^T) = \kappa_1 (A^H) . \end{split}$$

norm	CHARACTER*1. Must be '1' or '0' or 'I'. If <i>norm</i> = '1' or '0', then the routine estimates $\kappa_1(A)$. If <i>norm</i> = 'I', then the routine estimates $\kappa_{\infty}(A)$.
uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether A is upper or lower triangular: If $uplo = 'U'$, the array ap stores the upper triangle of A in packed form. If $uplo = 'L'$, the array ap stores the lower triangle of A in packed form.
diag	CHARACTER*1. Must be 'N' or 'U'. If $diag = 'N'$, then A is not a unit triangular matrix. If $diag = 'U'$, then A is unit triangular: diagonal elements are assumed to be 1 and not referenced in the array <i>ab</i> .
п	INTEGER . The order of the matrix $A \ (n \ge 0)$.
kd	INTEGER. The number of super-diagonals or sub-diagonals in the matrix $A \ (kd \ge 0)$.

ab, work	REAL for stbcon
	DOUBLE PRECISION for dtbcon
	COMPLEX for ctbcon
	DOUBLE COMPLEX for ztbcon.
	Arrays: ab(ldab,*), work(*).
	The array <i>ab</i> contains the band matrix A.
	The second dimension of ab must be at least max $(1,n)$.
	The array <i>work</i> is a workspace for the routine.
	The dimension of work must be at least $max(1, 3*n)$ for
	real flavors and $max(1, 2*n)$ for complex flavors.
ldab	INTEGER . The first dimension of the array <i>ab</i> .
	$(1dab \ge kd + 1).$
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, n)$.
rwork	REAL for ctbcon
	DOUBLE PRECISION for ztbcon.
	Workspace array, DIMENSION at least $max(1, n)$.

rcond	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal of the condition number.
	The routine sets $rcond = 0$ if the estimate underflows; in
	this case the matrix is singular (to working precision).
	However, anytime <i>rcond</i> is small compared to 1.0,
	for the working precision, the matrix may be poorly
	conditioned or even singular.
info	INTEGER. If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The computed *rcond* is never less than ρ (the reciprocal of the true condition number) and in practice is nearly always less than 10 ρ . A call to this routine involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately 2n(kd + 1) floating-point operations for real flavors and 8n(kd + 1) operations for complex flavors.

Refining the Solution and Estimating Its Error

This section describes the LAPACK routines for refining the computed solution of a system of linear equations and estimating the solution error. You can call these routines after factorizing the matrix of the system of equations and computing the solution (see <u>Routines for Matrix</u> Factorization and <u>Routines for Solving Systems of Linear Equations</u>).

?gerfs

Refines the solution of a system of linear equations with a general matrix and estimates its error.

call sgerfs	<pre>(trans,n,nrhs,a,lda,af,ldaf,ipiv,b,ldb, x,ldx,ferr,berr,work,iwork,info)</pre>
call dgerfs	<pre>(trans,n,nrhs,a,lda,af,ldaf,ipiv,b,ldb, x,ldx,ferr,berr,work,iwork,info)</pre>
call cgerfs	<pre>(trans,n,nrhs,a,lda,af,ldaf,ipiv,b,ldb, x,ldx,ferr,berr,work,rwork,info)</pre>
call zgerfs	<pre>(trans,n,nrhs,a,lda,af,ldaf,ipiv,b,ldb, x,ldx,ferr,berr,work,rwork,info)</pre>

Discussion

This routine performs an iterative refinement of the solution to a system of linear equations AX = B or $A^TX = B$ or $A^HX = B$ with a general matrix A, with multiple right-hand sides. For each computed solution vector x, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of A and b such that x is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|, \quad |\delta b_i| / |b_i| \leq \beta |b_i| \text{ such that } (A + \delta A)x = (b + \delta b).$

Finally, the routine estimates the *component-wise forward error* in the computed solution $||x - x_e|| ||| ||x|| |||_{\infty}$ (here x_e is the exact solution).

Before calling this routine:

- call the factorization routine <u>?getrf</u>
- call the solver routine <u>?getrs</u>.

```
CHARACTER*1. Must be 'N' or 'T' or 'C'.
trans
                  Indicates the form of the equations:
                  If trans = 'N', the system has the form AX = B.
                  If trans = 'T', the system has the form A^T X = B.
                  If trans = 'C', the system has the form A^{H}X = B.
                  INTEGER. The order of the matrix A \ (n \ge 0).
п
nrhs
                  INTEGER. The number of right-hand sides (nrhs \geq 0).
a, af, b, x, work
                          REAL for sgerfs
                          DOUBLE PRECISION for dgerfs
                          COMPLEX for cgerfs
                          DOUBLE COMPLEX for zgerfs.
                  Arrays:
                  a (1da, *) contains the original matrix A, as supplied
                  to ?getrf.
                  af (ldaf, *) contains the factored matrix A, as returned
                  by <u>?getrf</u>.
                  b(1db, *) contains the right-hand side matrix B.
                  x(ldx, *) contains the solution matrix X.
                  work (*) is a workspace array.
                  The second dimension of a and af must be at least
                  \max(1,n); the second dimension of b and x must be at
                  least max(1,nrhs); the dimension of work must be at
                  least max(1, 3*n) for real flavors and max(1, 2*n) for
                  complex flavors.
lda
                  INTEGER. The first dimension of a; 1da \ge max(1, n).
                  INTEGER. The first dimension of af; ldaf \ge max(1, n).
ldaf
ldb
                  INTEGER. The first dimension of b; ldb \ge max(1, n).
ldx
                  INTEGER. The first dimension of x; 1dx \ge max(1, n).
```

ipiv	INTEGER. Array, DIMENSION at least max(1, <i>n</i>). The <i>ipiv</i> array, as returned by <u>?getrf</u> .
iwork	INTEGER. Workspace array, DIMENSION at least $\max(1, n)$.
	workspace array, DIMENSION at least $\max(1, n)$.
rwork	REAL for cgerfs
	DOUBLE PRECISION for zgerfs.
	Workspace array, DIMENSION at least max(1, <i>n</i>).

x	The refined solution matrix <i>X</i> .
ferr, berr	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the
	component-wise forward and backward errors,
	respectively, for each solution vector.
info	INTEGER.
	If <i>info</i> = 0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

For each right-hand side, computation of the backward error involves a minimum of $4n^2$ floating-point operations (for real flavors) or $16n^2$ operations (for complex flavors). In addition, each step of iterative refinement involves $6n^2$ operations (for real flavors) or $24n^2$ operations (for complex flavors); the number of iterations may range from 1 to 5. Estimating the forward error involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors or $8n^2$ for complex flavors.

?gbrfs

Refines the solution of a system of linear equations with a general band matrix and estimates its error.

call sgbrfs	<pre>(trans,n,kl,ku,nrhs,ab,ldab,afb,ldafb,ipiv, b,ldb,x,ldx,ferr,berr,work,iwork,info)</pre>
call dgbrfs	<pre>(trans,n,kl,ku,nrhs,ab,ldab,afb,ldafb,ipiv, b,ldb,x,ldx,ferr,berr,work,iwork,info)</pre>
call cgbrfs	<pre>(trans,n,kl,ku,nrhs,ab,ldab,afb,ldafb,ipiv, b,ldb,x,ldx,ferr,berr,work,rwork,info)</pre>
call zgbrfs	<pre>(trans,n,kl,ku,nrhs,ab,ldab,afb,ldafb,ipiv, b,ldb,x,ldx,ferr,berr,work,rwork,info)</pre>

Discussion

This routine performs an iterative refinement of the solution to a system of linear equations AX = B or $A^TX = B$ or $A^HX = B$ with a band matrix A, with multiple right-hand sides. For each computed solution vector x, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of A and b such that x is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|$, $|\delta b_i| / |b_i| \leq \beta |b_i|$ such that $(A + \delta A)x = (b + \delta b)$. Finally, the routine estimates the *component-wise forward error* in the computed solution $||x - x_e|| \leq ||x|| \leq (here x_e \text{ is the exact solution})$. Before calling this routine:

- call the factorization routine <u>?gbtrf</u>
- call the solver routine <u>?gbtrs</u>.

input l'arantetere	
trans	CHARACTER*1. Must be 'N' or 'T' or 'C'.
	Indicates the form of the equations:
	If <i>trans</i> = 'N', the system has the form $AX = B$.
	If trans = T' , the system has the form $A^T X = B$.
	If <i>trans</i> = 'C', the system has the form $A^H X = B$.
п	INTEGER. The order of the matrix $A (n \ge 0)$.
kl	INTEGER. The number of sub-diagonals within the band
	of A ($k l \ge 0$).
ku	INTEGER. The number of super-diagonals within the
	band of A ($ku \ge 0$).
nrhs	INTEGER. The number of right-hand sides $(nrhs \ge 0)$.
ab,afb,b,x,wo	
	DOUBLE PRECISION for dgbrfs
	COMPLEX for cgbrfs
	DOUBLE COMPLEX for zgbrfs.
	Arrays:
	ab(ldab, *) contains the original band matrix A, as
	supplied to <u>?gbtrf</u> , but stored in rows from 1 to $kl + ku$
	+1.
	afb(ldafb, *) contains the factored band matrix A, as
	returned by <u>?gbtrf</u> .
	b(ldb, *) contains the right-hand side matrix B.
	x(ldx, *) contains the solution matrix X.
	work (*) is a workspace array.
	The second dimension of <i>ab</i> and <i>afb</i> must be at least
	$\max(1, n)$; the second dimension of b and x must be at
	least max(1, <i>nrhs</i>); the dimension of <i>work</i> must be at
	least max $(1, 3*n)$ for real flavors and max $(1, 2*n)$ for
	complex flavors.
ldab	INTEGER. The first dimension of <i>ab</i> .
ldafb	INTEGER. The first dimension of <i>afb</i> .
ldb	INTEGER. The first dimension of b; $ldb \ge max(1, n)$.
ldx	INTEGER . The first dimension of x ; $ldx \ge max(1, n)$.

ipiv	INTEGER.
	Array, DIMENSION at least max(1, <i>n</i>).
	The <i>ipiv</i> array, as returned by <u>?gbtrf</u> .
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, n)$.
rwork	REAL for cgbrfs
	DOUBLE PRECISION for zgbrfs
	Workspace array, DIMENSION at least $max(1, n)$.

x	The refined solution matrix X.
ferr, berr	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the
	component-wise forward and backward errors,
	respectively, for each solution vector.
info	INTEGER.
	If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

For each right-hand side, computation of the backward error involves a minimum of 4n(kl + ku) floating-point operations (for real flavors) or 16n(kl + ku) operations (for complex flavors). In addition, each step of iterative refinement involves 2n(4kl + 3ku) operations (for real flavors) or 8n(4kl + 3ku) operations (for complex flavors); the number of iterations may range from 1 to 5. Estimating the forward error involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors or $8n^2$ for complex flavors.

?gtrfs

Refines the solution of a system of linear equations with a tridiagonal matrix and estimates its error.

Discussion

This routine performs an iterative refinement of the solution to a system of linear equations AX = B or $A^TX = B$ or $A^HX = B$ with a tridiagonal matrix A, with multiple right-hand sides. For each computed solution vector x, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of A and b such that x is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|, \quad |\delta b_i| / |b_i| \leq \beta |b_i| \text{ such that } (A + \delta A)x = (b + \delta b).$

Finally, the routine estimates the *component-wise forward error* in the computed solution $||x - x_e|| \ll ||x|| \approx$ (here x_e is the exact solution).

Before calling this routine:

- call the factorization routine <u>?gttrf</u>
- call the solver routine <u>?gttrs</u>.

Input Parameters

trans

```
CHARACTER*1. Must be 'N' or 'T' or 'C'.
Indicates the form of the equations:
If trans = 'N', the system has the form AX = B.
If trans = 'T', the system has the form A^TX = B.
If trans = 'C', the system has the form A^HX = B.
```

```
INTEGER. The order of the matrix A (n \ge 0).
n
nrhs
                   INTEGER. The number of right-hand sides, i.e., the
                  number of columns of the matrix B (nrhs \ge 0).
dl,d,du,dlf,df,
duf,du2,b,x,work REAL for sqtrfs
                       DOUBLE PRECISION for dqtrfs
                       COMPLEX for cqtrfs
                       DOUBLE COMPLEX for zqtrfs.
                  Arrays:
                  d1, dimension (n - 1), contains the subdiagonal
                  elements of A.
                  d, dimension (n), contains the diagonal elements of A.
                  du, dimension (n - 1), contains the superdiagonal
                  elements of A.
                  dlf, dimension (n - 1), contains the (n - 1) multipliers
                  that define the matrix L from the LU factorization of A
                  as computed by <u>?gttrf</u>.
                  df, dimension (n), contains the n diagonal elements
                  of the upper triangular matrix U from the LU
                  factorization of A.
                  duf, dimension (n - 1), contains the (n - 1) elements
                  of the first super-diagonal of U.
                  du2, dimension (n - 2), contains the (n - 2) elements
                  of the second super-diagonal of U.
                  b(ldb, nrhs) contains the right-hand side matrix B.
                  x(ldx, nrhs) contains the solution matrix X, as
                  computed by <u>?gttrs</u>.
                  work (*) is a workspace array;
                   the dimension of work must be at least max(1, 3*n) for
                  real flavors and max(1, 2*n) for complex flavors.
ldb
                   INTEGER. The first dimension of b; ldb \ge max(1, n).
ldx
                   INTEGER. The first dimension of x; 1dx \ge max(1, n).
ipiv
                   INTEGER.
                   Array, DIMENSION at least max(1,n).
                   The ipiv array, as returned by <u>?gttrf</u>.
```

iwork	INTEGER.
	Workspace array, DIMENSION (<i>n</i>). Used for real
	flavors only.
rwork	REAL for cgtrfs
	DOUBLE PRECISION for zgtrfs.
	Workspace array, DIMENSION (<i>n</i>). Used for complex
	flavors only.

X	The refined solution matrix <i>X</i> .
ferr, berr	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the
	component-wise forward and backward errors,
	respectively, for each solution vector.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

?porfs

Refines the solution of a system of linear equations with a symmetric (Hermitian) positive-definite matrix and estimates its error.

call sporfs	<pre>(uplo,n,nrhs,a,lda,af,ldaf,b,ldb, x,ldx,ferr,berr,work,iwork,info)</pre>
call dporfs	<pre>(uplo,n,nrhs,a,lda,af,ldaf,b,ldb, x,ldx,ferr,berr,work,iwork,info)</pre>
call cporfs	<pre>(uplo,n,nrhs,a,lda,af,ldaf,b,ldb, x,ldx,ferr,berr,work,rwork,info)</pre>
call zporfs	<pre>(uplo,n,nrhs,a,lda,af,ldaf,b,ldb, x,ldx,ferr,berr,work,rwork,info)</pre>

Discussion

This routine performs an iterative refinement of the solution to a system of linear equations AX = B with a symmetric (Hermitian) positive definite matrix *A*, with multiple right-hand sides. For each computed solution vector *x*, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of *A* and *b* such that *x* is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|$, $|\delta b_i| / |b_i| \leq \beta |b_i|$ such that $(A + \delta A)x = (b + \delta b)$. Finally, the routine estimates the *component-wise forward error* in the computed solution $||x - x_e|| \leq ||x|| \leq (here x_e \text{ is the exact solution})$.

Before calling this routine:

- call the factorization routine <u>?potrf</u>
- call the solver routine <u>?potrs</u>.

input Paramet	
uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates how the input matrix A has been factored:
	If $uplo = 'U'$, the array <i>af</i> stores the factor U of the
	Cholesky factorization $A = U^H U$.
	If $uplo = 'L'$, the array <i>af</i> stores the factor L of the
	Cholesky factorization $A = LL^H$.
n	INTEGER . The order of the matrix $A (n \ge 0)$.
nrhs	INTEGER . The number of right-hand sides $(nrhs \ge 0)$.
a, af, b, x,	work REAL for sporfs
	DOUBLE PRECISION for dporfs
	COMPLEX for cporfs
	DOUBLE COMPLEX for zporfs.
	Arrays:
	a(lda, *) contains the original matrix A, as supplied
	to <u>?potrf</u> .
	af (ldaf, *) contains the factored matrix A, as returned
	by <u>?potrf</u> .
	b(1db, *) contains the right-hand side matrix B.
	x(ldx, *) contains the solution matrix X.
	work (*) is a workspace array.
	The second dimension of a and af must be at least
	$\max(1,n)$; the second dimension of <i>b</i> and x must be at
	least max(1, <i>nrhs</i>); the dimension of <i>work</i> must be at
	least max $(1, 3*n)$ for real flavors and max $(1, 2*n)$ for
	complex flavors.
lda	INTEGER . The first dimension of a; $1 da \ge max(1, n)$.
ldaf	INTEGER. The first dimension of <i>af</i> ; $1daf \ge max(1, n)$.
ldb	INTEGER . The first dimension of b; $ldb \ge max(1, n)$.
ldx	INTEGER. The first dimension of x ; $ldx \ge max(1, n)$.
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, n)$.
rwork	REAL for cporfs
	DOUBLE PRECISION for zporfs
	Workspace array, DIMENSION at least $max(1, n)$.

The refined solution matrix <i>X</i> .
REAL for single precision flavors.
DOUBLE PRECISION for double precision flavors.
Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the
component-wise forward and backward errors,
respectively, for each solution vector.
INTEGER.
If $info = 0$, the execution is successful.
If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

For each right-hand side, computation of the backward error involves a minimum of $4n^2$ floating-point operations (for real flavors) or $16n^2$ operations (for complex flavors). In addition, each step of iterative refinement involves $6n^2$ operations (for real flavors) or $24n^2$ operations (for complex flavors); the number of iterations may range from 1 to 5. Estimating the forward error involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors or $8n^2$ for complex flavors.

?pprfs

Refines the solution of a system of linear equations with a packed symmetric (Hermitian) positive-definite matrix and estimates its error.

call spprfs	(uplo,n,nrhs,ap,afp,b,ldb,x,ldx, ferr,berr,work,iwork,info)
call dpprfs	<pre>(uplo,n,nrhs,ap,afp,b,ldb,x,ldx, ferr,berr,work,iwork,info)</pre>
call cpprfs	(uplo,n,nrhs,ap,afp,b,ldb,x,ldx, ferr,berr,work,rwork,info)
call zpprfs	

Discussion

This routine performs an iterative refinement of the solution to a system of linear equations AX = B with a packed symmetric (Hermitian) positive definite matrix *A*, with multiple right-hand sides. For each computed solution vector *x*, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of *A* and *b* such that *x* is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|, \quad |\delta b_i| / |b_i| \leq \beta |b_i| \text{ such that } (A + \delta A)x = (b + \delta b).$

Finally, the routine estimates the *component-wise forward error* in the computed solution $||x - x_e|| ||| ||x|| ||_{\infty}$ (here x_e is the exact solution).

Before calling this routine:

- call the factorization routine <u>?pptrf</u>
- call the solver routine <u>?pptrs</u>.

Input Parameters

uplo

CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix *A* has been factored:

	If $uplo = U'$, the array <i>afp</i> stores the packed factor U of the Cholesky factorization $A = U^H U$.
	If $uplo = 'L'$, the array afp stores the packed factor L of the Cholesky factorization $A = LL^{H}$.
п	INTEGER . The order of the matrix $A (n \ge 0)$.
nrhs	INTEGER . The number of right-hand sides $(nrhs \ge 0)$.
ap, afp, b, x	, work REAL for spprfs
	DOUBLE PRECISION for dpprfs
	COMPLEX for cpprfs
	DOUBLE COMPLEX for zpprfs.
	Arrays:
	ap(*) contains the original packed matrix A, as supplied to <u>?pptrf</u> .
	<i>afp</i> (*) contains the factored packed matrix A, as returned by <u>?pptrf</u> .
	b(1db, *) contains the right-hand side matrix B.
	x(ldx, *) contains the solution matrix X.
	work (*) is a workspace array.
	The dimension of arrays ap and afp must be at least
	$\max(1, n(n+1)/2)$; the second dimension of b and x must
	be at least max(1, <i>nrhs</i>); the dimension of <i>work</i> must be
	at least $\max(1, 3^*n)$ for real flavors and $\max(1, 2^*n)$ for
	complex flavors.
ldb	INTEGER. The first dimension of b; $ldb \ge max(1, n)$.
ldx	INTEGER . The first dimension of <i>x</i> ; $1dx \ge max(1, n)$.
iwork	INTEGER.
1	Workspace array, DIMENSION at least $\max(1, n)$.
rwork	REAL for cpprfs DOUBLE PRECISION for zpprfs
	Workspace array, DIMENSION at least $\max(1, n)$.
	torrespace analy, Dimenoron at least max(1, 11).

x The refined solution matrix *X*.

ferr, berr	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the
	component-wise forward and backward errors,
	respectively, for each solution vector.
info	INTEGER. If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

For each right-hand side, computation of the backward error involves a minimum of $4n^2$ floating-point operations (for real flavors) or $16n^2$ operations (for complex flavors). In addition, each step of iterative refinement involves $6n^2$ operations (for real flavors) or $24n^2$ operations (for complex flavors); the number of iterations may range from 1 to 5.

Estimating the forward error involves solving a number of systems of linear equations Ax = b; the number of systems is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors or $8n^2$ for complex flavors.

?pbrfs

Refines the solution of a system of linear equations with a band symmetric (Hermitian) positive-definite matrix and estimates its error.

call	spbrfs	<pre>(uplo,n,kd,nrhs,ab,ldab,afb,ldafb, b,ldb,x,ldx,ferr,berr,work,iwork,info)</pre>
call	dpbrfs	<pre>(uplo,n,kd,nrhs,ab,ldab,afb,ldafb, b,ldb,x,ldx,ferr,berr,work,iwork,info)</pre>
call	cpbrfs	(uplo,n,kd,nrhs,ab,ldab,afb,ldafb, b,ldb,x,ldx,ferr,berr,work,rwork,info)
call	zpbrfs	<pre>(uplo,n,kd,nrhs,ab,ldab,afb,ldafb, b,ldb,x,ldx,ferr,berr,work,rwork,info)</pre>

Discussion

This routine performs an iterative refinement of the solution to a system of linear equations AX = B with a symmetric (Hermitian) positive definite band matrix *A*, with multiple right-hand sides. For each computed solution vector *x*, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of *A* and *b* such that *x* is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|, |\delta b_i| / |b_i| \leq \beta |b_i|$ such that $(A + \delta A)x = (b + \delta b)$.

Before calling this routine:

- call the factorization routine <u>?pbtrf</u>
- call the solver routine <u>?pbtrs</u>.

Input Parameters

uplo

CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix *A* has been factored:

	If $uplo = 'U'$, the array <i>afb</i> stores the factor U of the Cholesky factorization $A = U^H U$.
	If $uplo = 'L'$, the array <i>afb</i> stores the factor <i>L</i> of the
	Cholesky factorization $A = LL^H$.
n	INTEGER . The order of the matrix $A (n \ge 0)$.
kd	INTEGER . The number of super-diagonals or
	sub-diagonals in the matrix $A (kd \ge 0)$.
nrhs	INTEGER . The number of right-hand sides $(nrhs \ge 0)$.
ab,afb,b,x,wo	-
	DOUBLE PRECISION for dpbrfs
	COMPLEX for cpbrfs
	DOUBLE COMPLEX for zpbrfs.
	Arrays:
	<i>ab</i> (<i>ldab</i> , *) contains the original band matrix <i>A</i> , as supplied to <u>?pbtrf</u> .
	afb(ldafb, *) contains the factored band matrix A, as
	returned by <u>?pbtrf</u> .
	b(ldb, *) contains the right-hand side matrix B.
	x(ldx, *) contains the solution matrix X.
	work (*) is a workspace array.
	The second dimension of <u>ab</u> and <u>afb</u> must be at least
	$\max(1,n)$; the second dimension of b and x must be at
	least max(1, <i>nrhs</i>); the dimension of <i>work</i> must be at
	least max $(1, 3*n)$ for real flavors and max $(1, 2*n)$ for
	complex flavors.
ldab	INTEGER. The first dimension of <i>ab</i> ; $1dab \ge kd + 1$.
ldafb	INTEGER. The first dimension of <i>afb</i> ; $ldafb \ge kd + 1$.
ldb	INTEGER. The first dimension of b; $ldb \ge max(1, n)$.
ldx	INTEGER . The first dimension of <i>x</i> ; $ldx \ge max(1, n)$.
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, n)$.
rwork	REAL for cpbrfs
	DOUBLE PRECISION for zpbrfs
	Workspace array, DIMENSION at least $max(1, n)$.

The refined solution matrix <i>X</i> .
REAL for single precision flavors.
DOUBLE PRECISION for double precision flavors.
Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the
component-wise forward and backward errors,
respectively, for each solution vector.
INTEGER.
If $info = 0$, the execution is successful.
If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

For each right-hand side, computation of the backward error involves a minimum of 8n*kd floating-point operations (for real flavors) or 32n*kd operations (for complex flavors). In addition, each step of iterative refinement involves 12n*kd operations (for real flavors) or 48n*kd operations (for complex flavors); the number of iterations may range from 1 to 5.

Estimating the forward error involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately 4n*kd floating-point operations for real flavors or 16n*kd for complex flavors.

?ptrfs

Refines the solution of a system of linear equations with a symmetric (Hermitian) positive-definite tridiagonal matrix and estimates its error.

Discussion

This routine performs an iterative refinement of the solution to a system of linear equations AX = B with a symmetric (Hermitian) positive definite tridiagonal matrix *A*, with multiple right-hand sides. For each computed solution vector *x*, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of *A* and *b* such that *x* is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|$, $|\delta b_i| / |b_i| \leq \beta |b_i|$ such that $(A + \delta A)x = (b + \delta b)$. Finally, the routine estimates the *component-wise forward error* in the computed solution $||x - x_e|| \leq ||x|| \leq (here x_e \text{ is the exact solution}).$

Before calling this routine:

- call the factorization routine <u>?pttrf</u>
- call the solver routine <u>?pttrs</u>.

Input Parameters

uplo

CHARACTER*1. Used for complex flavors only. Must be 'U' or 'L'. Specifies whether the superdiagonal or the subdiagonal of the tridiagonal matrix A is stored and how A is factored:

	If $uplo = 'U'$, the array e stores the superdiagonal of A ,
	and A is factored as $U^H D U$;
	If $uplo = 'L'$, the array e stores the subdiagonal of A , and A is factored as LDL^{H} .
п	INTEGER . The order of the matrix $A \ (n \ge 0)$.
nrhs	INTEGER . The number of right-hand sides $(nrhs \ge 0)$.
d,df,rwork	REAL for single precision flavors
	DOUBLE PRECISION for double precision flavors
	Arrays: $d(n)$, $df(n)$, $rwork(n)$.
	The array d contains the n diagonal elements of the
	tridiagonal matrix A.
	The array df contains the <i>n</i> diagonal elements of the
	diagonal matrix D from the factorization of A as
	computed by <u>?pttrf</u> .
	The array <i>rwork</i> is a workspace array used for complex
	flavors only.
e,ef,b,x,work	REAL for sptrfs
	DOUBLE PRECISION for dptrfs
	COMPLEX for cptrfs
	DOUBLE COMPLEX for zptrfs.
	Arrays: $e(n-1)$, $ef(n-1)$, $b(ldb,nrhs)$,
	x(ldx,nrhs), work(*).
	The array e contains the $(n - 1)$ off-diagonal elements
	of the tridiagonal matrix A (see $uplo$). The error f contains the (-1) off diagonal elements
	The array ef contains the $(n - 1)$ off-diagonal elements of the unit bidiagonal factor U or L from the
	factorization computed by <u>?pttrf</u> (see <u>uplo</u>).
	The array b contains the matrix B whose columns are
	the right-hand sides for the systems of equations.
	The array \mathbf{x} contains the solution matrix X as computed
	by <u>?pttrs</u> .
	The array <i>work</i> is a workspace array. The dimension of
	work must be at least $2*n$ for real flavors, and at least
	<i>n</i> for complex flavors.
ldb	INTEGER. The leading dimension of <i>b</i> ; $ldb \ge max(1, n)$.
ldx	INTEGER. The leading dimension of x ; $ldx \ge max(1, n)$.

x ferr, berr	The refined solution matrix <i>X</i> . REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. Arrays DIMENSION et least may (1 marks). Contain the
info	Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the component-wise forward and backward errors, respectively, for each solution vector. INTEGER.
	If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value.

?syrfs

Refines the solution of a system of linear equations with a symmetric matrix and estimates its error.

call ssyrfs	<pre>(uplo,n,nrhs,a,lda,af,ldaf,ipiv,b,ldb, x,ldx,ferr,berr,work,iwork,info)</pre>
call dsyrfs	<pre>(uplo,n,nrhs,a,lda,af,ldaf,ipiv,b,ldb, x,ldx,ferr,berr,work,iwork,info)</pre>
call csyrfs	<pre>(uplo,n,nrhs,a,lda,af,ldaf,ipiv,b,ldb, x,ldx,ferr,berr,work,rwork,info)</pre>
call zsyrfs	(uplo,n,nrhs,a,lda,af,ldaf,ipiv,b,ldb, x,ldx,ferr,berr,work,rwork,info)

Discussion

This routine performs an iterative refinement of the solution to a system of linear equations AX = B with a symmetric full-storage matrix A, with multiple right-hand sides. For each computed solution vector x, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of A and b such that x is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|, \quad |\delta b_i| / |b_i| \leq \beta |b_i| \text{ such that } (A + \delta A)x = (b + \delta b).$

Finally, the routine estimates the *component-wise forward error* in the computed solution $||x - x_e|| ||| ||x|| |||_{\infty}$ (here x_e is the exact solution).

Before calling this routine:

- call the factorization routine <u>?sytrf</u>
- call the solver routine <u>?sytrs</u>.

Input Parameters

uplo

CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix *A* has been factored:

	If $uplo = 'U'$, the array <i>af</i> stores the Bunch-Kaufman
	factorization $A = PUDU^T P^T$.
	If $uplo = 'L'$, the array <i>af</i> stores the Bunch-Kaufman factorization $A = PLDL^T P^T$.
n	INTEGER . The order of the matrix $A (n \ge 0)$.
nrhs	INTEGER. The number of right-hand sides $(nrhs \ge 0)$.
a, af, b, x,	work REAL for ssyrfs
	DOUBLE PRECISION for dsyrfs
	COMPLEX for csyrfs
	DOUBLE COMPLEX for zsyrfs.
	Arrays:
	a(1da, *) contains the original matrix A, as supplied
	to <u>?sytrf</u> .
	af (ldaf, *) contains the factored matrix A, as returned
	by <u>?sytrf</u> .
	b(1db, *) contains the right-hand side matrix B.
	x(ldx, *) contains the solution matrix X.
	work (*) is a workspace array.
	The second dimension of a and af must be at least
	$\max(1,n)$; the second dimension of <i>b</i> and <i>x</i> must be at
	least max(1, <i>nrhs</i>); the dimension of <i>work</i> must be at
	least max $(1, 3*n)$ for real flavors and max $(1, 2*n)$ for
	complex flavors.
lda	INTEGER . The first dimension of a ; $1da \ge max(1, n)$.
ldaf	INTEGER. The first dimension of <i>af</i> ; $1daf \ge max(1, n)$.
ldb	INTEGER . The first dimension of b; $ldb \ge max(1, n)$.
ldx	INTEGER. The first dimension of x ; $ldx \ge max(1, n)$.
ipiv	INTEGER.
	Array, DIMENSION at least $\max(1, n)$.
	The <i>ipiv</i> array, as returned by <u>?sytrf</u> .
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, n)$.
rwork	REAL for csyrfs
	DOUBLE PRECISION for zsyrfs.
	Workspace array, DIMENSION at least $\max(1, n)$.

The refined solution matrix <i>X</i> .
REAL for single precision flavors.
DOUBLE PRECISION for double precision flavors.
Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the
component-wise forward and backward errors,
respectively, for each solution vector.
INTEGER.
If $info = 0$, the execution is successful.
If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

For each right-hand side, computation of the backward error involves a minimum of $4n^2$ floating-point operations (for real flavors) or $16n^2$ operations (for complex flavors). In addition, each step of iterative refinement involves $6n^2$ operations (for real flavors) or $24n^2$ operations (for complex flavors); the number of iterations may range from 1 to 5. Estimating the forward error involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors or $8n^2$ for complex flavors.

?herfs

Refines the solution of a system of linear equations with a complex Hermitian matrix and estimates its error.

> call cherfs (uplo, n, nrhs, a, lda, af, ldaf, ipiv, b, ldb, x,ldx,ferr,berr,work,rwork,info) call zherfs (uplo, n, nrhs, a, lda, af, ldaf, ipiv, b, ldb, x, ldx, ferr, berr, work, rwork, info)

Discussion

This routine performs an iterative refinement of the solution to a system of linear equations AX = B with a complex Hermitian full-storage matrix A, with multiple right-hand sides. For each computed solution vector *x*, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of A and b such that x is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|, |\delta b_j| / |b_j| \leq \beta |b_j|$ such that $(A + \delta A)x = (b + \delta b)$.

Finally, the routine estimates the *component-wise forward error* in the computed solution $||x - x_e|| \leq ||x|| \leq (here x_e is the exact solution).$

Before calling this routine:

- call the factorization routine ?hetrf
- call the solver routine ?hetrs.

uplo	CHARACTER*1. Must be 'U' or 'L'.
-	Indicates how the input matrix A has been factored:
	If $uplo = 'U'$, the array <i>af</i> stores the Bunch-Kaufman
	factorization $A = PUDU^{H}P^{T}$.
	If <u>uplo</u> = 'L', the array <u>af</u> stores the Bunch-Kaufman
	factorization $A = PLDL^{H}P^{T}$.
n	INTEGER . The order of the matrix $A (n \ge 0)$.

nrhs	INTEGER. The number of right-hand sides (<i>nrhs</i> \geq 0).
a, af, b, x,	work COMPLEX for cherfs DOUBLE COMPLEX for zherfs.
	Arrays:
	a (<i>lda</i> , *) contains the original matrix A, as supplied to <u>?hetrf</u> .
	af (ldaf, $*$) contains the factored matrix A, as returned by <u>?hetrf</u> .
	b(ldb, *) contains the right-hand side matrix B.
	x(ldx, *) contains the solution matrix X.
	work (*) is a workspace array.
	The second dimension of <i>a</i> and <i>af</i> must be at least $max(1,n)$; the second dimension of <i>b</i> and <i>x</i> must be at least $max(1,nrhs)$; the dimension of <i>work</i> must be at least $max(1, 2*n)$.
lda	INTEGER. The first dimension of a ; $1da \ge max(1, n)$.
ldaf	INTEGER. The first dimension of <i>af</i> ; $1daf \ge max(1, n)$.
ldb	INTEGER. The first dimension of b; $ldb \ge max(1, n)$.
ldx	INTEGER. The first dimension of x ; $ldx \ge max(1, n)$.
ipiv	INTEGER.
	Array, DIMENSION at least max $(1,n)$. The <i>ipiv</i> array, as returned by <u>?hetrf</u> .
rwork	REAL for cherfs
	DOUBLE PRECISION for zherfs. Workspace array, DIMENSION at least max(1, <i>n</i>).

x ferr, berr	The refined solution matrix X. REAL for cherfs DOUBLE PRECISION for zherfs.
	Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the component-wise forward and backward errors, respectively, for each solution vector.
info	INTEGER. If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

For each right-hand side, computation of the backward error involves a minimum of $16n^2$ operations. In addition, each step of iterative refinement involves $24n^2$ operations; the number of iterations may range from 1 to 5.

Estimating the forward error involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $8n^2$ floating-point operations.

The real counterpart of this routine is **ssyrfs** / **dsyrfs**.

?sprfs

Refines the solution of a system of linear equations with a packed symmetric matrix and estimates the solution error.

call ssp	fs (uplo,n,nrhs,ap,afp,ipiv,b,ldb,x,ldx, ferr,berr,work,iwork,info)
call dsp	fs (uplo,n,nrhs,ap,afp,ipiv,b,ldb,x,ldx, ferr,berr,work,iwork,info)
call csp	fs (uplo,n,nrhs,ap,afp,ipiv,b,ldb,x,ldx, ferr,berr,work,rwork,info)
call zsp	<pre>fs (uplo,n,nrhs,ap,afp,ipiv,b,ldb,x,ldx,</pre>

Discussion

This routine performs an iterative refinement of the solution to a system of linear equations AX = B with a packed symmetric matrix A, with multiple right-hand sides. For each computed solution vector x, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of A and b such that x is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|, \quad |\delta b_i| / |b_i| \leq \beta |b_i| \text{ such that } (A + \delta A)x = (b + \delta b).$

Before calling this routine:

- call the factorization routine <u>?sptrf</u>
- call the solver routine <u>?sptrs</u>.

Input Parameters

uplo

CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix *A* has been factored:

	If $uplo = 'U'$, the array <i>afp</i> stores the packed Bunch-Kaufman factorization $A = PUDU^TP^T$. If $uplo = 'L'$, the array <i>afp</i> stores the packed Bunch-Kaufman factorization $A = PLDL^TP^T$.
2	INTEGER. The order of the matrix A ($n \ge 0$).
n	
nrhs	INTEGER . The number of right-hand sides $(nrhs \ge 0)$.
ap, afp, b, x	, work REAL for ssprfs
	DOUBLE PRECISION for dsprfs
	COMPLEX for csprfs
	DOUBLE COMPLEX for zsprfs.
	Arrays:
	ap(*) contains the original packed matrix A, as supplied to <u>2sptrf</u> .
	afp(*) contains the factored packed matrix A, as
	returned by <u>?sptrf</u> .
	b(1db, *) contains the right-hand side matrix B.
	x(ldx, *) contains the solution matrix X.
	work (*) is a workspace array.
	The dimension of arrays ap and afp must be at least $\max(1, n(n+1)/2)$; the second dimension of b and x must be at least $\max(1, nrhs)$; the dimension of work must be at least $\max(1, 3*n)$ for real flavors and $\max(1, 2*n)$ for complex flavors.
ldb	INTEGER. The first dimension of b; $ldb \ge max(1, n)$.
ldx	INTEGER . The first dimension of <i>x</i> ; $ldx \ge max(1, n)$.
ipiv	INTEGER.
	Array, DIMENSION at least $max(1,n)$. The <i>ipiv</i> array, as returned by <u>?sptrf</u> .
iwork	INTEGER.
	Workspace array, DIMENSION at least max(1, <i>n</i>).
rwork	REAL for csprfs
	DOUBLE PRECISION for zsprfs
	Workspace array, DIMENSION at least $max(1, n)$.

The refined solution matrix <i>X</i> .
REAL for single precision flavors.
DOUBLE PRECISION for double precision flavors.
Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the
component-wise forward and backward errors,
respectively, for each solution vector.
INTEGER.
If $info = 0$, the execution is successful.
If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

For each right-hand side, computation of the backward error involves a minimum of $4n^2$ floating-point operations (for real flavors) or $16n^2$ operations (for complex flavors). In addition, each step of iterative refinement involves $6n^2$ operations (for real flavors) or $24n^2$ operations (for complex flavors); the number of iterations may range from 1 to 5.

Estimating the forward error involves solving a number of systems of linear equations Ax = b; the number of systems is usually 4 or 5 and never more than 11. Each solution requires approximately $2n^2$ floating-point operations for real flavors or $8n^2$ for complex flavors.

?hprfs

Refines the solution of a system of linear equations with a packed complex Hermitian matrix and estimates the solution error.

Discussion

This routine performs an iterative refinement of the solution to a system of linear equations AX = B with a packed complex Hermitian matrix A, with multiple right-hand sides. For each computed solution vector x, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of A and b such that x is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|, \quad |\delta b_i| / |b_i| \leq \beta |b_i| \text{ such that } (A + \delta A)x = (b + \delta b).$

Finally, the routine estimates the *component-wise forward error* in the computed solution $||x - x_e|| \ll ||x|| \approx$ (here x_e is the exact solution).

Before calling this routine:

- call the factorization routine <u>?hptrf</u>
- call the solver routine <u>?hptrs</u>.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates how the input matrix A has been factored:
	If $uplo = 'U'$, the array <i>afp</i> stores the packed
	Bunch-Kaufman factorization $A = PUDU^{H}P^{T}$.
	If $uplo = 'L'$, the array <i>afp</i> stores the packed
	Bunch-Kaufman factorization $A = PLDL^{H}P^{T}$.
п	INTEGER . The order of the matrix $A (n \ge 0)$.
nrhs	INTEGER . The number of right-hand sides (<i>nrhs</i> \geq 0).

ap, afp, b, x	, work COMPLEX for chprfs DOUBLE COMPLEX for zhprfs.
	Arrays:
	ap(*) contains the original packed matrix A, as supplied to <u>?hptrf</u> .
	afp(*) contains the factored packed matrix A, as returned by <u>?hptrf</u> .
	b(1db, *) contains the right-hand side matrix B.
	x(ldx, *) contains the solution matrix X.
	work (*) is a workspace array.
	The dimension of arrays ap and afp must be at least max $(1,n(n+1)/2)$; the second dimension of b and x must be at least max $(1,nrhs)$; the dimension of work must be at least max $(1, 2*n)$.
ldb	INTEGER. The first dimension of b; $ldb \ge max(1, n)$.
ldx	INTEGER. The first dimension of x ; $ldx \ge max(1, n)$.
ipiv	INTEGER. Array, DIMENSION at least max $(1,n)$. The <i>ipiv</i> array, as returned by <u>?hptrf</u> .
rwork	REAL for chprfs DOUBLE PRECISION for zhprfs Workspace array, DIMENSION at least max(1, n).

x	The refined solution matrix <i>X</i> .
ferr, berr	REAL for chprfs.
	DOUBLE PRECISION for zhprfs.
	Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the component-wise forward and backward errors, respectively, for each solution vector.
info	INTEGER. If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

For each right-hand side, computation of the backward error involves a minimum of $16n^2$ operations. In addition, each step of iterative refinement involves $24n^2$ operations; the number of iterations may range from 1 to 5.

Estimating the forward error involves solving a number of systems of linear equations Ax = b; the number is usually 4 or 5 and never more than 11. Each solution requires approximately $8n^2$ floating-point operations.

The real counterpart of this routine is **ssprfs** / **dsprfs**.

?trrfs

Estimates the error in the solution of a system of linear equations with a triangular matrix.

call strrfs	(uplo,trans,diag,n,nrhs,a,lda,b,ldb, x,ldx,ferr,berr,work,iwork,info)
call dtrrfs	<pre>(uplo,trans,diag,n,nrhs,a,lda,b,ldb, x,ldx,ferr,berr,work,iwork,info)</pre>
call ctrrfs	<pre>(uplo,trans,diag,n,nrhs,a,lda,b,ldb, x,ldx,ferr,berr,work,rwork,info)</pre>
call ztrrfs	(uplo,trans,diag,n,nrhs,a,lda,b,ldb,

Discussion

This routine estimates the errors in the solution to a system of linear equations AX = B or $A^TX = B$ or $A^HX = B$ with a triangular matrix A, with multiple right-hand sides. For each computed solution vector x, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of A and b such that x is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|, |\delta b_i| / |b_i| \leq \beta |b_i| \text{ such that } (A + \delta A)x = (b + \delta b).$

The routine also estimates the *component-wise forward error* in the computed solution $||x - x_e|| \ll ||x|| \approx$ (here x_e is the exact solution). Before calling this routine, call the solver routine <u>?trtrs</u>.

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<i>B</i> .
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ne array a.
<mark>s</mark> ≥ 0).
r matrix A,
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ax(1, <i>n</i>); ast e at least for

lda	INTEGER. The first dimension of a ; $1da \ge max(1, n)$.
ldb	INTEGER. The first dimension of <i>b</i> ; $ldb \ge max(1, n)$.
ldx	INTEGER . The first dimension of x ; $ldx \ge max(1, n)$.
iwork	INTEGER.
	Workspace array, DIMENSION at least max(1, n).
rwork	REAL for ctrrfs
	DOUBLE PRECISION for ztrrfs
	Workspace array, DIMENSION at least $max(1, n)$.

ferr, berr	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	Arrays, DIMENSION at least $max(1, nrhs)$. Contain the
	component-wise forward and backward errors,
	respectively, for each solution vector.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

A call to this routine involves, for each right-hand side, solving a number of systems of linear equations Ax = b; the number of systems is usually 4 or 5 and never more than 11. Each solution requires approximately n^2 floating-point operations for real flavors or $4n^2$ for complex flavors.

?tprfs

Estimates the error in the solution of a system of linear equations with a packed triangular matrix.

call stprfs	<pre>(uplo,trans,diag,n,nrhs,ap,b,ldb, x,ldx,ferr,berr,work,iwork,info)</pre>
call dtprfs	<pre>(uplo,trans,diag,n,nrhs,ap,b,ldb, x,ldx,ferr,berr,work,iwork,info)</pre>
call ctprfs	<pre>(uplo,trans,diag,n,nrhs,ap,b,ldb, x,ldx,ferr,berr,work,rwork,info)</pre>
call ztprfs	<pre>(uplo,trans,diag,n,nrhs,ap,b,ldb, x,ldx,ferr,berr,work,rwork,info)</pre>

Discussion

This routine estimates the errors in the solution to a system of linear equations AX = B or $A^TX = B$ or $A^HX = B$ with a packed triangular matrix A, with multiple right-hand sides. For each computed solution vector x, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of A and b such that x is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|$, $|\delta b_i| / |b_i| \leq \beta |b_i|$ such that $(A + \delta A)x = (b + \delta b)$. The routine also estimates the *component-wise forward error* in the computed solution $||x - x_e|| \leq ||x|| \leq (here x_e \text{ is the exact solution})$. Before calling this routine, call the solver routine <u>?tptrs</u>.

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uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether A is upper or lower triangular:
	If $uplo = 'U'$, then A is upper triangular.
	If $uplo = 'L'$, then A is lower triangular.
trans	CHARACTER*1. Must be 'N' or 'T' or 'C'.
	Indicates the form of the equations:
	If $trans = 'N'$, the system has the form $AX = B$.
	If $trans = 'T'$, the system has the form $A^T X = B$.
	If $trans = 'C'$, the system has the form $A^H X = B$.
diag	CHARACTER*1. Must be 'N' or 'U'.
	If $diag = 'N'$, A is not a unit triangular matrix.
	If $diag = U'$, A is unit triangular: diagonal elements of A
	are assumed to be 1 and not referenced in the array ap.
n	INTEGER. The order of the matrix $A (n \ge 0)$.
nrhs	INTEGER . The number of right-hand sides $(nrhs \ge 0)$.
ap, b, x, wo	ork REAL for strrfs
	DOUBLE PRECISION for dtrrfs
	COMPLEX for ctrrfs
	DOUBLE COMPLEX for ztrrfs.
	Arrays:
	ap(*) contains the upper or lower triangular matrix A, as
	specified by uplo.
	b(ldb, *) contains the right-hand side matrix B.
	x(ldx, *) contains the solution matrix X.
	work (*) is a workspace array.
	The dimension of <i>ap</i> must be at least $max(1,n(n+1)/2)$;
	the second dimension of b and x must be at least
	max(1, <i>nrhs</i>); the dimension of <i>work</i> must be at least
	$\max(1, 3*n)$ for real flavors and $\max(1, 2*n)$ for complex
	flavors.
ldb	INTEGER. The first dimension of b ; $1db \ge max(1, n)$.
ldx	INTEGER . The first dimension of x ; $1dx \ge max(1, n)$.
iwork	INTEGER.
	Workspace array, DIMENSION at least max(1, <i>n</i>).

rwork REAL for ctrrfs DOUBLE PRECISION for ztrrfs Workspace array, DIMENSION at least max(1, n).

Output Parameters

ferr, berr	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the
	component-wise forward and backward errors,
	respectively, for each solution vector.
info	INTEGER.
	If <i>info</i> = 0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

A call to this routine involves, for each right-hand side, solving a number of systems of linear equations Ax = b; the number of systems is usually 4 or 5 and never more than 11. Each solution requires approximately n^2 floating-point operations for real flavors or $4n^2$ for complex flavors.

?tbrfs

Estimates the error in the solution of a system of linear equations with a triangular band matrix.

call stbrfs	<pre>(uplo,trans,diag,n,kd,nrhs,ab,ldab,b,ldb, x,ldx,ferr,berr,work,iwork,info)</pre>
call dtbrfs	<pre>(uplo,trans,diag,n,kd,nrhs,ab,ldab,b,ldb, x,ldx,ferr,berr,work,iwork,info)</pre>
call ctbrfs	<pre>(uplo,trans,diag,n,kd,nrhs,ab,ldab,b,ldb, x,ldx,ferr,berr,work,rwork,info)</pre>
call ztbrfs	<pre>(uplo,trans,diag,n,kd,nrhs,ab,ldab,b,ldb, x,ldx,ferr,berr,work,rwork,info)</pre>

Discussion

This routine estimates the errors in the solution to a system of linear equations AX = B or $A^TX = B$ or $A^HX = B$ with a triangular band matrix A, with multiple right-hand sides. For each computed solution vector x, the routine computes the *component-wise backward error* β . This error is the smallest relative perturbation in elements of A and b such that x is the exact solution of the perturbed system:

 $|\delta a_{ij}| / |a_{ij}| \leq \beta |a_{ij}|$, $|\delta b_i| / |b_i| \leq \beta |b_i|$ such that $(A + \delta A)x = (b + \delta b)$. The routine also estimates the *component-wise forward error* in the computed solution $||x - x_e|| \leq ||x|| \leq \beta$ (here x_e is the exact solution).

Before calling this routine, call the solver routine <u>?tbtrs</u>.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether A is upper or lower triangular:
	If $uplo = 'U'$, then A is upper triangular.
	If $uplo = 'L'$, then A is lower triangular.
trans	CHARACTER*1. Must be 'N' or 'T' or 'C'.
	Indicates the form of the equations:
	If $trans = 'N'$, the system has the form $AX = B$.
	If <i>trans</i> = 'T', the system has the form $A^T X = B$.
	If $trans = 'C'$, the system has the form $A^H X = B$.
diag	CHARACTER*1. Must be 'N' or 'U'.
	If $diag = 'N'$, A is not a unit triangular matrix.
	If $diag = 'U'$, A is unit triangular: diagonal elements of A
	are assumed to be 1 and not referenced in the array <i>ab</i> .
п	INTEGER. The order of the matrix $A (n \ge 0)$.
kd	INTEGER . The number of super-diagonals or
	sub-diagonals in the matrix A $(kd \ge 0)$.
nrhs	INTEGER. The number of right-hand sides $(nrhs \ge 0)$.
ab, b, x,	
	DOUBLE PRECISION for dtbrfs
	COMPLEX for ctbrfs
	DOUBLE COMPLEX for ztbrfs.
	DOUBLE COMPLEX for ztbrfs. Arrays:
	Arrays:
	Arrays: ab(ldab, *) contains the upper or lower triangular matrix
	Arrays: ab(ldab,*) contains the upper or lower triangular matrix <i>A</i> , as specified by <i>uplo</i> , in band storage format.
	Arrays: ab(ldab,*) contains the upper or lower triangular matrix <i>A</i> , as specified by <i>uplo</i> , in band storage format. b(ldb,*) contains the right-hand side matrix <i>B</i> .
	 Arrays: ab(ldab,*) contains the upper or lower triangular matrix A, as specified by uplo, in band storage format. b(ldb,*) contains the right-hand side matrix B. x(ldx,*) contains the solution matrix X.
	 Arrays: ab(ldab,*) contains the upper or lower triangular matrix A, as specified by uplo, in band storage format. b(ldb,*) contains the right-hand side matrix B. x(ldx,*) contains the solution matrix X. work (*) is a workspace array.
	 Arrays: ab(ldab,*) contains the upper or lower triangular matrix A, as specified by uplo, in band storage format. b(ldb,*) contains the right-hand side matrix B. x(ldx,*) contains the solution matrix X. work (*) is a workspace array. The second dimension of a must be at least max(1,n);
	 Arrays: ab(ldab,*) contains the upper or lower triangular matrix A, as specified by uplo, in band storage format. b(ldb,*) contains the right-hand side matrix B. x(ldx,*) contains the solution matrix X. work (*) is a workspace array. The second dimension of a must be at least max(1,n); the second dimension of b and x must be at least
	 Arrays: ab(ldab,*) contains the upper or lower triangular matrix A, as specified by uplo, in band storage format. b(ldb,*) contains the right-hand side matrix B. x(ldx,*) contains the solution matrix X. work (*) is a workspace array. The second dimension of a must be at least max(1,n); the second dimension of b and x must be at least max(1,nrhs).
ldab	 Arrays: ab(ldab,*) contains the upper or lower triangular matrix A, as specified by uplo, in band storage format. b(ldb,*) contains the right-hand side matrix B. x(ldx,*) contains the solution matrix X. work (*) is a workspace array. The second dimension of a must be at least max(1,n); the second dimension of b and x must be at least max(1,nrhs). The dimension of work must be at least max(1, 3*n) for
ldab	 Arrays: ab(ldab,*) contains the upper or lower triangular matrix A, as specified by uplo, in band storage format. b(ldb,*) contains the right-hand side matrix B. x(ldx,*) contains the solution matrix X. work (*) is a workspace array. The second dimension of a must be at least max(1,n); the second dimension of b and x must be at least max(1,nrhs). The dimension of work must be at least max(1, 3*n) for real flavors and max(1, 2*n) for complex flavors.

ldb	INTEGER. The first dimension of b; $ldb \ge max(1, n)$.
ldx	INTEGER. The first dimension of x ; $ldx \ge max(1, n)$.
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, n)$.
rwork	REAL for ctbrfs
	DOUBLE PRECISION for ztbrfs
	Workspace array, DIMENSION at least max(1, n).

ferr, berr	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the
	component-wise forward and backward errors,
	respectively, for each solution vector.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.

Application Notes

The bounds returned in *ferr* are not rigorous, but in practice they almost always overestimate the actual error.

A call to this routine involves, for each right-hand side, solving a number of systems of linear equations Ax = b; the number of systems is usually 4 or 5 and never more than 11. Each solution requires approximately 2n kd floating-point operations for real flavors or 8n kd operations for complex flavors.

Routines for Matrix Inversion

It is seldom necessary to compute an explicit inverse of a matrix. In particular, do not attempt to solve a system of equations Ax = b by first computing A^{-1} and then forming the matrix-vector product $x = A^{-1}b$. Call a solver routine instead (see <u>Routines for Solving Systems of Linear</u> Equations); this is more efficient and more accurate.

However, matrix inversion routines are provided for the rare occasions when an explicit inverse matrix is needed.

?getri

Computes the inverse of an LU-factored general matrix.

call	sgetri	(<i>n</i> ,	a,	lda,	ipiv,	work,	lwork,	info)
call	dgetri	(n,	a,	lda,	ipiv,	work,	lwork,	info)
call	cgetri	(n,	a,	lda,	ipiv,	work,	lwork,	info)
call	zgetri	(n,	a,	lda,	ipiv,	work,	lwork,	info)

Discussion

This routine computes the inverse (A^{-1}) of a general matrix *A*. Before calling this routine, call <u>?getrf</u> to factorize *A*.

п	INTEGER . The order of the matrix $A (n \ge 0)$.
a, work	REAL for sgetri DOUBLE PRECISION for dgetri COMPLEX for cgetri
	DOUBLE COMPLEX for zgetri. Arrays: $a(lda, *)$, $work(lwork)$. a(lda, *) contains the factorization of the matrix A, as returned by <u>?getrf</u> : $A = PLU$. The second dimension of a must be at least max(1,n).
	work(lwork) is a workspace array.

lda	INTEGER . The first dimension of a ; $1 da \ge max(1, n)$.
ipiv	INTEGER.
	Array, DIMENSION at least $max(1,n)$.
	The <i>ipiv</i> array, as returned by <u>?getrf</u> .
lwork	INTEGER. The size of the <i>work</i> array $(lwork \ge n)$
	See <i>Application notes</i> for the suggested value of <i>lwork</i> .

a	Overwritten by the <i>n</i> by <i>n</i> matrix A^{-1} .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, the <i>i</i> th diagonal element of the factor <i>U</i> is zero, <i>U</i> is singular, and the inversion could not be completed.

Application Notes

For better performance, try using *lwork* = n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work(1)* and use this value for subsequent runs.

The computed inverse *X* satisfies the following error bound:

 $|XA - I| \le c(\mathbf{n})\varepsilon |X|P|L||U|$

where c(n) is a modest linear function of n; ε is the machine precision; I denotes the identity matrix; P, L, and U are the factors of the matrix factorization A = PLU.

The total number of floating-point operations is approximately $(4/3)n^3$ for real flavors and $(16/3)n^3$ for complex flavors.

?potri

Computes the inverse of a symmetric (Hermitian) positive-definite matrix.

call	spotri	(uplo,	n,	a,	lda,	info)
call	dpotri	(uplo,	n,	a,	lda,	info)
call	cpotri	(uplo,	n,	a,	lda,	info)
call	zpotri	(uplo,	n,	a,	lda,	info)

Discussion

This routine computes the inverse (A^{-1}) of a symmetric positive definite or, for complex flavors, Hermitian positive-definite matrix *A*. Before calling this routine, call <u>?potrf</u> to factorize *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix <i>A</i> has been factored: If $uplo = 'U'$, the array a stores the factor <i>U</i> of the Cholesky factorization $A = U^H U$. If $uplo = 'L'$, the array a stores the factor <i>L</i> of the Cholesky factorization $A = LL^H$.
n	INTEGER . The order of the matrix $A \ (n \ge 0)$.
a	REAL for spotri DOUBLE PRECISION for dpotri COMPLEX for cpotri DOUBLE COMPLEX for zpotri. Array: a(lda,*).
	Contains the factorization of the matrix A , as returned by <u>?potrf</u> .
	The second dimension of a must be at least $\max(1,n)$.
lda	INTEGER. The first dimension of a; $1 da \ge max(1, n)$.

a	Overwritten by the n by n matrix A^{-1} .
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = i, the ith diagonal element of the Cholesky factor (and hence the factor itself) is zero, and the inversion could not be completed.</pre>

Application Notes

The computed inverse *X* satisfies the following error bounds:

 $\|XA - I\|_2 \le c(\mathbf{n}) \varepsilon \kappa_2(A), \quad \|AX - I\|_2 \le c(\mathbf{n}) \varepsilon \kappa_2(A)$

where c(n) is a modest linear function of n, and ε is the machine precision; *I* denotes the identity matrix.

The 2-norm $||A||_2$ of a matrix A is defined by $||A||_2 = \max_{x:x=1} (Ax \cdot Ax)^{1/2}$, and the condition number $\kappa_2(A)$ is defined by $\kappa_2(A) = ||A||_2 ||A^{-1}||_2$.

The total number of floating-point operations is approximately $(2/3)n^3$ for real flavors and $(8/3)n^3$ for complex flavors.

?pptri

Computes the inverse of a packed symmetric (Hermitian) positive-definite matrix

call spptri (uplo, n, ap, info)
call dpptri (uplo, n, ap, info)
call cpptri (uplo, n, ap, info)
call zpptri (uplo, n, ap, info)

Discussion

This routine computes the inverse (A^{-1}) of a symmetric positive definite or, for complex flavors, Hermitian positive-definite matrix *A* in *packed* form. Before calling this routine, call <u>?pptrf</u> to factorize *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix <i>A</i> has been factored: If $uplo = 'U'$, the array <i>ap</i> stores the packed factor <i>U</i> of the Cholesky factorization $A = U^H U$. If $uplo = 'L'$, the array <i>ap</i> stores the packed factor <i>L</i> of the Cholesky factorization $A = LL^H$.
n	INTEGER . The order of the matrix $A (n \ge 0)$.
ap	REAL for spptri DOUBLE PRECISION for dpptri COMPLEX for cpptri DOUBLE COMPLEX for zpptri. Array, DIMENSION at least $max(1,n(n+1)/2)$.
	Contains the factorization of the packed matrix <i>A</i> , as returned by <u>?pptrf</u> .
	The dimension ap must be at least max $(1,n(n+1)/2)$.

ap	Overwritten by the packed <i>n</i> by <i>n</i> matrix A^{-1} .
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = i, the ith diagonal element of the Cholesky factor (and hence the factor itself) is zero, and the inversion could not be completed.</pre>

Application Notes

The computed inverse *X* satisfies the following error bounds:

 $\|XA - I\|_2 \le c(\mathbf{n}) \varepsilon \kappa_2(A), \quad \|AX - I\|_2 \le c(\mathbf{n}) \varepsilon \kappa_2(A)$

where c(n) is a modest linear function of n, and ε is the machine precision; *I* denotes the identity matrix.

The 2-norm $||A||_2$ of a matrix A is defined by $||A||_2 = \max_{x:x=1} (Ax \cdot Ax)^{1/2}$, and the condition number $\kappa_2(A)$ is defined by $\kappa_2(A) = ||A||_2 ||A^{-1}||_2$.

The total number of floating-point operations is approximately $(2/3)n^3$ for real flavors and $(8/3)n^3$ for complex flavors.

?sytri

Computes the inverse of a symmetric matrix.

call ssytri (uplo, n, a, lda, ipiv, work, info) call dsytri (uplo, n, a, lda, ipiv, work, info) call csytri (uplo, n, a, lda, ipiv, work, info) call zsytri (uplo, n, a, lda, ipiv, work, info)

Discussion

This routine computes the inverse (A^{-1}) of a symmetric matrix *A*. Before calling this routine, call <u>?sytrf</u> to factorize *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix A has been factored: If $uplo = 'U'$, the array a stores the Bunch-Kaufman factorization $A = PUDU^TP^T$. If $uplo = 'L'$, the array a stores the Bunch-Kaufman factorization $A = PLDL^TP^T$.
n	INTEGER. The order of the matrix $A (n \ge 0)$.
a, work	REAL for ssytri DOUBLE PRECISION for dsytri COMPLEX for csytri DOUBLE COMPLEX for zsytri. Arrays:
	a(1da, *) contains the factorization of the matrix A, as returned by <u>?sytrf</u> . The second dimension of a must be at least max(1,n).
	work(*) is a workspace array. The dimension of work must be at least $\max(1,2*n)$.
lda	INTEGER. The first dimension of <i>a</i> ; $lda \ge max(1, n)$.

ipiv

INTEGER.

Array, DIMENSION at least max(1,n). The *ipiv* array, as returned by <u>?sytrf</u>.

Output Parameters

a	Overwritten by the <i>n</i> by <i>n</i> matrix A^{-1} .
info	INTEGER. If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, the <i>i</i> th diagonal element of D is zero, D is provide a subscription or planet by complete d
	singular, and the inversion could not be completed.

Application Notes

The computed inverse *X* satisfies the following error bounds:

$$|DU^{T}P^{T}XPU - I| \leq c(\mathbf{n})\varepsilon (|D||U^{T}|P^{T}|X|P|U| + |D||D^{-1}|)$$

for uplo = 'U', and

$$\left| DL^{T}P^{T}XPL - I \right| \leq c(\mathbf{n})\varepsilon \left(|D| |L^{T}|P^{T}|X|P|L| + |D| |D^{-1}| \right)$$

for uplo = 'L'. Here c(n) is a modest linear function of n, and ε is the machine precision; I denotes the identity matrix.

The total number of floating-point operations is approximately $(2/3)n^3$ for real flavors and $(8/3)n^3$ for complex flavors.

?hetri

Computes the inverse of a complex Hermitian matrix.

call chetri (uplo, n, a, lda, ipiv, work, info)
call zhetri (uplo, n, a, lda, ipiv, work, info)

Discussion

This routine computes the inverse (A^{-1}) of a complex Hermitian matrix *A*. Before calling this routine, call <u>?hetrf</u> to factorize *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix A has been factored: If $uplo = 'U'$, the array a stores the Bunch-Kaufman factorization $A = PUDU^H P^T$. If $uplo = 'L'$, the array a stores the Bunch-Kaufman factorization $A = PLDL^H P^T$.
n	INTEGER. The order of the matrix $A (n \ge 0)$.
a, work	COMPLEX for chetri DOUBLE COMPLEX for zhetri. Arrays:
	 a(lda,*) contains the factorization of the matrix A, as returned by <u>?hetrf</u>. The second dimension of a must be at least max(1,n).
	<pre>work(*) is a workspace array. The dimension of work must be at least max(1,n).</pre>
lda	INTEGER. The first dimension of <i>a</i> ; $lda \ge max(1, n)$.
ipiv	INTEGER. Array, DIMENSION at least $max(1,n)$. The <i>ipiv</i> array, as returned by <u>?hetrf</u> .

a	Overwritten by the <i>n</i> by <i>n</i> matrix A^{-1} .
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = i, the ith diagonal element of D is zero, D is singular, and the inversion could not be completed.</pre>

Application Notes

The computed inverse *X* satisfies the following error bounds:

$$|DU^{H}P^{T}XPU - I| \leq c(\mathbf{n})\varepsilon (|D||U^{H}|P^{T}|X|P|U| + |D||D^{-1}|)$$

for uplo = 'U', and

$$\left|DL^{H}P^{T}XPL - I\right| \leq c(\mathbf{n})\varepsilon \left(\left|D\right|\left|L^{H}\right|P^{T}|X|P|L| + \left|D\right|\left|D^{-1}\right|\right)\right)$$

for uplo = 'L'. Here c(n) is a modest linear function of n, and ε is the machine precision; I denotes the identity matrix.

The total number of floating-point operations is approximately $(2/3)n^3$ for real flavors and $(8/3)n^3$ for complex flavors.

The real counterpart of this routine is ?sytri.

?sptri

Computes the inverse of a symmetric matrix using packed storage.

call ssptri (uplo, n, ap, ipiv, work, info) call dsptri (uplo, n, ap, ipiv, work, info) call csptri (uplo, n, ap, ipiv, work, info) call zsptri (uplo, n, ap, ipiv, work, info)

Discussion

This routine computes the inverse (A^{-1}) of a packed symmetric matrix *A*. Before calling this routine, call <u>?sptrf</u> to factorize *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix A has been factored: If $uplo = 'U'$, the array ap stores the Bunch-Kaufman factorization $A = PUDU^T P^T$. If $uplo = 'L'$, the array ap stores the Bunch-Kaufman factorization $A = PLDL^T P^T$.
п	INTEGER . The order of the matrix $A \ (n \ge 0)$.
ap, work	REAL for ssptri DOUBLE PRECISION for dsptri COMPLEX for csptri DOUBLE COMPLEX for zsptri. Arrays:
	ap(*) contains the factorization of the matrix A, as returned by <u>?sptrf</u> . The dimension of ap must be at least $max(1,n(n+1)/2)$.
	<pre>work(*) is a workspace array. The dimension of work must be at least max(1,n).</pre>

ipiv

INTEGER.

Array, **DIMENSION** at least max(1,*n*). The *ipiv* array, as returned by <u>?sptrf</u>.

Output Parameters

ap	Overwritten by the <i>n</i> by <i>n</i> matrix A^{-1} in packed form.
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.
	If $info = i$, the <i>i</i> th diagonal element of D is zero, D is
	singular, and the inversion could not be completed.

Application Notes

The computed inverse *X* satisfies the following error bounds:

$$|DU^{T}P^{T}XPU - I| \leq c(\mathbf{n})\varepsilon (|D||U^{T}|P^{T}|X|P|U| + |D||D^{-1}|)$$

for uplo = 'U', and

$$\left|DL^{T}P^{T}XPL - I\right| \leq c(\mathbf{n})\varepsilon \left(\left|D\right|\left|L^{T}\right|P^{T}\left|X\right|P\left|L\right| + \left|D\right|\left|D^{-1}\right|\right)$$

for uplo = 'L'. Here c(n) is a modest linear function of n, and ε is the machine precision; I denotes the identity matrix.

The total number of floating-point operations is approximately $(2/3)n^3$ for real flavors and $(8/3)n^3$ for complex flavors.

?hptri

Computes the inverse of a complex Hermitian matrix using packed storage.

call chptri (uplo, n, ap, ipiv, work, info)
call zhptri (uplo, n, ap, ipiv, work, info)

Discussion

This routine computes the inverse (A^{-1}) of a complex Hermitian matrix *A* using packed storage. Before calling this routine, call <u>?hptrf</u> to factorize *A*.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates how the input matrix A has been factored: If $uplo = 'U'$, the array ap stores the packed Bunch-Kaufman factorization $A = PUDU^{H}P^{T}$. If $uplo = 'L'$, the array ap stores the packed Bunch-Kaufman factorization $A = PLDL^{H}P^{T}$.
n	INTEGER . The order of the matrix $A \ (n \ge 0)$.
ар	COMPLEX for chptri DOUBLE COMPLEX for zhptri. Arrays:
	ap(*) contains the factorization of the matrix A, as returned by <u>?hptrf</u> . The dimension of ap must be at least $\max(1, n(n+1)/2)$.
	<pre>work(*) is a workspace array. The dimension of work must be at least max(1,n).</pre>
ipiv	INTEGER. Array, DIMENSION at least $\max(1, n)$. The <i>ipiv</i> array, as returned by <u>?hptrf</u> .

ар	Overwritten by the <i>n</i> by <i>n</i> matrix A^{-1} .
info	INTEGER. If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, the <i>i</i> th diagonal element of <i>D</i> is zero, <i>D</i> is singular, and the inversion could not be completed.

Application Notes

The computed inverse *X* satisfies the following error bounds:

$$|DU^{H}P^{T}XPU - I| \leq c(\mathbf{n})\varepsilon (|D||U^{H}|P^{T}|X|P|U| + |D||D^{-1}|)$$

for uplo = 'U', and

$$\left|DL^{H}P^{T}XPL - I\right| \leq c(\mathbf{n})\varepsilon \left(\left|D\right|\left|L^{H}\right|P^{T}|X|P|L| + \left|D\right|\left|D^{-1}\right|\right)\right)$$

for uplo = 'L'. Here c(n) is a modest linear function of n, and ε is the machine precision; I denotes the identity matrix.

The total number of floating-point operations is approximately $(2/3)n^3$ for real flavors and $(8/3)n^3$ for complex flavors.

The real counterpart of this routine is ?sptri.

?trtri

Computes the inverse of a triangular matrix.

call strtri (uplo, diag, n, a, lda, info) call dtrtri (uplo, diag, n, a, lda, info) call ctrtri (uplo, diag, n, a, lda, info) call ztrtri (uplo, diag, n, a, lda, info)

Discussion

This routine computes the inverse (A^{-1}) of a triangular matrix A.

uplo diag	CHARACTER*1. Must be 'U' or 'L'. Indicates whether A is upper or lower triangular: If $uplo = 'U'$, then A is upper triangular. If $uplo = 'L'$, then A is lower triangular. CHARACTER*1. Must be 'N' or 'U'. If $diag = 'N'$, then A is not a unit triangular matrix. If $diag = 'U'$, A is unit triangular: diagonal elements of A are assumed to be 1 and not referenced in the array a.
п	INTEGER. The order of the matrix $A \ (n \ge 0)$.
a	REAL for strtri DOUBLE PRECISION for dtrtri COMPLEX for ctrtri DOUBLE COMPLEX for ztrtri.
	Array: DIMENSION (<i>lda</i> , *). Contains the matrix <i>A</i> . The second dimension of a must be at least max(1, <i>n</i>).
lda	INTEGER . The first dimension of a ; $1da \ge max(1, n)$.

a	Overwritten by the <i>n</i> by <i>n</i> matrix A^{-1} .
info	INTEGER. If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, the <i>i</i> th diagonal element of <i>A</i> is zero, <i>A</i> is singular, and the inversion could not be completed.

Application Notes

The computed inverse *X* satisfies the following error bounds:

 $|XA - I| \le c(n)\varepsilon |X||A|$ $|X - A^{-1}| \le c(n)\varepsilon |A^{-1}||A||X|$

where c(n) is a modest linear function of n; ε is the machine precision; *I* denotes the identity matrix.

The total number of floating-point operations is approximately $(1/3)n^3$ for real flavors and $(4/3)n^3$ for complex flavors.

?tptri

Computes the inverse of a triangular matrix using packed storage.

call stptri (uplo, diag, n, ap, info)
call dtptri (uplo, diag, n, ap, info)
call ctptri (uplo, diag, n, ap, info)
call ztptri (uplo, diag, n, ap, info)

Discussion

This routine computes the inverse (A^{-1}) of a packed triangular matrix A.

Input Parameters

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether A is upper or lower triangular:
	If $uplo = 'U'$, then A is upper triangular.
	If $uplo = 'L'$, then A is lower triangular.
diag	CHARACTER*1. Must be 'N' or 'U'.
	If $diag = 'N'$, then A is not a unit triangular matrix.
	If $diag = 'U'$, A is unit triangular: diagonal elements of
	A are assumed to be 1 and not referenced in the array ap.
n	INTEGER. The order of the matrix $A (n \ge 0)$.
ap	REAL for stptri
	DOUBLE PRECISION for dtptri
	COMPLEX for ctptri
	DOUBLE COMPLEX for ztptri.
	Array: DIMENSION at least $\max(1, n(n+1)/2)$.
	Contains the packed triangular matrix A.

Output Parameters

ар	Overwritten by the packed <i>n</i> by <i>n</i> matrix A^{-1} .
info	INTEGER.
	If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.
	If $info = i$, the <i>i</i> th diagonal element of A is zero, A is
	singular, and the inversion could not be completed.

Application Notes

The computed inverse *X* satisfies the following error bounds:

$$|XA - I| \le c(n)\varepsilon |X||A|$$
$$|X - A^{-1}| \le c(n)\varepsilon |A^{-1}||A||X|$$

where c(n) is a modest linear function of n; ε is the machine precision; *I* denotes the identity matrix.

The total number of floating-point operations is approximately $(1/3)n^3$ for real flavors and $(4/3)n^3$ for complex flavors.

Routines for Matrix Equilibration

Routines described in this section are used to compute scaling factors needed to equilibrate a matrix. Note that these routines do not actually scale the matrices.

?geequ

Computes row and column scaling factors intended to equilibrate a matrix and reduce its condition number.

call sgeequ (m, n, a, lda, r, c, rowend, colend, amax, info) call dgeequ (m, n, a, lda, r, c, rowend, colend, amax, info) call egeequ (m, n, a, lda, r, c, rowend, colend, amax, info) call zgeequ (m, n, a, lda, r, c, rowend, colend, amax, info)

Discussion

This routine computes row and column scalings intended to equilibrate an *m*-by-*n* matrix *A* and reduce its condition number. The output array *r* returns the row scale factors and the array *c* the column scale factors. These factors are chosen to try to make the largest element in each row and column of the matrix B with elements $b_{ii}=r(i)*a_{ii}*c(j)$ have absolute value 1.

m	INTEGER . The number of rows of the matrix A, $m \ge 0$.
п	INTEGER. The number of columns of the matrix A,
	$n \geq 0.$
а	REAL for sgeequ
	DOUBLE PRECISION for dgeequ
	COMPLEX for cgeequ
	DOUBLE COMPLEX for zgeequ.

lda	Array: DIMENSION (lda ,*). Contains the <i>m</i> -by- <i>n</i> matrix <i>A</i> whose equilibration factors are to be computed. The second dimension of <i>a</i> must be at least max(1, <i>n</i>). INTEGER. The leading dimension of <i>a</i> ; $lda \ge max(1, m)$.		
Output Param	Output Parameters		
r, c	REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Arrays: $r(m)$, $c(n)$. If $info = 0$, or $info > m$, the array r contains the row scale factors of the matrix A . If $info = 0$, the array c contains the column scale factors of the matrix A .		
rowend	<pre>REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. If info = 0 or info > m, rowcnd contains the ratio of the smallest r(i) to the largest r(i).</pre>		
colcnd	REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. If <i>info</i> = 0, <i>colcnd</i> contains the ratio of the smallest c(i) to the largest $c(i)$.		
amax	REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Absolute value of the largest element of the matrix <i>A</i> .		
info	INTEGER. If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$ and $i \le m$, the <i>i</i> th row of A is exactly zero; i > m, the $(i-m)$ th column of A is exactly zero.		

Application Notes

All the components of r and c are restricted to be between SMLNUM = smallest safe number and BIGNUM = largest safe number. Use of these scaling factors is not guaranteed to reduce the condition number of A but works well in practice.

If $rowcnd \ge 0.1$ and amax is neither too large nor too small, it is not worth scaling by r. If $colend \ge 0.1$, it is not worth scaling by c.

If *amax* is very close to overflow or very close to underflow, the matrix *A* should be scaled.

?gbequ

Computes row and column scaling factors intended to equilibrate a band matrix and reduce its condition number.

call sgbequ (m, n, kl, ku, ab, ldab, r, c, rowcnd, colcnd,amax,info) call dgbequ (m, n, kl, ku, ab, ldab, r, c, rowcnd, colcnd,amax,info) call cgbequ (m, n, kl, ku, ab, ldab, r, c, rowcnd, colcnd,amax,info) call zgbequ (m, n, kl, ku, ab, ldab, r, c, rowcnd, colcnd,amax,info)

Discussion

This routine computes row and column scalings intended to equilibrate an *m*-by-*n* band matrix *A* and reduce its condition number. The output array *r* returns the row scale factors and the array *c* the column scale factors. These factors are chosen to try to make the largest element in each row and column of the matrix B with elements $b_{ij}=r(i)*a_{ij}*c(j)$ have absolute value 1.

m	INTEGER . The number of rows of the matrix A, $m \ge 0$.
n	INTEGER . The number of columns of the matrix A,
	$n \geq 0.$
kl	INTEGER. The number of sub-diagonals within the band
	of A (kl ≥ 0).
ku	INTEGER. The number of super-diagonals within the
	band of A ($ku \ge 0$).
ab	REAL for sgbequ
	DOUBLE PRECISION for dgbequ
	COMPLEX for cgbequ
	DOUBLE COMPLEX for zgbequ.
	Array, DIMENSION (1dab, *).
	Contains the original band matrix A stored in rows
	from 1 to $kl + ku + 1$.

	The second dimension of <i>ab</i> must be at least $max(1,n)$;
ldab	INTEGER . The leading dimension of <i>ab</i> ,
	$1dab \geq kl+ku+1.$
Output Param	neters
r, c	REAL for single precision flavors;
	DOUBLE PRECISION for double precision flavors.
	Arrays: $r(m)$, $c(n)$. If $info = 0$, or $info > m$, the array r contains the row
	scale factors of the matrix A .
	If $info = 0$, the array c contains the column scale
	factors of the matrix A.
rowcnd	REAL for single precision flavors;
	DOUBLE PRECISION for double precision flavors. If $info = 0$ or $info > m$, rowcnd contains the ratio of
	the smallest $\mathbf{r}(i)$ to the largest $\mathbf{r}(i)$.
colcnd	REAL for single precision flavors;
	DOUBLE PRECISION for double precision flavors.
	If <i>info</i> = 0, <i>colcnd</i> contains the ratio of the smallest
	c(i) to the largest $c(i)$.
amax	REAL for single precision flavors;
	DOUBLE PRECISION for double precision flavors. Absolute value of the largest element of the matrix A.
	, and the second s
info	INTEGER. If $info = 0$, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.
	If $info = i$ and
	$i \leq m$, the <i>i</i> th row of A is exactly zero;
	i > m, the $(i-m)$ th column of A is exactly zero.

Application Notes

All the components of r and c are restricted to be between SMLNUM = smallest safe number and BIGNUM = largest safe number. Use of these scaling factors is not guaranteed to reduce the condition number of A but works well in practice.

If rowend ≥ 0.1 and amax is neither too large nor too small, it is not worth scaling by r. If colend ≥ 0.1 , it is not worth scaling by c.

If *amax* is very close to overflow or very close to underflow, the matrix *A* should be scaled.

?poequ

Computes row and column scaling factors intended to equilibrate a symmetric (Hermitian) positive definite matrix and reduce its condition number.

call spoequ (n, a, lda, s, scond, amax, info)
call dpoequ (n, a, lda, s, scond, amax, info)
call cpoequ (n, a, lda, s, scond, amax, info)
call zpoequ (n, a, lda, s, scond, amax, info)

Discussion

This routine computes row and column scalings intended to equilibrate a symmetric (Hermitian) positive definite matrix A and reduce its condition number (with respect to the two-norm). The output array s returns scale factors computed as

$$s(i) = \frac{1}{\sqrt{a_{i, i}}}$$

These factors are chosen so that the scaled matrix B with elements $b_{ii}=s(i)*a_{ii}*s(j)$ has diagonal elements equal to 1.

This choice of s puts the condition number of B within a factor n of the smallest possible condition number over all possible diagonal scalings.

Input Parameters

n

INTEGER. The order of the matrix A, $n \ge 0$.

a	REAL for spoequ DOUBLE PRECISION for dpoequ COMPLEX for cpoequ DOUBLE COMPLEX for zpoequ.		
	Array: DIMENSION (lda , *). Contains the <i>n</i> -by- <i>n</i> symmetric or Hermitian positive definite matrix <i>A</i> whose scaling factors are to be computed. Only diagonal elements of <i>A</i> are referenced. The second dimension of <i>a</i> must be at least max(1, <i>n</i>).		
lda	INTEGER. The leading dimension of <i>a</i> ; $1da \ge max(1, m)$.		
Output Parameters			
S	<pre>REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Array, DIMENSION (n). If info = 0, the array s contains the scale factors for A.</pre>		
scond	<pre>REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. If info = 0, scond contains the ratio of the smallest s(i) to the largest s(i).</pre>		
amax	REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Absolute value of the largest element of the matrix <i>A</i> .		
info	INTEGER. If $info = 0$, the execution is successful.		

If info = -i, the *i*th parameter had an illegal value. If info = i, the *i*th diagonal element of A is nonpositive.

Application Notes

If $scond \ge 0.1$ and amax is neither too large nor too small, it is not worth scaling by s.

If *amax* is very close to overflow or very close to underflow, the matrix *A* should be scaled.

?ppequ

Computes row and column scaling factors intended to equilibrate a symmetric (Hermitian) positive definite matrix in packed storage and reduce its condition number.

> call sppequ (uplo, n, ap, s, scond, amax, info) call dppequ (uplo, n, ap, s, scond, amax, info) call cppequ (uplo, n, ap, s, scond, amax, info) call zppequ (uplo, n, ap, s, scond, amax, info)

Discussion

This routine computes row and column scalings intended to equilibrate a symmetric (Hermitian) positive definite matrix *A* in packed storage and reduce its condition number (with respect to the two-norm). The output array *s* returns scale factors computed as

$$s(i) = \frac{1}{\sqrt{a_{i, i}}}$$

These factors are chosen so that the scaled matrix B with elements $b_{ij} = \mathbf{s}(\mathbf{i}) * a_{ij} * \mathbf{s}(\mathbf{j})$ has diagonal elements equal to 1.

This choice of s puts the condition number of B within a factor n of the smallest possible condition number over all possible diagonal scalings.

Input Parameters

uplo

CHARACTER*1. Must be 'U' or 'L'. Indicates whether the upper or lower triangular part of A is packed in the array ap: If uplo = 'U', the array ap stores the upper triangular part of the matrix A. If uplo = 'L', the array ap stores the lower triangular part of the matrix A.

n	INTEGER. The order of matrix A ($n \ge 0$).
ар	REAL for sppequ
	DOUBLE PRECISION for dppequ
	COMPLEX for cppequ
	DOUBLE COMPLEX for zppequ.
	Array, DIMENSION at least $\max(1, n(n+1)/2)$.
	The array <i>ap</i> contains either the upper or the lower
	triangular part of the matrix A (as specified by uplo) in
	packed storage (see Matrix Storage Schemes).

S	 REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Array, DIMENSION (n). If <i>info</i> = 0, the array <i>s</i> contains the scale factors for <i>A</i>.
scond	REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. If <i>info</i> = 0, <i>scond</i> contains the ratio of the smallest <i>s</i> (i) to the largest <i>s</i> (i).
amax	REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Absolute value of the largest element of the matrix <i>A</i> .
info	INTEGER. If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, the <i>i</i> th diagonal element of <i>A</i> is nonpositive.

Application Notes

If $scond \ge 0.1$ and amax is neither too large nor too small, it is not worth scaling by s.

If *amax* is very close to overflow or very close to underflow, the matrix *A* should be scaled.

?pbequ

Computes row and column scaling factors intended to equilibrate a symmetric (Hermitian) positive definite band matrix and reduce its condition number.

call spbequ (uplo, n, kd, ab, ldab, s, scond, amax, info) call dpbequ (uplo, n, kd, ab, ldab, s, scond, amax, info) call cpbequ (uplo, n, kd, ab, ldab, s, scond, amax, info) call zpbequ (uplo, n, kd, ab, ldab, s, scond, amax, info)

Discussion

This routine computes row and column scalings intended to equilibrate a symmetric (Hermitian) positive definite matrix *A* in packed storage and reduce its condition number (with respect to the two-norm). The output array *s* returns scale factors computed as

$$s(i) = \frac{1}{\sqrt{a_{i, i}}}$$

These factors are chosen so that the scaled matrix B with elements $b_{ij}=s(i)*a_{ij}*s(j)$ has diagonal elements equal to 1. This choice of a pute the condition number of B within a factor n of the scaled matrix $B = a_{ij} + a_{ij}$

This choice of s puts the condition number of B within a factor n of the smallest possible condition number over all possible diagonal scalings.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether the upper or lower triangular part of A
	is packed in the array <i>ab</i> :
	If $uplo = 'U'$, the array <i>ab</i> stores the upper triangular
	part of the matrix A.
	If <u>uplo</u> = 'L', the array <u>ab</u> stores the lower triangular
	part of the matrix A.
п	INTEGER. The order of matrix A $(n \ge 0)$.
kd	INTEGER. The number of super-diagonals or
	sub-diagonals in the matrix A $(kd \ge 0)$.

ab	REAL for spbequ
	DOUBLE PRECISION for dpbequ
	COMPLEX for cpbequ
	DOUBLE COMPLEX for zpbequ.
	Array, DIMENSION (<i>ldab</i> ,*).
	The array <i>ap</i> contains either the upper or the lower
	triangular part of the matrix A (as specified by uplo) in
	band storage (see Matrix Storage Schemes).
	The second dimension of ab must be at least max(1, n).
ldab	INTEGER. The leading dimension of the array <i>ab</i> .
	$(1dab \ge kd + 1).$

S	<pre>REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Array, DIMENSION (n). If info = 0, the array s contains the scale factors for A.</pre>
scond	REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. If <i>info</i> = 0, <i>scond</i> contains the ratio of the smallest <i>s</i> (i) to the largest <i>s</i> (i).
amax	REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Absolute value of the largest element of the matrix <i>A</i> .
info	INTEGER. If $info = 0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, the <i>i</i> th diagonal element of <i>A</i> is nonpositive.

Application Notes

If $scond \ge 0.1$ and amax is neither too large nor too small, it is not worth scaling by s.

If *amax* is very close to overflow or very close to underflow, the matrix *A* should be scaled.

Driver Routines

<u>Table 4-3</u> lists the LAPACK driver routines for solving systems of linear equations with real or complex matrices.

Table 4-3 Driver Routines for Solving Systems of Linear Equations

Matrix type, storage scheme	Simple Driver	Expert Driver
general	?gesv	?gesvx
general band	?gbsv	?gbsvx
general tridiagonal	?gtsv	?gtsvx
symmetric/Hermitian positive-definite	?posv	?posvx
symmetric/Hermitian positive-definite, packed storage	?psv	?ppsvx
symmetric/Hermitian positive-definite, band	?pbsv	?pbsvx
symmetric/Hermitian positive-definite, tridiagonal	<u>?ptsv</u>	?ptsvx
symmetric/Hermitian indefinite	<u>?sysv/?hesv</u>	<u>?sysvx</u> / <u>?hesvx</u>
symmetric/Hermitian indefinite, packed storage	<u>?spsv</u> /?hpsv	?spsvx/?hpsvx
complex symmetric	?sysv	?sysvx
complex symmetric, packed storage	?spsv	?spsvx

In this table **?** stands for **s** (single precision real), **d** (double precision real), **c** (single precision complex), or **z** (double precision complex).

?gesv

Computes the solution to the system of linear equations with a square matrix A and multiple right-hand sides.

call	sgesv	(n,	nrhs,	a,	lda,	ipiv,	b,	ldb,	info)
call	dgesv	(n,	nrhs,	a,	lda,	ipiv,	b,	ldb,	info)
call	cgesv	(n,	nrhs,	a,	lda,	ipiv,	b,	ldb,	info)
call	zgesv	(n,	nrhs,	a,	lda,	ipiv,	b,	ldb,	info)

Discussion

This routine solves for X the system of linear equations AX = B, where A is an *n*-by-*n* matrix, the columns of matrix *B* are individual right-hand sides, and the columns of X are the corresponding solutions.

The *LU* decomposition with partial pivoting and row interchanges is used to factor *A* as A = P L U, where *P* is a permutation matrix, *L* is unit lower triangular, and *U* is upper triangular. The factored form of *A* is then used to solve the system of equations AX = B.

n	INTEGER. The order of <i>A</i> ; the number of rows in <i>B</i> $(n \ge 0)$.
nrhs	INTEGER. The number of right-hand sides; the number of columns in <i>B</i> (<i>nrhs</i> \ge 0).
a, b	REAL for sgesv DOUBLE PRECISION for dgesv COMPLEX for cgesv DOUBLE COMPLEX for zgesv. Arrays: a(lda,*), b(ldb,*).
	The array <i>a</i> contains the matrix <i>A</i> . The array <i>b</i> contains the matrix <i>B</i> whose columns are the right-hand sides for the systems of equations. The second dimension of <i>a</i> must be at least $\max(1,n)$, the second dimension of <i>b</i> at least $\max(1,nrhs)$.

lda	INTEGER. The first dimension of a ; $1da \ge max(1, n)$.
ldb	INTEGER. The first dimension of b ; $1db \ge max(1, n)$.
Output Paran	neters
a	Overwritten by the factors L and U from the factorization of $A = P L U$; the unit diagonal elements of L are not stored.
b	Overwritten by the solution matrix <i>X</i> .
ipiv	INTEGER. Array, DIMENSION at least $max(1,n)$. The pivot indices that define the permutation matrix <i>P</i> ; row i of the matrix was interchanged with row $ipiv(i)$.
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$, the <i>i</i> th parameter had an illegal value. If <i>info</i> = <i>i</i> , $U(i,i)$ is exactly zero. The factorization has been completed, but the factor U is exactly singular, so the solution could not be computed.

?gesvx

Computes the solution to the system of linear equations with a square matrix A and multiple right-hand sides, and provides error bounds on the solution.

Discussion

This routine uses the *LU* factorization to compute the solution to a real or complex system of linear equations AX = B, where A is an *n*-by-*n* matrix, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

Error bounds on the solution and a condition estimate are also provided.

The routine **?gesvx** performs the following steps:

1. If fact = 'E', real scaling factors r and c are computed to equilibrate the system:

trans = 'N':	$\operatorname{diag}(\mathbf{r}) * A * \operatorname{diag}(\mathbf{c}) * \operatorname{diag}(\mathbf{c})^{-1} * X = \operatorname{diag}(\mathbf{r}) * B$
trans = 'T':	$(\operatorname{diag}(\mathbf{r}) * A * \operatorname{diag}(\mathbf{c}))^{\mathrm{T}} * \operatorname{diag}(\mathbf{r})^{-1} * X = \operatorname{diag}(\mathbf{c}) * B$
<i>trans</i> = 'C':	$(\operatorname{diag}(\mathbf{r})^*A^*\operatorname{diag}(\mathbf{c}))^H *\operatorname{diag}(\mathbf{r})^{-1}*X = \operatorname{diag}(\mathbf{c})^*B$

Whether or not the system will be equilibrated depends on the scaling of the matrix A, but if equilibration is used, A is overwritten by diag(r) * A * diag(c) and B by diag(r) * B (if trans='N') or diag(c) * B (if trans='T' or 'C').

2. If *fact* = 'N' or 'E', the *LU* decomposition is used to factor the matrix *A* (after equilibration if *fact* = 'E') as A = P L U, where *P* is a permutation matrix, *L* is a unit lower triangular matrix, and *U* is upper triangular.

3. If some $U_{i,i} = 0$, so that U is exactly singular, then the routine returns with *info* = i. Otherwise, the factored form of A is used to estimate the condition number of the matrix A. If the reciprocal of the condition number is less than machine precision, *info* = n + 1 is returned as a warning, but the routine still goes on to solve for X and compute error bounds as described below.

4. The system of equations is solved for *X* using the factored form of *A*.

5. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

6. If equilibration was used, the matrix X is premultiplied by diag(c) (if trans = 'N') or diag(r) (if trans = 'T' or 'C') so that it solves the original system before equilibration.

fact	CHARACTER*1. Must be 'F', 'N', or 'E'.
	Specifies whether or not the factored form of the matrix A is supplied on entry, and if not, whether the matrix A should be equilibrated before it is factored.
	If $fact = 'F'$: on entry, <i>af</i> and <i>ipiv</i> contain the factored form of <i>A</i> . If <i>equed</i> is not 'N', the matrix <i>A</i> has been equilibrated with scaling factors given by <i>r</i> and <i>c</i> . <i>a</i> , <i>af</i> , and <i>ipiv</i> are not modified.
	If <i>fact</i> = 'N', the matrix <i>A</i> will be copied to <i>af</i> and factored. If <i>fact</i> = 'E', the matrix <i>A</i> will be equilibrated if necessary, then copied to <i>af</i> and factored.
trans	CHARACTER*1. Must be 'N', 'T', or 'C'.
	Specifies the form of the system of equations:
	If $trans = 'N'$, the system has the form $A X = B$ (No transpose); If $trans = 'T'$, the system has the form $A^T X = B$ (Transpose); If $trans = 'C'$, the system has the form $A^H X = B$ (Conjugate transpose);
п	INTEGER . The number of linear equations; the order of the matrix $A \ (n \ge 0)$.
nrhs	INTEGER . The number of right hand sides; the number of columns of the matrices <i>B</i> and X (<i>nrhs</i> \ge 0).
a,af,b,work	REAL for sgesvx DOUBLE PRECISION for dgesvx COMPLEX for cgesvx DOUBLE COMPLEX for zgesvx. Arrays: a(lda,*), af(ldaf,*), b(ldb,*), work(*). The array a contains the matrix A. If fact = 'F' and equed is not 'N', then A must have been equilibrated by the scaling factors in r and/or c. The second dimension

lda ldaf ldb ipiv

equed

of a must be at least max $(1,n)$. The array af is an input argument if $fact = 'F'$. It contains the factored form of the matrix A, i.e., the factors L and U from the factorization $A = P L U$ as computed by <u>?getrf</u> . If equed is not 'N', then af is the factored form of the equilibrated matrix A. The second dimension of af must be at least max $(1,n)$. The array b contains the matrix B whose columns are the right-hand sides for the systems of equations. The second dimension of b must be at least max $(1,nrhs)$.
<pre>work(*) is a workspace array. The dimension of work must be at least $\max(1,4*n)$ for real flavors, and at least $\max(1,2*n)$ for complex flavors.</pre>
INTEGER. The first dimension of a ; $1da \ge max(1, n)$.
INTEGER. The first dimension of <i>af</i> ; $1daf \ge max(1, n)$.
INTEGER. The first dimension of b ; $1db \ge max(1, n)$.
INTEGER. Array, DIMENSION at least max(1, <i>n</i>). The array <i>ipiv</i> is an input argument if <i>fact</i> = 'F'. It contains the pivot indices from the factorization A = P L U as computed by <u>?getrf;</u> row i of the matrix was interchanged with row <i>ipiv</i> (i).
CHARACTER*1. Must be 'N', 'R', 'C', or 'B'. equed is an input argument if $fact = 'F'$. It specifies the form of equilibration that was done: If equed = 'N', no equilibration was done (always true if $fact = 'N'$); If equed = 'R', row equilibration was done and A has been premultiplied by diag(r); If equed = 'C', column equilibration was done and A has been postmultiplied by diag(c); If equed = 'B', both row and column equilibration was done; A has been replaced by diag(r)*A*diag(c).

r, c	REAL for single precision flavors;
	DOUBLE PRECISION for double precision flavors.
	Arrays: $r(n)$, $c(n)$.
	 The array r contains the row scale factors for A, and the array c contains the column scale factors for A. These arrays are input arguments if <i>fact</i> = 'F' only; otherwise they are output arguments. If <i>equed</i> = 'R' or 'B', A is multiplied on the left by diag(r); if <i>equed</i> = 'N' or 'C', r is not accessed. If <i>fact</i> = 'F' and <i>equed</i> = 'R' or 'B', each element of r must be positive.
	If equed = 'C' or 'B', A is multiplied on the right by diag(c); if equed = 'N' or 'R', c is not accessed. If fact = 'F' and equed = 'C' or 'B', each element of c must be positive.
ldx	INTEGER. The first dimension of the output array x ; $ldx \ge max(1, n)$.
iwork	INTEGER . Workspace array, DIMENSION at least max(1, <i>n</i>); used
rwork	in real flavors only. REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Workspace array, DIMENSION at least max(1, 2* <i>n</i>); used in complex flavors only.

x

REAL for sgesvx DOUBLE PRECISION for dgesvx COMPLEX for cgesvx DOUBLE COMPLEX for zgesvx. Array, DIMENSION (*ldx*,*).

If info = 0 or info = n+1, the array x contains the solution matrix X to the *original* system of equations. Note that A and B are modified on exit if *equed* \neq 'N', and the solution to the *equilibrated* system is: diag(c)⁻¹*X, if *trans* = 'N' and *equed* = 'C' or 'B';

	diag $(r)^{-1} * X$, if <i>trans</i> = 'T' or 'C' and <i>equed</i> = 'R' or 'B'. The second dimension of x must be at least max $(1,nrhs)$.
a	Array a is not modified on exit if $fact = 'F'$ or 'N', or if fact = 'E' and $equed = 'N'$. If $equed \neq 'N'$, A is scaled on exit as follows: equed = 'R': $A = diag(r)*Aequed = 'C'$: $A = A*diag(c)equed = 'B'$: $A = diag(r)*A*diag(c)$
af	If $fact = 'N'$ or 'E', then af is an output argument and on exit returns the factors L and U from the factorization A = P L U of the original matrix $A(if fact = 'N')$ or of the equilibrated matrix A (if $fact = 'E'$). See the description of a for the form of the equilibrated matrix.
Ь	Overwritten by diag(r)* B if trans = 'N' and equed = 'R' or 'B'; overwritten by diag(c)*B if trans = 'T' and equed = 'C' or 'B'; not changed if equed = 'N'.
r, c	These arrays are output arguments if $fact \neq 'F'$. See the description of r , c in <i>Input Arguments</i> section.
rcond	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. An estimate of the reciprocal condition number of the matrix <i>A</i> after equilibration (if done). The routine sets <i>rcond</i> =0 if the estimate underflows; in this case the matrix is singular (to working precision). However, anytime <i>rcond</i> is small compared to 1.0, for the working precision, the matrix may be poorly conditioned or even singular.
ferr, berr	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the component-wise forward and relative backward errors, respectively, for each solution vector.

ipiv	If $fact = 'N'$ or 'E', then <i>ipiv</i> is an output argument and on exit contains the pivot indices from the factorization $A = P L U$ of the original matrix $A(if fact$ = 'N') or of the equilibrated matrix A (if $fact = 'E'$).
equed	If $fact \neq 'F'$, then <i>equed</i> is an output argument. It specifies the form of equilibration that was done (see the description of <i>equed</i> in <i>Input Arguments</i> section).
work, rwork	On exit, work(1) for real flavors, or rwork(1) for complex flavors, contains the reciprocal pivot growth factor norm(A)/norm(U). The "max absolute element" norm is used. If work(1) for real flavors, or rwork(1) for complex flavors is much less than 1, then the stability of the LU factorization of the (equilibrated) matrix A could be poor. This also means that the solution x, condition estimator rcond, and forward error bound ferr could be unreliable. If factorization fails with $0 < info \leq n$, then work(1) for real flavors, or rwork(1) for complex flavors contains the reciprocal pivot growth factor for the leading <i>info</i> columns of A.
info	INTEGER. If $info=0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, and $i \leq n$, then $U(i,i)$ is exactly zero. The factorization has been completed, but the factor <i>U</i> is exactly singular, so the solution and error bounds could not be computed; <i>rcond</i> = 0 is returned. If $info = i$, and $i = n + 1$, then <i>U</i> is nonsingular, but <i>rcond</i> is less than machine precision, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of <i>rcond</i> would suggest.

?gbsv

Computes the solution to the system of linear equations with a band matrix A and multiple right-hand sides.

call sgbsv (n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info) call dgbsv (n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info) call cgbsv (n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info) call zgbsv (n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)

Discussion

This routine solves for *X* the real or complex system of linear equations AX = B, where A is an *n*-by-*n* band matrix with *k*1 subdiagonals and *ku* superdiagonals, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

The *LU* decomposition with partial pivoting and row interchanges is used to factor *A* as A = L U, where *L* is a product of permutation and unit lower triangular matrices with *kl* subdiagonals, and *U* is upper triangular with *kl+ku* superdiagonals. The factored form of *A* is then used to solve the system of equations AX = B.

п	INTEGER. The order of <i>A</i> ; the number of rows in <i>B</i> $(n \ge 0)$.
kl	INTEGER. The number of sub-diagonals within the band of A ($kl \ge 0$).
ku	INTEGER. The number of super-diagonals within the band of A ($ku \ge 0$).
nrhs	INTEGER. The number of right-hand sides; the number of columns in <i>B</i> (<i>nrhs</i> \ge 0).
ab, b	REAL for sgbsv DOUBLE PRECISION for dgbsv COMPLEX for cgbsv

	DOUBLE COMPLEX for zgbsv.
	Arrays: $ab(ldab, *)$, $b(ldb, *)$.
	The array <i>ab</i> contains the matrix <i>A</i> in band storage
	(see Matrix Storage Schemes).
	The second dimension of ab must be at least max $(1, n)$. The array b contains the matrix B whose columns are the right-hand sides for the systems of equations. The second dimension of b must be at least
	max(1, <i>nrhs</i>).
ldab	INTEGER. The first dimension of the array <i>ab</i> . $(1dab \ge 2kl + ku + 1)$
ldb	INTEGER. The first dimension of b; $ldb \ge max(1, n)$.
Output Parame	ters
ab	Overwritten by L and U. The diagonal and $kl + ku$ super-diagonals of U are stored in the first $l + kl + ku$ rows of <i>ab</i> . The multipliers used to form L are stored in the next <i>kl</i> rows.
b	Overwritten by the solution matrix <i>X</i> .
ipiv	INTEGER. Array, DIMENSION at least max(1, <i>n</i>). The pivot indices: row <i>i</i> was interchanged with row <i>ipiv(i)</i> .
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$, the <i>i</i> th parameter had an illegal value. If <i>info</i> = i , $U(i,i)$ is exactly zero. The factorization

has been completed, but the factor U is exactly singular, so the solution could not be computed.

?gbsvx

Computes the solution to the real or complex system of linear equations with a band matrix A and multiple right-hand sides, and provides error bounds on the solution.

Discussion

This routine uses the *LU* factorization to compute the solution to a real or complex system of linear equations AX = B, $A^TX = B$, or $A^HX = B$, where A is a band matrix of order *n* with *k*l subdiagonals and *ku* superdiagonals, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

Error bounds on the solution and a condition estimate are also provided.

The routine **?gbsvx** performs the following steps:

1. If *fact* = 'E', real scaling factors r and c are computed to equilibrate the system:

 $trans = 'N': \quad \operatorname{diag}(r) * A * \operatorname{diag}(c) * \operatorname{diag}(c)^{-1} * X = \operatorname{diag}(r) * B$ $trans = 'T': \quad (\operatorname{diag}(r) * A * \operatorname{diag}(c))^{T} * \operatorname{diag}(r)^{-1} * X = \operatorname{diag}(c) * B$ $trans = 'C': \quad (\operatorname{diag}(r) * A * \operatorname{diag}(c))^{H} * \operatorname{diag}(r)^{-1} * X = \operatorname{diag}(c) * B$

Whether or not the system will be equilibrated depends on the scaling of the matrix A, but if equilibration is used, A is overwritten by diag(r)*A*diag(c) and B by diag(r)*B (if trans='N') or diag(c)*B (if trans = 'T' or 'C').

2. If fact = 'N' or 'E', the *LU* decomposition is used to factor the matrix *A* (after equilibration if fact = 'E') as A = L U, where *L* is a product of permutation and unit lower triangular matrices with *kl* subdiagonals, and *U* is upper triangular with kl+ku superdiagonals.

3. If some $U_{i,i} = 0$, so that *U* is exactly singular, then the routine returns with *info* = i. Otherwise, the factored form of *A* is used to estimate the condition number of the matrix *A*. If the reciprocal of the condition number is less than machine precision, *info* = n + 1 is returned as a warning, but the routine still goes on to solve for *X* and compute error bounds as described below.

4. The system of equations is solved for *X* using the factored form of *A*.

5. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

6. If equilibration was used, the matrix X is premultiplied by diag(c) (if trans = 'N') or diag(r) (if trans = 'T' or 'C') so that it solves the original system before equilibration.

Input Parameters

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fact
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CHARACTER*1. Must be 'F', 'N', or 'E'.

Specifies whether or not the factored form of the matrix *A* is supplied on entry, and if not, whether the matrix *A* should be equilibrated before it is factored.

If fact = 'F': on entry, *afb* and *ipiv* contain the factored form of *A*. If *equed* is not 'N', the matrix *A* has been equilibrated with scaling factors given by *r* and *c*. *ab*, *afb*, and *ipiv* are not modified.

If fact = 'N', the matrix A will be copied to afb and factored.

If fact = 'E', the matrix A will be equilibrated if necessary, then copied to *afb* and factored.

trans CHARACTER*1. Must be 'N', 'T', or 'C'.

Specifies the form of the system of equations:

	-Former of the system of the s
	If $trans = 'N'$, the system has the form $A X = B$ (No transpose);
	If $trans = 'T'$, the system has the form $A^T X = B$ (Transpose);
	If $transpose$, If $trans = 'C'$, the system has the form $A^H X = B$ (Conjugate transpose);
n	INTEGER. The number of linear equations; the order of the matrix A ($n \ge 0$).
kl	INTEGER. The number of sub-diagonals within the band of A ($kl \ge 0$).
ku	INTEGER. The number of super-diagonals within the band of A ($ku \ge 0$).
nrhs	INTEGER. The number of right hand sides; the number of columns of the matrices <i>B</i> and <i>X</i> (<i>nrhs</i> \ge 0).
ab,afb,b,work	REAL for sgesvx DOUBLE PRECISION for dgesvx COMPLEX for cgesvx DOUBLE COMPLEX for zgesvx. Arrays: a(lda,*), af(ldaf,*), b(ldb,*), work(*). The array ab contains the matrix A in band storage (see <u>Matrix Storage Schemes</u>). The second dimension of ab must be at least max(1, n). If fact = 'F' and equed is not 'N', then A must have been equilibrated by the scaling factors in r and/or c.
	The array <i>afb</i> is an input argument if <i>fact</i> = 'F'. The second dimension of <i>afb</i> must be at least max(1, <i>n</i>). It contains the factored form of the matrix A, i.e., the factors L and U from the factorization $A = L U$ as computed by <u>?gbtrf</u> . U is stored as an upper triangular band matrix with $kl + ku$ super-diagonals in the first 1 + kl + ku rows of <i>afb</i> . The multipliers used during

	the factorization are stored in the next kl rows. If <i>equed</i> is not 'N', then <i>afb</i> is the factored form of the equilibrated matrix A.
	The array b contains the matrix B whose columns are the right-hand sides for the systems of equations. The second dimension of b must be at least max $(1,nrhs)$.
	<i>work</i> (*) is a workspace array. The dimension of <i>work</i> must be at least $max(1,3*n)$ for real flavors, and at least $max(1,2*n)$ for complex flavors.
ldab	INTEGER. The first dimension of <i>ab</i> ; $1dab \ge k1+ku+1$.
ldafb	INTEGER. The first dimension of <i>afb</i> ; $ldafb \ge 2*kl+ku+1$.
ldb	INTEGER . The first dimension of <i>b</i> ; $1db \ge max(1, n)$.
ipiv	INTEGER. Array, DIMENSION at least max $(1,n)$. The array <i>ipiv</i> is an input argument if <i>fact</i> = 'F'. It contains the pivot indices from the factorization A = L U as computed by <u>?gbtrf</u> ; row i of the matrix was interchanged with row <i>ipiv</i> (i).
equed	CHARACTER*1. Must be 'N', 'R', 'C', or 'B'. equed is an input argument if $fact = 'F'$. It specifies the form of equilibration that was done: If equed = 'N', no equilibration was done (always true if $fact = 'N'$); If equed = 'R', row equilibration was done and A has been premultiplied by diag(r); If equed = 'C', column equilibration was done and A has been postmultiplied by diag(c); If equed = 'B', both row and column equilibration was done; A has been replaced by diag(r):A*diag(c).
r, c	REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Arrays: $r(n)$, $c(n)$. The array r contains the row scale factors for A , and the

	array c contains the column scale factors for A. These
	arrays are input arguments if <i>fact</i> = 'F' only; otherwise
	they are output arguments.
	If $equed = 'R'$ or 'B', A is multiplied on the left by
	diag(r); if equed = 'N' or 'C', r is not accessed.
	If $fact = F'$ and $equed = R'$ or B', each element of
	<i>r</i> must be positive.
	If $equed = 'C'$ or 'B', A is multiplied on the right by
	diag(c); if $equed = 'N'$ or 'R', c is not accessed.
	If $fact = 'F'$ and $equed = 'C'$ or 'B', each element of
	<i>c</i> must be positive.
ldx	INTEGER. The first dimension of the output array \mathbf{x} ;
	$ldx \ge max(1, n).$
iwork	INTEGER.
	Workspace array, DIMENSION at least max(1, <i>n</i>); used
	in real flavors only.
rwork	REAL for single precision flavors;
	DOUBLE PRECISION for double precision flavors.
	Workspace array, DIMENSION at least max(1, <i>n</i>); used
	in complex flavors only.

Output Parameters

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REAL for sgbsvx DOUBLE PRECISION for dgbsvx COMPLEX for cgbsvx DOUBLE COMPLEX for zgbsvx. Array, DIMENSION (*ldx*,*).

If info = 0 or info = n+1, the array x contains the solution matrix X to the *original* system of equations. Note that A and B are modified on exit if $equed \neq 'N'$, and the solution to the *equilibrated* system is: $diag(c)^{-1}*X$, if trans = 'N' and equed = 'C' or 'B'; $diag(r)^{-1}*X$, if trans = 'T' or 'C' and equed = 'R' or 'B'.

The second dimension of x must be at least max(1,*nrhs*).

ab	Array <i>ab</i> is not modified on exit if $fact = 'F'$ or 'N', or if $fact = 'E'$ and $equed = 'N'$.
	If $equed \neq 'N'$, A is scaled on exit as follows:
	equed = 'R': A = diag(r)*A equed = 'C': A = A*diag(c)
	equed = 'B': $A = diag(r) * A * diag(c)$
afb	If $fact = 'N'$ or $'E'$, then afb is an output argument and on exit returns details of the <i>LU</i> factorization of the original matrix $A(if fact = 'N')$ or of the equilibrated matrix A (if $fact = 'E'$). See the description of ab for the form of the equilibrated matrix.
b	Overwritten by $diag(r)^{*b}$ if $trans = 'N'$ and
	equed = 'R' or 'B';
	<pre>overwritten by diag(c)*b if trans = 'T' and equed = 'C' or 'B';</pre>
	not changed if $equed = 'N'$.
r, c	These arrays are output arguments if $fact \neq 'F'$.
1, 0	See the description of r , c in <i>Input Arguments</i> section.
rcond	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	An estimate of the reciprocal condition number of the matrix <i>A</i> after equilibration (if done).
	If <i>rcond</i> is less than the machine precision (in
	particular, if $rcond = 0$), the matrix is singular to
	working precision. This condition is indicated by a
ferr, berr	return code of $info > 0$. REAL for single precision flavors.
ieii, Deii	DOUBLE PRECISION for double precision flavors.
	Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the
	component-wise forward and relative backward errors,
	respectively, for each solution vector.
ipiv	If $fact = 'N'$ or 'E', then <i>ipiv</i> is an output argument and on exit contains the pivot indices from the
	factorization $A = L U$ of the original matrix $A(\text{if } fact = bt)$ or of the equilibrated matrix $A(\text{if } fact = bt)$
	'N') or of the equilibrated matrix A (if $fact = 'E'$).

equed	If $fact \neq 'F'$, then equed is an output argument. It specifies the form of equilibration that was done (see the description of equed in <i>Input Arguments</i> section).
work, rwork	On exit, $work(1)$ for real flavors, or $rwork(1)$ for complex flavors, contains the reciprocal pivot growth factor norm(A)/norm(U). The "max absolute element" norm is used. If $work(1)$ for real flavors, or $rwork(1)$ for complex flavors is much less than 1, then the stability of the LU factorization of the (equilibrated) matrix A could be poor. This also means that the solution x, condition estimator $rcond$, and forward error bound ferr could be unreliable. If factorization fails with $0 < info \leq n$, then $work(1)$ for real flavors, or $rwork(1)$ for complex flavors contains the reciprocal pivot growth factor for the leading $info$ columns of A .
info	INTEGER. If $info=0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, and $i \leq n$, then $U(i,i)$ is exactly zero. The factorization has been completed, but the factor <i>U</i> is exactly singular, so the solution and error bounds could not be computed; $rcond = 0$ is returned. If $info = i$, and $i = n + 1$, then <i>U</i> is nonsingular, but $rcond$ is less than machine precision, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of $rcond$ would suggest.

?gtsv

Computes the solution to the system of linear equations with a tridiagonal matrix A and multiple right-hand sides.

call sgtsv (n, nrhs, dl, d, du, b, ldb, info)
call dgtsv (n, nrhs, dl, d, du, b, ldb, info)
call cgtsv (n, nrhs, dl, d, du, b, ldb, info)
call zgtsv (n, nrhs, dl, d, du, b, ldb, info)

Discussion

This routine solves for *X* the system of linear equations AX = B, where A is an *n*-by-*n* tridiagonal matrix, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions. The routine uses Gaussian elimination with partial pivoting.

Note that the equation $A^{T}X = B$ may be solved by interchanging the order of the arguments *du* and *dl*.

n	INTEGER . The order of <i>A</i> ; the number of rows in <i>B</i> $(n \ge 0)$.
nrhs	INTEGER. The number of right-hand sides; the number of columns in <i>B</i> (<i>nrhs</i> \ge 0).
dl, d, du, b	REAL for sgtsv DOUBLE PRECISION for dgtsv COMPLEX for cgtsv DOUBLE COMPLEX for zgtsv. Arrays: $dl(n - 1)$, $d(n)$, $du(n - 1)$, $b(ldb, *)$. The array dl contains the $(n - 1)$ subdiagonal elements of A . The array d contains the diagonal elements of A . The array du contains the $(n - 1)$ superdiagonal elements of A .

	The array <i>b</i> contains the matrix <i>B</i> whose columns are the right-hand sides for the systems of equations. The second dimension of <i>b</i> must be at least max(1,nrhs).
ldb	INTEGER. The first dimension of b ; $1db \ge max(1, n)$.
Output Parame	eters
dl	Overwritten by the $(n-2)$ elements of the second superdiagonal of the upper triangular matrix U from the LU factorization of A. These elements are stored in $dl(1), \dots, dl(n-2)$.
d	Overwritten by the n diagonal elements of U .
du	Overwritten by the $(n-1)$ elements of the first superdiagonal of U .
b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$, the <i>i</i> th parameter had an illegal value. If <i>info</i> = i , $U(i,i)$ is exactly zero, and the solution has not been computed. The factorization has not been completed unless $i = n$.

?gtsvx

Computes the solution to the real or complex system of linear equations with a tridiagonal matrix A and multiple right-hand sides, and provides error bounds on the solution.

Discussion

This routine uses the *LU* factorization to compute the solution to a real or complex system of linear equations AX = B, $A^TX = B$, or $A^HX = B$, where A is a tridiagonal matrix of order *n*, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

Error bounds on the solution and a condition estimate are also provided.

The routine **?gtsvx** performs the following steps:

1. If *fact* = 'N', the *LU* decomposition is used to factor the matrix *A* as A = LU, where *L* is a product of permutation and unit lower bidiagonal matrices and *U* is an upper triangular matrix with nonzeroes in only the main diagonal and first two superdiagonals.

2. If some $U_{i,i} = 0$, so that *U* is exactly singular, then the routine returns with *info* = i. Otherwise, the factored form of *A* is used to estimate the condition number of the matrix *A*. If the reciprocal of the condition number

is less than machine precision, info = n + 1 is returned as a warning, but the routine still goes on to solve for X and compute error bounds as described below.

3. The system of equations is solved for X using the factored form of A.

4. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

fact	CHARACTER*1. Must be 'F' or 'N'.
	Specifies whether or not the factored form of the matrix <i>A</i> has been supplied on entry.
	If fact = 'F': on entry, dlf, df, duf, du2, and ipiv contain the factored form of A; arrays dl, d, du, dlf, df, duf, du2, and ipiv will not be modified.
	If $fact = 'N'$, the matrix A will be copied to dlf , df , and duf and factored.
trans	CHARACTER*1. Must be 'N', 'T', or 'C'.
	Specifies the form of the system of equations:
	If $trans = 'N'$, the system has the form $A X = B$ (No transpose);
	If <i>trans</i> = 'T', the system has the form $A^{T}X = B$
	(Transpose); If <i>trans</i> = 'C', the system has the form $A^{H}X = B$
	(Conjugate transpose);
n	INTEGER . The number of linear equations; the order of the matrix $A \ (n \ge 0)$.
nrhs	INTEGER . The number of right hand sides; the number of columns of the matrices <i>B</i> and <i>X</i> (<i>nrhs</i> \ge 0).
dl,d,du,dlf,d	
duf,du2,b,x,w	ork REAL for sgtsvx
	DOUBLE PRECISION for dgtsvx
	COMPLEX for cgtsvx DOUBLE COMPLEX for zgtsvx.
	Arrays:
	1 11 a y 5.

	d1, dimension $(n - 1)$, contains the subdiagonal elements of A.
	d, dimension (n) , contains the diagonal elements of A.
	du, dimension $(n - 1)$, contains the superdiagonal elements of A .
	<i>dlf</i> , dimension $(n - 1)$. If <i>fact</i> = 'F', then <i>dlf</i> is an input argument and on entry contains the $(n - 1)$ multipliers that define the matrix <i>L</i> from the <i>LU</i> factorization of <i>A</i> as computed by <u>?gttrf</u> .
	<i>df</i> , dimension (<i>n</i>). If <i>fact</i> = 'F', then <i>df</i> is an input argument and on entry contains the <i>n</i> diagonal elements of the upper triangular matrix <i>U</i> from the <i>LU</i> factorization of <i>A</i> .
	<i>duf</i> , dimension $(n - 1)$. If <i>fact</i> = 'F', then <i>duf</i> is an input argument and on entry contains the $(n - 1)$ elements of the first super-diagonal of U .
	<i>du2</i> , dimension $(n - 2)$. If <i>fact</i> = 'F', then <i>du2</i> is an input argument and on entry contains the $(n - 2)$ elements of the second super-diagonal of <i>U</i> .
	b(1db, *) contains the right-hand side matrix <i>B</i> . The second dimension of <i>b</i> must be at least max $(1,nrhs)$.
	x(ldx, *) contains the solution matrix X. The second dimension of x must be at least max $(1, nrhs)$.
	work $(*)$ is a workspace array; the dimension of work must be at least max $(1, 3*n)$ for real flavors and max $(1, 2*n)$ for complex flavors.
ldb	INTEGER. The first dimension of b; $ldb \ge max(1, n)$.
ldx	INTEGER . The first dimension of x ; $1dx \ge max(1, n)$.
ipiv	INTEGER. Array, DIMENSION at least $max(1,n)$. If <i>fact</i> = 'F', then <i>ipiv</i> is an input argument and on entry contains the pivot indices, as returned by <u>?gttrf</u> .
iwork	INTEGER. Workspace array, DIMENSION (<i>n</i>). Used for real flavors only.

REAL for cgtsvx rwork DOUBLE PRECISION for zgtsvx. Workspace array, **DIMENSION** (*n*). Used for complex flavors only. **Output Parameters** REAL for sqtsvx x DOUBLE PRECISION for dgtsvx COMPLEX for cqtsvx DOUBLE COMPLEX for zqtsvx. Array, DIMENSION (ldx, *). If info = 0 or info = n+1, the array x contains the solution matrix X. The second dimension of \mathbf{x} must be at least max(1, nrhs). If fact = 'N', then dlf is an output argument and on dlf exit contains the (n - 1) multipliers that define the matrix L from the LU factorization of A. df If fact = 'N', then df is an output argument and on exit contains the n diagonal elements of the upper triangular matrix U from the LU factorization of A. duf If fact = 'N', then *duf* is an output argument and on exit contains the (n - 1) elements of the first super-diagonal of U. du2 If fact = N', then du2 is an output argument and on exit contains the (n - 2) elements of the second super-diagonal of U. The array *ipiv* is an output argument if fact = 'N' and, ipiv on exit, contains the pivot indices from the factorization A = L U; row *i* of the matrix was interchanged with row *ipiv*(*i*). The value of *ipiv*(*i*) will always be either *i* or i+1; ipiv(i)=i indicates a row interchange was not required. **REAL** for single precision flavors. rcond

DOUBLE PRECISION for double precision flavors. An estimate of the reciprocal condition number of the matrix A.

	If <i>rcond</i> is less than the machine precision (in particular, if <i>rcond</i> = 0), the matrix is singular to working precision. This condition is indicated by a return code of <i>info</i> > 0 .
ferr, berr	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the component-wise forward and backward errors, respectively, for each solution vector.
info	INTEGER. If $info=0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, and $i \leq n$, then $U(i,i)$ is exactly zero. The factorization has not been completed unless $i = n$, but the factor <i>U</i> is exactly singular, so the solution and error bounds could not be computed; $rcond = 0$ is returned. If $info = i$, and $i = n + 1$, then <i>U</i> is nonsingular, but $rcond$ is less than machine precision, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of $rcond$ would suggest.

?posv

Computes the solution to the system of linear equations with a symmetric or Hermitian positive definite matrix A and multiple right-hand sides.

call	sposv	(uplo,	n,	nrhs,	a,	lda,	b,	ldb,	info)
call	dposv	(uplo,	n,	nrhs,	a,	lda,	b,	ldb,	info)
call	cposv	(uplo,	n,	nrhs,	a,	lda,	b,	ldb,	info)
call	zposv	(uplo,	n,	nrhs,	a,	lda,	b,	ldb,	info)

Discussion

This routine solves for *X* the real or complex system of linear equations AX = B, where A is an *n*-by-*n* symmetric/Hermitian positive definite matrix, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

The Cholesky decomposition is used to factor A as $A = U^{H}U$ if uplo = U'

or $A = LL^H$ if uplo = L', where U is an upper triangular matrix and L is a lower triangular matrix. The factored form of A is then used to solve the system of equations AX = B.

uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether the upper or lower triangular part of A
	is stored and how A is factored:
	If $uplo = U'$, the array a stores the upper triangular part of the matrix A, and A is factored as $U^H U$.
	If $uplo = 'L'$, the array a stores the lower triangular part of the matrix A; A is factored as LL^H .
n	INTEGER. The order of matrix $A (n \ge 0)$.
nrhs	INTEGER. The number of right-hand sides; the number of columns in B (<i>nrhs</i> ≥ 0).

a, b	REAL for sposy
	DOUBLE PRECISION for dposv
	COMPLEX for cposv
	DOUBLE COMPLEX for zposv.
	Arrays: $a(lda, *), b(ldb, *).$
	The array a contains either the upper or the lower
	triangular part of the matrix A (see uplo).
	The second dimension of a must be at least $max(1, n)$.
	The array b contains the matrix B whose columns are
	the right-hand sides for the systems of equations.
	The second dimension of <i>b</i> must be at least
	max(1, <i>nrhs</i>).
lda	INTEGER . The first dimension of <i>a</i> ; $1da \ge max(1, n)$.
ldb	INTEGER. The first dimension of <i>b</i> ; $1db \ge max(1, n)$.
Output Pa	rameters
а	If <i>info</i> =0, the upper or lower triangular part of <i>a</i> is
	overwritten by the Cholesky factor U or L, as specified
	by uplo.
b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER. If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.
	If <i>info</i> = <i>i</i> , the leading minor of order <i>i</i> (and hence the
	matrix A itself) is not positive definite, so the
	factorization could not be completed, and the solution
	has not been computed.

?posvx

Uses the Cholesky factorization to compute the solution to the system of linear equations with a symmetric or Hermitian positive definite matrix A, and provides error bounds on the solution.

Discussion

This routine uses the Cholesky factorization $A = U^H U$ or $A = LL^H$ to compute the solution to a real or complex system of linear equations AX = B, where A is a *n*-by-*n* real symmetric/Hermitian positive definite matrix, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

Error bounds on the solution and a condition estimate are also provided.

The routine **?posvx** performs the following steps:

1. If *fact* = 'E', real scaling factors *s* are computed to equilibrate the system:

 $\operatorname{diag}(s) * A * \operatorname{diag}(s) * \operatorname{diag}(s)^{-1} * X = \operatorname{diag}(s) * B$

Whether or not the system will be equilibrated depends on the scaling of the matrix *A*, but if equilibration is used, *A* is overwritten by diag(s)*A*diag(s) and *B* by diag(s)*B.

2. If fact = 'N' or 'E', the Cholesky decomposition is used to factor the matrix A (after equilibration if fact = 'E') as

 $A = U^{H} U, \text{ if } uplo = `U', \text{ or}$ $A = L L^{H}, \text{ if } uplo = `L',$

where U is an upper triangular matrix and L is a lower triangular matrix.

3. If the leading *i*-by-*i* principal minor is not positive definite, then the routine returns with info = i. Otherwise, the factored form of A is used to estimate the condition number of the matrix A. If the reciprocal of the condition number is less than machine precision, info = n + 1 is returned as a warning, but the routine still goes on to solve for X and compute error bounds as described below.

4. The system of equations is solved for *X* using the factored form of *A*.

5. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

6. If equilibration was used, the matrix X is premultiplied by diag(s) so that it solves the original system before equilibration.

fact	CHARACTER*1. Must be 'F', 'N', or 'E'.
	Specifies whether or not the factored form of the matrix A is supplied on entry, and if not, whether the matrix A should be equilibrated before it is factored.
	If <i>fact</i> = 'F': on entry, <i>af</i> contains the factored form of <i>A</i> . If <i>equed</i> = 'Y', the matrix <i>A</i> has been equilibrated with scaling factors given by <i>s</i> . <i>a</i> and <i>af</i> will not be modified.
	If $fact = 'N'$, the matrix A will be copied to af and factored. If $fact = 'E'$, the matrix A will be equilibrated if necessary, then copied to af and factored.
uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether the upper or lower triangular part of A is stored and how A is factored: If $uplo = 'U'$, the array a stores the upper triangular part of the matrix A, and A is factored as $U^H U$. If $uplo = 'L'$, the array a stores the lower triangular part of the matrix A; A is factored as LL^H .

п	INTEGER. The order of matrix $A (n \ge 0)$.
nrhs	INTEGER. The number of right-hand sides; the number of columns in <i>B</i> (<i>nrhs</i> \ge 0).
a,af,b,work	<pre>REAL for sposvx DOUBLE PRECISION for dposvx COMPLEX for cposvx DOUBLE COMPLEX for zposvx. Arrays: a(lda,*), af(ldaf,*), b(ldb,*), work(*).</pre>
	The array <i>a</i> contains the matrix <i>A</i> as specified by <i>uplo</i> . If <i>fact</i> = 'F' and <i>equed</i> = 'Y', then <i>A</i> must have been equilibrated by the scaling factors in <i>s</i> , and <i>a</i> must contain the equilibrated matrix diag(<i>s</i>)* <i>A</i> *diag(<i>s</i>). The second dimension of <i>a</i> must be at least max(1, <i>n</i>).
	The array <i>af</i> is an input argument if <i>fact</i> = 'F'. It contains the triangular factor <i>U</i> or <i>L</i> from the Cholesky factorization of <i>A</i> in the same storage format as <i>A</i> . If <i>equed</i> is not 'N', then <i>af</i> is the factored form of the equilibrated matrix $diag(s)*A*diag(s)$. The second dimension of <i>af</i> must be at least $max(1,n)$.
	The array <i>b</i> contains the matrix <i>B</i> whose columns are the right-hand sides for the systems of equations. The second dimension of <i>b</i> must be at least $max(1,nrhs)$.
	<pre>work(*) is a workspace array. The dimension of work must be at least $max(1,3*n)$ for real flavors, and at least $max(1,2*n)$ for complex flavors.</pre>
lda	INTEGER . The first dimension of <i>a</i> ; $1da \ge max(1, n)$.
ldaf	INTEGER. The first dimension of af ; $ldaf \ge max(1, n)$.
ldb	INTEGER. The first dimension of b; $1db \ge max(1, n)$.
equed	CHARACTER*1. Must be 'N' or 'Y'. equed is an input argument if fact = 'F'. It specifies the form of equilibration that was done: If equed = 'N', no equilibration was done (always

	true if $fact = 'N'$; If $equed = 'Y'$, equilibration was done and A has been replaced by diag(s)*A*diag(s).
S	REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Array, DIMENSION (<i>n</i>). The array <i>s</i> contains the scale factors for <i>A</i> . This array is an input argument if <i>fact</i> = 'F' only; otherwise it is an output argument. If <i>equed</i> = 'N', <i>s</i> is not accessed.
	If $fact = 'F'$ and $equed = 'Y'$, each element of s must be positive.
ldx	INTEGER. The first dimension of the output array x ; $ldx \ge max(1, n)$.
iwork	INTEGER. Workspace array, DIMENSION at least $max(1, n)$; used in real flavors only.
rwork	REAL for cposvx; DOUBLE PRECISION for zposvx. Workspace array, DIMENSION at least max(1, n); used in complex flavors only.

Output Parameters

Y	
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REAL for sposvx DOUBLE PRECISION for dposvx COMPLEX for cposvx DOUBLE COMPLEX for zposvx. Array, DIMENSION (*ldx*,*).

> If info = 0 or info = n+1, the array x contains the solution matrix X to the *original* system of equations. Note that if *equed* = 'Y', A and B are modified on exit, and the solution to the equilibrated system is $diag(s)^{-1} * X$. The second dimension of x must be at least max(1,nrhs).

a	Array a is not modified on exit if $fact = 'F'$ or 'N', or if fact = 'E' and $equed = 'N'$. If $fact = 'E'$ and $equed = 'Y'$, A is overwritten by diag(s)*A*diag(s)
af	If $fact = 'N'$ or 'E', then af is an output argument and on exit returns the triangular factor U or L from the Cholesky factorization $A=U^{H}U$ or $A=LL^{H}$ of the original matrix $A(if fact = 'N')$, or of the equilibrated matrix A (if fact = 'E'). See the description of a for the form of the equilibrated matrix.
b	Overwritten by diag(s)* B , if equed = 'Y'; not changed if equed = 'N'.
S	This array is an output argument if $fact \neq F'$. See the description of <i>s</i> in <i>Input Arguments</i> section.
rcond ferr, berr	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. An estimate of the reciprocal condition number of the matrix <i>A</i> after equilibration (if done). If <i>rcond</i> is less than the machine precision (in particular, if <i>rcond</i> = 0), the matrix is singular to working precision. This condition is indicated by a return code of <i>info</i> > 0. REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the component-wise forward and relative backward errors,
	respectively, for each solution vector.
equed	If $fact \neq 'F'$, then equed is an output argument. It specifies the form of equilibration that was done (see the description of equed in <i>Input Arguments</i> section).
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$, the <i>i</i> th parameter had an illegal value. If <i>info</i> = <i>i</i> , and <i>i</i> \leq <i>n</i> , the leading minor of order <i>i</i> (and hence the matrix <i>A</i> itself) is not positive definite, so the factorization could not be completed, and the solution and error bounds could not be computed; <i>rcond</i> = 0 is

returned.

If info = i, and i = n + 1, then *U* is nonsingular, but *rcond* is less than machine precision, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of *rcond* would suggest.

?ppsv

Computes the solution to the system of linear equations with a symmetric (Hermitian) positive definite packed matrix A and multiple right-hand sides.

call	sppsv	(uplo,	n,	nrhs,	ap,	b,	ldb,	info)
call	dppsv	(uplo,	n,	nrhs,	ap,	b,	ldb,	info)
call	cppsv	(uplo,	n,	nrhs,	ap,	b,	ldb,	info)
call	zppsv	(uplo,	n,	nrhs,	ap,	b,	ldb,	info)

Discussion

This routine solves for X the real or complex system of linear equations AX = B, where A is an *n*-by-*n* real symmetric/Hermitian positive definite matrix stored in packed format, the columns of matrix *B* are individual right-hand sides, and the columns of X are the corresponding solutions.

The Cholesky decomposition is used to factor A as $A = U^{H}U$ if uplo = U'or $A = LL^{H}$ if uplo = L', where U is an upper triangular matrix and L is a lower triangular matrix. The factored form of A is then used to solve the system of equations AX = B.

Input Parameters

uplo CHARACTER*1. Must be 'U' or 'L'.

п	Indicates whether the upper or lower triangular part of <i>A</i> is stored and how <i>A</i> is factored: If $uplo = 'U'$, the array <i>a</i> stores the upper triangular part of the matrix <i>A</i> , and <i>A</i> is factored as $U^H U$. If $uplo = 'L'$, the array <i>a</i> stores the lower triangular part of the matrix <i>A</i> ; <i>A</i> is factored as LL^H . INTEGER. The order of matrix <i>A</i> ($n \ge 0$).
nrhs	INTEGER . The number of right-hand sides; the number of columns in <i>B</i> (<i>nrhs</i> \ge 0).
ap, b	REAL for sppsv DOUBLE PRECISION for dppsv COMPLEX for cppsv DOUBLE COMPLEX for zppsv. Arrays: $ap(*)$, $b(ldb, *)$. The array ap contains either the upper or the lower triangular part of the matrix A (as specified by $uplo$) in <i>packed storage</i> (see <u>Matrix Storage Schemes</u>). The dimension of ap must be at least max $(1,n(n+1)/2)$. The array b contains the matrix B whose columns are the right-hand sides for the systems of equations. The second dimension of b must be at least max $(1,nrhs)$.
ldb	INTEGER . The first dimension of b ; $1db \ge max(1, n)$.
Output Parame	eters
ap	If $info=0$, the upper or lower triangular part of A in packed storage is overwritten by the Cholesky factor U or L, as specified by uplo.
b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER. If $info=0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, the leading minor of order <i>i</i> (and hence the matrix <i>A</i> itself) is not positive definite, so the factorization could not be completed, and the solution has not been computed.

?ppsvx

Uses the Cholesky factorization to compute the solution to the system of linear equations with a symmetric (Hermitian) positive definite packed matrix A, and provides error bounds on the solution.

Discussion

This routine uses the Cholesky factorization $A = U^H U$ or $A = LL^H$ to compute the solution to a real or complex system of linear equations AX = B, where A is a *n*-by-*n* symmetric or Hermitian positive definite matrix stored in packed format, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

Error bounds on the solution and a condition estimate are also provided.

The routine **?ppsvx** performs the following steps:

1. If *fact* = 'E', real scaling factors *s* are computed to equilibrate the system:

 $\operatorname{diag}(s) * A * \operatorname{diag}(s) * \operatorname{diag}(s)^{-1} * X = \operatorname{diag}(s) * B$

Whether or not the system will be equilibrated depends on the scaling of the matrix *A*, but if equilibration is used, *A* is overwritten by diag(s) * A * diag(s) and *B* by diag(s) * B.

2. If $fact = |\mathbf{N}|$ or $|\mathbf{E}|$, the Cholesky decomposition is used to factor the matrix A (after equilibration if $fact = |\mathbf{E}|$) as

 $\begin{aligned} A &= U^H U, \text{ if } uplo = `U', \text{ or} \\ A &= L L^H, \text{ if } uplo = `L', \end{aligned}$

where U is an upper triangular matrix and L is a lower triangular matrix.

3. If the leading *i*-by-*i* principal minor is not positive definite, then the routine returns with info = i. Otherwise, the factored form of A is used to estimate the condition number of the matrix A. If the reciprocal of the condition number is less than machine precision, info = n + 1 is returned as a warning, but the routine still goes on to solve for X and compute error bounds as described below.

4. The system of equations is solved for *X* using the factored form of *A*.

5. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

6. If equilibration was used, the matrix X is premultiplied by diag(s) so that it solves the original system before equilibration.

fact	CHARACTER*1. Must be 'F', 'N', or 'E'.
	Specifies whether or not the factored form of the matrix <i>A</i> is supplied on entry, and if not, whether the matrix <i>A</i> should be equilibrated before it is factored.
	If $fact = 'F'$: on entry, afp contains the factored form of A. If $equed = 'Y'$, the matrix A has been equilibrated with scaling factors given by s . ap and afp will not be modified.
	If $fact = 'N'$, the matrix A will be copied to afp and factored. If $fact = 'E'$, the matrix A will be equilibrated if necessary, then copied to afp and factored.
uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether the upper or lower triangular part of A is stored and how A is factored: If $uplo = 'U'$, the array ap stores the upper triangular part of the matrix A, and A is factored as $U^H U$. If $uplo = 'L'$, the array ap stores the lower triangular part of the matrix A; A is factored as LL^H .

п	INTEGER. The order of matrix A ($n \ge 0$).
nrhs	INTEGER. The number of right-hand sides; the number of columns in B (<i>nrhs</i> \ge 0).
ap,afp,b,wor	<pre>k REAL for sppsvx DOUBLE PRECISION for dppsvx COMPLEX for cppsvx DOUBLE COMPLEX for zppsvx. Arrays: ap(*), afp(*), b(ldb,*), work (*).</pre>
	The array <i>ap</i> contains the upper or lower triangle of the original symmetric/Hermitian matrix A in <i>packed</i> storage (see Matrix Storage Schemes). In case when $fact = 'F'$ and $equed = 'Y'$, <i>ap</i> must contain the equilibrated matrix diag(<i>s</i>)* <i>A</i> *diag(<i>s</i>). The array <i>afp</i> is an input argument if <i>fact</i> = 'F' and contains the triangular factor <i>U</i> or <i>L</i> from the Cholesky factorization of <i>A</i> in the same storage format as <i>A</i> . If <i>equed</i> is not 'N', then <i>afp</i> is the factored form of the equilibrated matrix <i>A</i> . The array <i>b</i> contains the matrix <i>B</i> whose columns are the right-hand sides for the systems of equations. <i>work</i> (*) is a workspace array. The dimension of arrays <i>ap</i> and <i>afp</i> must be at least max(1, <i>n</i> (<i>n</i> +1)/2); the second dimension of <i>work</i> must be at least max(1, 3* <i>n</i>) for real flavors and max(1, 2* <i>n</i>) for complex flavors.
ldb	INTEGER . The first dimension of <i>b</i> ; $1db \ge max(1, n)$.
equed	CHARACTER*1. Must be 'N' or 'Y'. equed is an input argument if $fact = 'F'$. It specifies the form of equilibration that was done: If equed = 'N', no equilibration was done (always true if $fact = 'N'$); If equed = 'Y', equilibration was done and A has been replaced by diag(s)*A*diag(s).

S	REAL for single precision flavors;
	DOUBLE PRECISION for double precision flavors.
	Array, DIMENSION (n).
	The array s contains the scale factors for A . This array
	is an input argument if <i>fact</i> = 'F' only; otherwise it is an
	output argument.
	If $equed = 'N'$, s is not accessed.
	If $fact = 'F'$ and $equed = 'Y'$, each element of s must
	be positive.
ldx	INTEGER. The first dimension of the output array \mathbf{x} ;
	$ldx \ge max(1, n).$
iwork	INTEGER.
	Workspace array, DIMENSION at least max(1, <i>n</i>); used
	in real flavors only.
rwork	REAL for cppsvx;
	DOUBLE PRECISION for zppsvx.
	Workspace array, DIMENSION at least $max(1, n)$; used
	in complex flavors only.

Output Parameters

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REAL for sppsvx DOUBLE PRECISION for dppsvx COMPLEX for cppsvx DOUBLE COMPLEX for zppsvx. Array, DIMENSION (*ldx*,*).

If info = 0 or info = n+1, the array x contains the solution matrix X to the *original* system of equations. Note that if *equed* = 'Y', A and B are modified on exit, and the solution to the equilibrated system is diag(s)⁻¹*X. The second dimension of x must be at least max(1,nrhs). Array *ap* is not modified on exit if *fact* = 'F' or 'N', or if *fact* = 'E' and *equed* = 'N'.

If fact = 'E' and equed = 'Y', A is overwritten by diag(s)*A*diag(s)

afp	If $fact = 'N'$ or 'E', then afp is an output argument and on exit returns the triangular factor U or L from the Cholesky factorization $A=U^{H}U$ or $A=LL^{H}$ of the original matrix $A(if fact = 'N')$, or of the equilibrated matrix A (if $fact = 'E'$). See the description of ap for the form of the equilibrated matrix.
b	Overwritten by $diag(s) * B$, if $equed = 'Y'$; not changed if $equed = 'N'$.
S	This array is an output argument if $fact \neq 'F'$. See the description of <i>s</i> in <i>Input Arguments</i> section.
rcond	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. An estimate of the reciprocal condition number of the matrix <i>A</i> after equilibration (if done). If <i>rcond</i> is less than the machine precision (in particular, if <i>rcond</i> = 0), the matrix is singular to working precision. This condition is indicated by a return code of <i>info</i> > 0.
ferr, berr	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the component-wise forward and relative backward errors, respectively, for each solution vector.
equed	If $fact \neq 'F'$, then <i>equed</i> is an output argument. It specifies the form of equilibration that was done (see the description of <i>equed</i> in <i>Input Arguments</i> section).
info	INTEGER. If $info=0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, and $i \leq n$, the leading minor of order <i>i</i> (and hence the matrix <i>A</i> itself) is not positive definite, so the factorization could not be completed, and the solution and error bounds could not be computed; rcond = 0 is returned. If $info = i$, and $i = n + 1$, then <i>U</i> is nonsingular, but rcond is less than machine precision, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of $rcond$
	would suggest.

?pbsv

Computes the solution to the system of linear equations with a symmetric or Hermitian positive definite band matrix A and multiple right-hand sides.

call	spbsv	(uplo,	n,	kd,	nrhs,	ab,	ldab,	b,	ldb,	info)
call	dpbsv	(uplo,	n,	kd,	nrhs,	ab,	ldab,	b,	ldb,	info)
call	cpbsv	(uplo,	n,	kd,	nrhs,	ab,	ldab,	b,	ldb,	info)
call	zpbsv	(uplo,	n,	kd,	nrhs,	ab,	ldab,	b,	ldb,	info)

Discussion

This routine solves for *X* the real or complex system of linear equations AX = B, where A is an *n*-by-*n* symmetric/Hermitian positive definite band matrix, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

The Cholesky decomposition is used to factor A as $A = U^{H}U$ if uplo = U'

or $A = LL^H$ if uplo = 'L', where U is an upper triangular band matrix and L is a lower triangular band matrix, with the same number of superdiagonals or subdiagonals as A. The factored form of A is then used to solve the system of equations AX = B.

Input Parameters

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether the upper or lower triangular part of A
	is stored in the array <i>ab</i> , and how A is factored:
	If $uplo = 'U'$, the array <i>ab</i> stores the upper triangular
	part of the matrix A, and A is factored as $U^{H}U$.
	If $uplo = 'L'$, the array <i>ab</i> stores the lower triangular
	part of the matrix A; A is factored as LL^{H} .
п	INTEGER. The order of matrix $A (n \ge 0)$.

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kd	INTEGER. The number of superdiagonals of the matrix A if $uplo = 'U'$, or the number of subdiagonals if $uplo = 'L'$ ($kd \ge 0$).
nrhs	INTEGER. The number of right-hand sides; the number of columns in <i>B</i> (<i>nrhs</i> \ge 0).
ab, b	REAL for spbsv
	DOUBLE PRECISION for dpbsv
	COMPLEX for cpbsv
	DOUBLE COMPLEX for zpbsv.
	Arrays: $ab(1dab, *), b(1db, *).$
	The array <i>ab</i> contains either the upper or the lower
	triangular part of the matrix A (as specified by uplo) in
	band storage (see Matrix Storage Schemes).
	The second dimension of ab must be at least max $(1, n)$.
	The array <i>b</i> contains the matrix <i>B</i> whose columns are
	the right-hand sides for the systems of equations.
	The second dimension of <i>b</i> must be at least
	$\max(1, nrhs).$
ldab	INTEGER. The first dimension of the array <i>ab</i> .
	$(1dab \ge kd + 1)$
ldb	INTEGER. The first dimension of b ; $1db \ge max(1, n)$.
Output Parame	ters
ab	The upper or lower triangular part of <i>A</i> (in band storage)
	is overwritten by the Cholesky factor U or L , as
	specified by <u>uplo</u> , in the same storage format as A.

b	
info	

INTEGER. If *info*=0, the execution is successful. If *info* = -i, the *i*th parameter had an illegal value. If *info* = i, the leading minor of order i (and hence the matrix A itself) is not positive definite, so the factorization could not be completed, and the solution has not been computed.

Overwritten by the solution matrix *X*.

?pbsvx

Uses the Cholesky factorization to compute the solution to the system of linear equations with a symmetric (Hermitian) positive definite band matrix A, and provides error bounds on the solution.

Discussion

This routine uses the Cholesky factorization $A = U^H U$ or $A = LL^H$ to compute the solution to a real or complex system of linear equations AX = B, where A is a *n*-by-*n* symmetric or Hermitian positive definite band matrix, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

Error bounds on the solution and a condition estimate are also provided.

The routine **?pbsvx** performs the following steps:

1. If *fact* = 'E', real scaling factors *s* are computed to equilibrate the system:

 $\operatorname{diag}(s) * A * \operatorname{diag}(s) * \operatorname{diag}(s)^{-1} * X = \operatorname{diag}(s) * B$

Whether or not the system will be equilibrated depends on the scaling of the matrix *A*, but if equilibration is used, *A* is overwritten by diag(s)*A*diag(s) and *B* by diag(s)*B.

2. If fact = 'N' or 'E', the Cholesky decomposition is used to factor the matrix A (after equilibration if fact = 'E') as

 $\begin{aligned} A &= U^H U, \text{ if } uplo = `U', \text{ or} \\ A &= L L^H, \text{ if } uplo = `L', \end{aligned}$

where U is an upper triangular band matrix and L is a lower triangular band matrix.

3. If the leading *i*-by-*i* principal minor is not positive definite, then the routine returns with *info* = *i*. Otherwise, the factored form of *A* is used to estimate the condition number of the matrix *A*. If the reciprocal of the condition number is less than machine precision, *info* = n + 1 is returned as a warning, but the routine still goes on to solve for *X* and compute error bounds as described below.

4. The system of equations is solved for *X* using the factored form of *A*.

5. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

6. If equilibration was used, the matrix X is premultiplied by diag(s) so that it solves the original system before equilibration.

fact	CHARACTER*1. Must be 'F', 'N', or 'E'.
	Specifies whether or not the factored form of the matrix <i>A</i> is supplied on entry, and if not, whether the matrix <i>A</i> should be equilibrated before it is factored.
	If <i>fact</i> = 'F': on entry, <i>afb</i> contains the factored form of A. If <i>equed</i> = 'Y', the matrix A has been equilibrated with scaling factors given by <i>s</i> . <i>ab</i> and <i>afb</i> will not be modified.
	If $fact = 'N'$, the matrix A will be copied to afb and factored. If $fact = 'E'$, the matrix A will be equilibrated if
	necessary, then copied to <i>afb</i> and factored.
uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether the upper or lower triangular part of A is stored and how A is factored:

n kd	If $uplo = 'U'$, the array <i>ab</i> stores the upper triangular part of the matrix A, and A is factored as $U^H U$. If $uplo = 'L'$, the array <i>ab</i> stores the lower triangular part of the matrix A; A is factored as LL^H . INTEGER. The order of matrix A $(n \ge 0)$. INTEGER. The number of super-diagonals or sub-diagonals in the matrix A $(kd \ge 0)$.
nrhs	INTEGER. The number of right-hand sides; the number of columns in <i>B</i> (<i>nrhs</i> \ge 0).
ab,afb,b,work	REAL for spbsvx DOUBLE PRECISION for dpbsvx COMPLEX for cpbsvx DOUBLE COMPLEX for zpbsvx. Arrays: $ab(ldab,*)$, $afb(ldab,*)$, $b(ldb,*)$, work(*). The array ab contains the upper or lower triangle of the matrix A in band storage (see <u>Matrix Storage Schemes</u>). If $fact = 'F'$ and $equed = 'Y'$, then ab must contain the equilibrated matrix $diag(s)*A*diag(s)$. The second dimension of ab must be at least max(1, n). The array afb is an input argument if $fact = 'F'$. It contains the triangular factor U or L from the Cholesky factorization of the band matrix A in the same storage format as A . If $equed = 'Y'$, then afb is the factored form of the equilibrated matrix A . The second dimension of afb must be at least max(1, n).
	The array b contains the matrix B whose columns are the right-hand sides for the systems of equations. The second dimension of b must be at least max $(1,nrhs)$.
	<pre>work(*) is a workspace array. The dimension of work must be at least $\max(1,3*n)$ for real flavors, and at least $\max(1,2*n)$ for complex flavors.</pre>
ldab	INTEGER. The first dimension of <i>ab</i> ; $1dab \ge kd+1$.
ldafb	INTEGER. The first dimension of <i>afb</i> ; $ldafb \ge kd+1$.

ldb	INTEGER. The first dimension of b; $1db \ge max(1, n)$.
equed	CHARACTER*1. Must be 'N' or 'Y'. equed is an input argument if fact = 'F'. It specifies the form of equilibration that was done: If equed = 'N', no equilibration was done (always true if fact = 'N'); If equed = 'Y', equilibration was done and A has been replaced by diag(s)*A*diag(s).
5	REAL for single precision flavors; DOUBLE PRECISION for double precision flavors. Array, DIMENSION (<i>n</i>). The array <i>s</i> contains the scale factors for <i>A</i> . This array is an input argument if <i>fact</i> = 'F' only; otherwise it is an output argument. If <i>equed</i> = 'N', <i>s</i> is not accessed. If <i>fact</i> = 'F' and <i>equed</i> = 'Y', each element of <i>s</i> must be positive.
ldx	INTEGER. The first dimension of the output array x ; $ldx \ge max(1, n)$.
iwork	INTEGER . Workspace array, DIMENSION at least max(1, <i>n</i>); used in real flavors only.
rwork	REAL for cpbsvx; DOUBLE PRECISION for zpbsvx. Workspace array, DIMENSION at least max(1, n); used in complex flavors only.

X	REAL for spbsvx
	DOUBLE PRECISION for dpbsvx
	COMPLEX for cpbsvx
	DOUBLE COMPLEX for zpbsvx.
	Array, DIMENSION (ldx, *).

	If $info = 0$ or $info = n+1$, the array x contains the solution matrix X to the <i>original</i> system of equations. Note that if <i>equed</i> = 'Y', A and B are modified on exit, and the solution to the equilibrated system is $diag(s)^{-1} * X$. The second dimension of x must be at least $max(1,nrhs)$.
ab	On exit, if $fact = 'E'$ and $equed = 'Y'$, A is overwritten by diag(s)*A*diag(s)
afb	If $fact = 'N'$ or 'E', then <i>afb</i> is an output argument and on exit returns the triangular factor U or L from the Cholesky factorization $A=U^{H}U$ or $A=LL^{H}$ of the original matrix $A(if fact = 'N')$, or of the equilibrated matrix A (if fact = 'E'). See the description of <i>ab</i> for the form of the equilibrated matrix.
b	Overwritten by diag(s)* B , if equed = 'Y'; not changed if equed = 'N'.
S	This array is an output argument if $fact \neq 'F'$. See the description of <i>s</i> in <i>Input Arguments</i> section.
rcond	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. An estimate of the reciprocal condition number of the matrix <i>A</i> after equilibration (if done). If <i>rcond</i> is less than the machine precision (in particular, if <i>rcond</i> = 0), the matrix is singular to working precision. This condition is indicated by a return code of <i>info</i> > 0.
ferr, berr	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the component-wise forward and relative backward errors, respectively, for each solution vector.
equed	If $fact \neq 'F'$, then equed is an output argument. It specifies the form of equilibration that was done (see the description of equed in <i>Input Arguments</i> section).

INTEGER. If info=0, the execution is successful. If info = -i, the *i*th parameter had an illegal value. If info = i, and $i \le n$, the leading minor of order *i* (and hence the matrix *A* itself) is not positive definite, so the factorization could not be completed, and the solution and error bounds could not be computed; *rcond* = 0 is returned. If *info* = *i*, and *i* = *n* +1, then *U* is nonsingular, but *rcond* is less than machine precision, meaning that the

matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of *rcond* would suggest.

?ptsv

Computes the solution to the system of linear equations with a symmetric or Hermitian positive definite tridiagonal matrix A and multiple right-hand sides.

info

call sptsv (n, nrhs, d, e, b, ldb, info)
call dptsv (n, nrhs, d, e, b, ldb, info)
call cptsv (n, nrhs, d, e, b, ldb, info)
call zptsv (n, nrhs, d, e, b, ldb, info)

Discussion

This routine solves for *X* the real or complex system of linear equations AX = B, where A is an *n*-by-*n* symmetric/Hermitian positive definite tridiagonal matrix, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

A is factored as $A = L D L^{H}$, and the factored form of A is then used to solve the system of equations AX = B.

Input Parameters

п	INTEGER. The order of matrix $A (n \ge 0)$.
nrhs	INTEGER . The number of right-hand sides; the number
	of columns in B (<i>nrhs</i> \geq 0).
d	REAL for single precision flavors.
	DOUBLE PRECISION for double precision flavors.
	Array, dimension at least $max(1, n)$. Contains the
	diagonal elements of the tridiagonal matrix A.
e, b	REAL for sptsv
	DOUBLE PRECISION for dptsv
	COMPLEX for cptsv
	DOUBLE COMPLEX for zptsv.
	Arrays: $e(n-1)$, $b(ldb, *)$.
	The array e contains the $(n - 1)$ subdiagonal elements
	of A.
	The array b contains the matrix B whose columns are
	the right-hand sides for the systems of equations.
	The second dimension of b must be at least
	max(1, <i>nrhs</i>).
ldb	INTEGER. The first dimension of b ; $ldb \ge max(1, n)$.

d	Overwritten by the <i>n</i> diagonal elements of the diagonal matrix <i>D</i> from the LDL^{H} factorization of A.
е	Overwritten by the $(n - 1)$ subdiagonal elements of the unit bidiagonal factor <i>L</i> from the factorization of A.
b	Overwritten by the solution matrix <i>X</i> .
info	INTEGER. If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$, the <i>i</i> th parameter had an illegal value. If <i>info</i> = <i>i</i> , the leading minor of order <i>i</i> (and hence the matrix <i>A</i> itself) is not positive definite, and the solution has not been computed. The factorization has not been completed unless <i>i</i> = <i>n</i> .

?ptsvx

Uses the factorization $A=LDL^{H}$ to compute the solution to the system of linear equations with a symmetric (Hermitian) positive definite tridiagonal matrix A, and provides error bounds on the solution.

Discussion

This routine uses the Cholesky factorization $A=L D L^H$ to compute the solution to a real or complex system of linear equations AX=B, where A is a *n*-by-*n* symmetric or Hermitian positive definite tridiagonal matrix, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

Error bounds on the solution and a condition estimate are also provided.

The routine **?ptsvx** performs the following steps:

1. If *fact* = 'N', the matrix A is factored as $A = L D L^{H}$, where L is a unit lower bidiagonal matrix and D is diagonal. The factorization can also be regarded as having the form $A = U^{H} D U$.

2. If the leading *i*-by-*i* principal minor is not positive definite, then the routine returns with info = i. Otherwise, the factored form of A is used to estimate the condition number of the matrix A. If the reciprocal of the condition number is less than machine precision, info = n + 1 is returned as a warning, but the routine still goes on to solve for X and compute error bounds as described below.

3. The system of equations is solved for *X* using the factored form of *A*.

4. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

fact	CHARACTER*1. Must be 'F' or 'N'.
	Specifies whether or not the factored form of the matrix <i>A</i> is supplied on entry.
	If <i>fact</i> = 'F': on entry, <i>df</i> and <i>ef</i> contain the factored form of <i>A</i> . Arrays <i>d</i> , <i>e</i> , <i>df</i> , and <i>ef</i> will not be modified.
	If $fact = 'N'$, the matrix A will be copied to df and ef and factored.
п	INTEGER. The order of matrix $A (n \ge 0)$.
nrhs	INTEGER. The number of right-hand sides; the number of columns in <i>B</i> (<i>nrhs</i> \ge 0).
d,df,rwork	REAL for single precision flavors DOUBLE PRECISION for double precision flavors Arrays: $d(n)$, $df(n)$, $rwork(n)$. The array d contains the n diagonal elements of the tridiagonal matrix A. The array df is an input argument if $fact = 'F'$ and on entry contains the n diagonal elements of the diagonal matrix D from the $L D L^H$ factorization of A. The array <i>rwork</i> is a workspace array used for complex flavors only.
e,ef,b,work	REAL for sptsvx DOUBLE PRECISION for dptsvx COMPLEX for cptsvx DOUBLE COMPLEX for zptsvx. Arrays: $e(n-1)$, $ef(n-1)$, $b(ldb,*)$, $work(*)$. The array e contains the $(n-1)$ subdiagonal elements of the tridiagonal matrix A .

	The array ef is an input argument if $fact = 'F'$ and
	on entry contains the $(n - 1)$ subdiagonal elements of
	the unit bidiagonal factor L from the $L D L^{H}$
	factorization of A.
	The array b contains the matrix B whose columns are
	the right-hand sides for the systems of equations.
	The array <i>work</i> is a workspace array. The dimension of
	work must be at least 2*n for real flavors, and at least
	<i>n</i> for complex flavors.
ldb	INTEGER. The leading dimension of <i>b</i> ; $1db \ge max(1, n)$.
ldx	INTEGER . The leading dimension of x ; $ldx \ge max(1, n)$.

x	REAL for sptsvx DOUBLE PRECISION for dptsvx COMPLEX for cptsvx DOUBLE COMPLEX for zptsvx. Array, DIMENSION (<i>ldx</i> ,*).
	If $info = 0$ or $info = n+1$, the array x contains the solution matrix X to the system of equations. The second dimension of x must be at least max $(1,nrhs)$.
df, ef	These arrays are output arguments if $fact = 'N'$. See the description of df , ef in <i>Input Arguments</i> section.
rcond	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. An estimate of the reciprocal condition number of the matrix <i>A</i> after equilibration (if done). If <i>rcond</i> is less than the machine precision (in particular, if <i>rcond</i> = 0), the matrix is singular to working precision. This condition is indicated by a return code of <i>info</i> > 0.
ferr, berr	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the component-wise forward and relative backward errors, respectively, for each solution vector.

info

INTEGER. If *info*=0, the execution is successful. If *info* = -i, the *i*th parameter had an illegal value. If *info* = i, and $i \leq n$, the leading minor of order i (and hence the matrix A itself) is not positive definite, so the factorization could not be completed, and the solution and error bounds could not be computed; *rcond* = 0 is returned.

If info = i, and i = n + 1, then U is nonsingular, but *rcond* is less than machine precision, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of *rcond* would suggest.

?sysv

Computes the solution to the system of linear equations with a real or complex symmetric matrix A and multiple right-hand sides.

call ssysv (uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info) call dsysv (uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info) call csysv (uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info) call zsysv (uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info)

Discussion

This routine solves for X the real or complex system of linear equations AX = B, where A is an *n*-by-*n* symmetric matrix, the columns of matrix *B* are individual right-hand sides, and the columns of X are the corresponding solutions.

The diagonal pivoting method is used to factor A as $A = U D U^T$ or $A = L D L^T$, where U (or L) is a product of permutation and unit upper (lower) triangular matrices, and D is symmetric and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

The factored form of *A* is then used to solve the system of equations AX = B.

uplo n	CHARACTER*1. Must be 'U' or 'L'. Indicates whether the upper or lower triangular part of <i>A</i> is stored and how <i>A</i> is factored: If $uplo = 'U'$, the array <i>a</i> stores the upper triangular part of the matrix <i>A</i> , and <i>A</i> is factored as UDU^{T} . If $uplo = 'L'$, the array <i>a</i> stores the lower triangular part of the matrix <i>A</i> ; <i>A</i> is factored as LDL^{T} . INTEGER. The order of matrix <i>A</i> ($n \ge 0$).
nrhs	INTEGER . The number of right-hand sides; the number of columns in B (<i>nrhs</i> \ge 0).
a, b, work	REAL for ssysv DOUBLE PRECISION for dsysv COMPLEX for csysv DOUBLE COMPLEX for zsysv. Arrays: $a(lda, *)$, $b(ldb, *)$, work(lwork). The array a contains either the upper or the lower triangular part of the symmetric matrix A (see uplo). The second dimension of a must be at least max(1, n). The array b contains the matrix B whose columns are the right-hand sides for the systems of equations. The second dimension of b must be at least max(1,nrhs). work(lwork) is a workspace array.
lda	INTEGER . The first dimension of a ; $1da \ge max(1, n)$.
ldb lwork	INTEGER. The first dimension of b; $1db \ge max(1, n)$. INTEGER. The size of the work array ($1work \ge 1$) See Application notes for the suggested value of $1work$.

a	If $info = 0$, a is overwritten by the block-diagonal matrix D and the multipliers used to obtain the factor U (or L) from the factorization of A as computed by <u>?sytrf</u> .
b	If $info = 0$, b is overwritten by the solution matrix X.
ipiv	INTEGER.
	Array, DIMENSION at least $max(1,n)$.
	Contains details of the interchanges and the block
	structure of <i>D</i> , as determined by <u>?sytrf</u> .
	If $ipiv(i) = k > 0$, then d_{ii} is a 1-by-1 diagonal block,
	and the <i>i</i> th row and column of A was interchanged with
	the <i>k</i> th row and column.
	If $uplo = 'U'$ and $ipiv(i) = ipiv(i-1) = -m < 0$,
	then D has a 2-by-2 block in rows/columns i and $i-1$,
	and $(i-1)$ th row and column of A was interchanged
	with the <i>m</i> th row and column.
	If $uplo = 'L'$ and $ipiv(i) = ipiv(i+1) = -m < 0$,
	then D has a 2-by-2 block in rows/columns i and $i+1$,
	and $(i+1)$ th row and column of A was interchanged
	with the <i>m</i> th row and column.
work(1)	If <i>info</i> =0, on exit <i>work</i> (1) contains the minimum
	value of <i>lwork</i> required for optimum performance. Use
	this <i>lwork</i> for subsequent runs.
info	INTEGER . If <i>info</i> =0, the execution is successful.
	If $info = -i$, the <i>i</i> th parameter had an illegal value.
	If $info = i$, d_{ii} is 0. The factorization has been
	completed, but D is exactly singular, so the solution
	could not be computed.

Application Notes

For better performance, try using lwork = n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use *lwork* =-1 for the first run. In this case, a workspace query is assumed; the routine only calculates the optimal size of the *work* array, returns this value as the first

entry *work*(1) of the *work* array, and no error message related to *lwork* is issued by XERBLA. On exit, examine *work*(1) and use this value for subsequent runs.

?sysvx

Uses the diagonal pivoting factorization to compute the solution to the system of linear equations with a real or complex symmetric matrix A, and provides error bounds on the solution.

Discussion

This routine uses the diagonal pivoting factorization to compute the solution to a real or complex system of linear equations AX = B, where A is a *n*-by-*n* symmetric matrix, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

Error bounds on the solution and a condition estimate are also provided.

The routine **?sysvx** performs the following steps:

1. If fact = 'N', the diagonal pivoting method is used to factor the matrix A. The form of the factorization is $A = UD U^T$ or $A = LD L^T$, where U (or L) is a product of permutation and unit upper (lower) triangular matrices, and D is symmetric and block diagonal with 1-by-1 and 2-by-2 diagonal blocks. 2. If some $d_{i,i} = 0$, so that *D* is exactly singular, then the routine returns with *info* = i. Otherwise, the factored form of *A* is used to estimate the condition number of the matrix *A*. If the reciprocal of the condition number is less than machine precision, *info* = n + 1 is returned as a warning, but the routine still goes on to solve for *X* and compute error bounds as described below.

3. The system of equations is solved for *X* using the factored form of *A*.

4. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

fact	CHARACTER*1. Must be 'F' or 'N'.
	Specifies whether or not the factored form of the matrix <i>A</i> has been supplied on entry.
	If <i>fact</i> = 'F': on entry, <i>af</i> and <i>ipiv</i> contain the factored form of <i>A</i> . Arrays <i>a</i> , <i>af</i> , and <i>ipiv</i> will not be modified.
	If $fact = 'N'$, the matrix A will be copied to af and factored.
uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether the upper or lower triangular part of A is stored and how A is factored:
	If $uplo = 'U'$, the array <i>a</i> stores the upper triangular part of the symmetric matrix <i>A</i> , and <i>A</i> is factored as UDU^{T} .
	If $uplo = 'L'$, the array <i>a</i> stores the lower triangular part of the symmetric matrix <i>A</i> ; <i>A</i> is factored as LDL^{T} .
n	INTEGER . The order of matrix $A (n \ge 0)$.
nrhs	INTEGER. The number of right-hand sides; the number of columns in <i>B</i> (<i>nrhs</i> \ge 0).
a,af,b,work	REAL for ssysvx DOUBLE PRECISION for dsysvx COMPLEX for csysvx

	DOUBLE COMPLEX for zsysvx. Arrays: a(lda,*), af(ldaf,*), b(ldb,*),
	work(*).
	The array <i>a</i> contains either the upper or the lower triangular part of the symmetric matrix A (see <i>uplo</i>). The second dimension of <i>a</i> must be at least max $(1,n)$.
	The array <i>af</i> is an input argument if <i>fact</i> = 'F'. It contains he block diagonal matrix <i>D</i> and the multipliers used to obtain the factor <i>U</i> or <i>L</i> from the factorization $A = UDU^T$ or $A = LDL^T$ as computed by <u>?sytrf</u> . The second dimension of <i>af</i> must be at least max(1, <i>n</i>).
	The array b contains the matrix B whose columns are the right-hand sides for the systems of equations. The second dimension of b must be at least max(1, <i>nrhs</i>).
	<pre>work(*) is a workspace array of dimension (lwork).</pre>
lda	INTEGER. The first dimension of a ; $1da \ge max(1, n)$.
ldaf	INTEGER. The first dimension of <i>af</i> ; $ldaf \ge max(1, n)$.
ldb	INTEGER. The first dimension of <i>b</i> ; $ldb \ge max(1, n)$.
ipiv	INTEGER.
	Array, DIMENSION at least $\max(1, n)$.
	The array <i>ipiv</i> is an input argument if $fact = 'F'$.
	It contains details of the interchanges and the block structure of <i>D</i> , as determined by <u>?sytrf</u> .
	If $ipiv(i) = k > 0$, then d_{ii} is a 1-by-1 diagonal block,
	and the <i>i</i> th row and column of A was interchanged with the <i>k</i> th row and column.
	If $uplo = 'U'$ and $ipiv(i) = ipiv(i-1) = -m < 0$, then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> -1,
	and $(i-1)$ th row and column of A was interchanged
	with the <i>m</i> th row and column.
	If $uplo = 'L'$ and $ipiv(i) = ipiv(i+1) = -m < 0$,
	then D has a 2-by-2 block in rows/columns i and $i+1$,
	and $(i+1)$ th row and column of A was interchanged
	with the <i>m</i> th row and column.

ldx	INTEGER. The leading dimension of the output array x ; $ldx \ge max(1, n)$.
	$IUX \geq IIIdX(1, II).$
lwork	INTEGER . The size of the <i>work</i> array.
	See Application notes for the suggested value of <i>lwork</i> .
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, n)$; used
	in real flavors only.
rwork	REAL for csysvx;
	DOUBLE PRECISION for zsysvx.
	Workspace array, DIMENSION at least max(1, <i>n</i>); used in complex flavors only.

x	REAL for ssysvx DOUBLE PRECISION for dsysvx COMPLEX for csysvx DOUBLE COMPLEX for zsysvx. Array, DIMENSION (<i>ldx</i> ,*).
	If $info = 0$ or $info = n+1$, the array x contains the solution matrix X to the system of equations. The second dimension of x must be at least max $(1,nrhs)$.
af, ipiv	These arrays are output arguments if $fact = 'N'$. See the description of <i>af</i> , <i>ipiv</i> in <i>Input Arguments</i> section.
rcond	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. An estimate of the reciprocal condition number of the matrix <i>A</i> . If <i>rcond</i> is less than the machine precision (in particular, if <i>rcond</i> = 0), the matrix is singular to working precision. This condition is indicated by a return code of <i>info</i> > 0.
ferr, berr	REAL for single precision flavors. DOUBLE PRECISION for double precision flavors. Arrays, DIMENSION at least max(1, <i>nrhs</i>). Contain the component-wise forward and relative backward errors, respectively, for each solution vector.

work(1)	If <i>info</i> =0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info=0$, the execution is successful. If $info = -i$, the <i>i</i> th parameter had an illegal value. If $info = i$, and $i \leq n$, then d_{ii} is exactly zero. The factorization has been completed, but the block diagonal matrix <i>D</i> is exactly singular, so the solution and error bounds could not be computed; <i>rcond</i> = 0 is returned. If $info = i$, and $i = n + 1$, then <i>D</i> is nonsingular, but <i>rcond</i> is less than machine precision, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of <i>rcond</i> would suggest.
	~~~

### **Application Notes**

For real flavors, *lwork* must be at least 3*n, and for complex flavors at least 2*n. For better performance, try using *lwork* = n*blocksize, where *blocksize* is the optimal block size for ?sytrf.

If you are in doubt how much workspace to supply, use *lwork* =-1 for the first run. In this case, a workspace query is assumed; the routine only calculates the optimal size of the *work* array, returns this value as the first entry *work(1)* of the *work* array, and no error message related to *lwork* is issued by XERBLA. On exit, examine *work(1)* and use this value for subsequent runs.

## ?hesvx

Uses the diagonal pivoting factorization to compute the solution to the complex system of linear equations with a Hermitian matrix A, and provides error bounds on the solution.

#### Discussion

This routine uses the diagonal pivoting factorization to compute the solution to a complex system of linear equations AX = B, where A is a *n*-by-*n* Hermitian matrix, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

Error bounds on the solution and a condition estimate are also provided.

The routine **?hesvx** performs the following steps:

1. If fact = N', the diagonal pivoting method is used to factor the matrix A. The form of the factorization is  $A = UDU^H$  or  $A = LDL^H$ , where U (or L) is a product of permutation and unit upper (lower) triangular matrices, and D is Hermitian and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

2. If some  $d_{i,i} = 0$ , so that *D* is exactly singular, then the routine returns with info = i. Otherwise, the factored form of *A* is used to estimate the condition number of the matrix *A*. If the reciprocal of the condition number is less than machine precision, info = n + 1 is returned as a warning, but the routine still goes on to solve for *X* and compute error bounds as described below.

3. The system of equations is solved for *X* using the factored form of *A*.

4. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

fact	CHARACTER*1. Must be 'F' or 'N'.
	Specifies whether or not the factored form of the matrix <i>A</i> has been supplied on entry.
	If <i>fact</i> = 'F': on entry, <i>af</i> and <i>ipiv</i> contain the factored form of <i>A</i> . Arrays <i>a</i> , <i>af</i> , and <i>ipiv</i> will not be modified.
	If $fact = 'N'$ , the matrix A will be copied to $af$ and factored.
uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether the upper or lower triangular part of $A$ is stored and how $A$ is factored:
	If $uplo = 'U'$ , the array <i>a</i> stores the upper triangular part of the Hermitian matrix <i>A</i> , and <i>A</i> is factored as $UDU^{H}$ .
n	If $uplo = 'L'$ , the array <i>a</i> stores the lower triangular part of the Hermitian matrix <i>A</i> ; <i>A</i> is factored as $LDL^H$ . INTEGER. The order of matrix <i>A</i> ( $n \ge 0$ ).
nrhs	<b>INTEGER.</b> The number of right-hand sides; the number of columns in <i>B</i> ( <i>nrhs</i> $\ge$ 0).
a,af,b,work	COMPLEX for chesvx DOUBLE COMPLEX for zhesvx. Arrays: a(lda,*), af(ldaf,*), b(ldb,*), work(*).
	The array <i>a</i> contains either the upper or the lower triangular part of the Hermitian matrix <i>A</i> (see <i>uplo</i> ). The second dimension of <i>a</i> must be at least $max(1,n)$ .
	The array <i>af</i> is an input argument if <i>fact</i> = 'F'. It contains he block diagonal matrix <i>D</i> and the multipliers used to obtain the factor <i>U</i> or <i>L</i> from the factorization $A = UDU^H$ or $A = LDL^H$ as computed by <u>?hetrf</u> .
	The second dimension of <i>af</i> must be at least $max(1,n)$ .

	The array $b$ contains the matrix $B$ whose columns are the right-hand sides for the systems of equations. The second dimension of $b$ must be at least max $(1,nrhs)$ .
	<pre>work(*) is a workspace array of dimension (lwork).</pre>
lda	<b>INTEGER</b> . The first dimension of <b>a</b> ; $1da \ge max(1, n)$ .
ldaf	<b>INTEGER.</b> The first dimension of <i>af</i> ; $ldaf \ge max(1, n)$ .
ldb	<b>INTEGER</b> . The first dimension of <i>b</i> ; $1db \ge max(1, n)$ .
ipiv	INTEGER. Array, DIMENSION at least max(1, <i>n</i> ). The array <i>ipiv</i> is an input argument if <i>fact</i> = 'F'. It contains details of the interchanges and the block structure of <i>D</i> , as determined by <u>?hetrf</u> . If <i>ipiv(i)</i> = $k > 0$ , then $d_{ii}$ is a 1-by-1 diagonal block, and the <i>i</i> th row and column of <i>A</i> was interchanged with the <i>k</i> th row and column. If <i>uplo</i> = 'U' and <i>ipiv(i)</i> = <i>ipiv(i-1)</i> = - <i>m</i> < 0, then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> -1, and ( <i>i</i> -1) th row and column. If <i>uplo</i> = 'L' and <i>ipiv(i)</i> = <i>ipiv(i+1)</i> = - <i>m</i> < 0, then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i+1</i> , and ( <i>i+1</i> ) th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column. If <i>uplo</i> = 'L' and <i>ipiv(i)</i> = <i>ipiv(i+1)</i> = - <i>m</i> < 0, then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i+1</i> , and ( <i>i+1</i> ) th row and column. INTEGER The leading dimension of the output array <i>x</i> :
ldx	<b>INTEGER.</b> The leading dimension of the output array $x$ ; $ldx \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array. See <i>Application notes</i> for the suggested value of <i>lwork</i> .
rwork	REAL for chesvx; DOUBLE PRECISION for zhesvx. Workspace array, DIMENSION at least max(1, n).

x

COMPLEX for chesvx DOUBLE COMPLEX for zhesvx. Array, DIMENSION (*ldx*,*).

	If $info = 0$ or $info = n+1$ , the array x contains the solution matrix X to the system of equations. The second dimension of x must be at least max $(1,nrhs)$ .
af, ipiv	These arrays are output arguments if <i>fact</i> = 'N'. See the description of <i>af</i> , <i>ipiv</i> in <i>Input Arguments</i> section.
rcond	REAL for chesvx; DOUBLE PRECISION for zhesvx. An estimate of the reciprocal condition number of the matrix <i>A</i> . If <i>rcond</i> is less than the machine precision (in particular, if <i>rcond</i> = 0), the matrix is singular to working precision. This condition is indicated by a return code of <i>info</i> > 0.
ferr, berr work(1)	REAL for chesvx; DOUBLE PRECISION for zhesvx. Arrays, DIMENSION at least max(1, <i>nrhs</i> ). Contain the component-wise forward and relative backward errors, respectively, for each solution vector. If <i>info</i> =0, on exit <i>work</i> (1) contains the minimum
WOIK(I)	value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$ , the <i>i</i> th parameter had an illegal value. If <i>info</i> = $i$ , and $i \leq n$ , then $d_{ii}$ is exactly zero. The factorization has been completed, but the block diagonal matrix $D$ is exactly singular, so the solution and error bounds could not be computed; <i>rcond</i> = 0 is returned. If <i>info</i> = $i$ , and $i = n + 1$ , then $D$ is nonsingular, but <i>rcond</i> is less than machine precision, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of <i>rcond</i> would suggest.

### **Application Notes**

The value of *lwork* must be at least 2*n. For better performance, try using *lwork* = n*blocksize, where *blocksize* is the optimal block size for ?hetrf.

If you are in doubt how much workspace to supply, use *lwork* =-1 for the first run. In this case, a workspace query is assumed; the routine only calculates the optimal size of the *work* array, returns this value as the first entry *work(1)* of the *work* array, and no error message related to *lwork* is issued by XERBLA. On exit, examine *work(1)* and use this value for subsequent runs.

## ?hesv

Computes the solution to the system of linear equations with a Hermitian matrix A and multiple right-hand sides.

call chesv (uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info) call zhesv (uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info)

### **Discussion**

This routine solves for X the real or complex system of linear equations AX = B, where A is an *n*-by-*n* symmetric matrix, the columns of matrix *B* are individual right-hand sides, and the columns of X are the corresponding solutions.

The diagonal pivoting method is used to factor A as  $A = U D U^H$  or  $A = L D L^H$ , where U (or L) is a product of permutation and unit upper (lower) triangular matrices, and D is Hermitian and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

The factored form of *A* is then used to solve the system of equations AX = B.

#### **Input Parameters**

uplo CHARACTER*1. Must be 'U' or 'L'.

n	Indicates whether the upper or lower triangular part of <i>A</i> is stored and how <i>A</i> is factored: If $uplo = 'U'$ , the array <i>a</i> stores the upper triangular part of the matrix <i>A</i> , and <i>A</i> is factored as $UDU^{H}$ . If $uplo = 'L'$ , the array <i>a</i> stores the lower triangular part of the matrix <i>A</i> ; <i>A</i> is factored as $LDL^{H}$ . INTEGER. The order of matrix <i>A</i> ( $n \ge 0$ ).
nrhs	<b>INTEGER.</b> The number of right-hand sides; the number of columns in <i>B</i> ( <i>nrhs</i> $\ge$ 0).
a, b, work	COMPLEX for chesv DOUBLE COMPLEX for zhesv. Arrays: $a(lda, *)$ , $b(ldb, *)$ , $work(lwork)$ . The array <i>a</i> contains either the upper or the lower triangular part of the Hermitian matrix <i>A</i> (see <i>uplo</i> ). The second dimension of <i>a</i> must be at least max(1, <i>n</i> ). The array <i>b</i> contains the matrix <i>B</i> whose columns are the right-hand sides for the systems of equations. The second dimension of <i>b</i> must be at least max(1, <i>nrhs</i> ). <i>work(lwork)</i> is a workspace array.
lda	<b>INTEGER.</b> The first dimension of <b>a</b> ; $1 da \ge max(1, n)$ .
ldb lwork	<b>INTEGER.</b> The first dimension of <i>b</i> ; $ldb \ge max(1, n)$ . <b>INTEGER.</b> The size of the <i>work</i> array ( <i>lwork</i> $\ge 1$ ) See <i>Application notes</i> for the suggested value of <i>lwork</i> .

a	If $info = 0$ , <i>a</i> is overwritten by the block-diagonal matrix <i>D</i> and the multipliers used to obtain the factor <i>U</i> (or <i>L</i> ) from the factorization of <i>A</i> as computed by <u>?hetrf</u> .
b	If $info = 0$ , b is overwritten by the solution matrix X.
ipiv	INTEGER. Array, DIMENSION at least $max(1,n)$ . Contains details of the interchanges and the block structure of $D$ , as determined by <u>?hetrf</u> .

	If $ipiv(i) = k > 0$ , then $d_{ii}$ is a 1-by-1 diagonal block, and the <i>i</i> th row and column of <i>A</i> was interchanged with the <i>k</i> th row and column.
	If $uplo = 'U'$ and $ipiv(i) = ipiv(i-1) = -m < 0$ ,
	then D has a 2-by-2 block in rows/columns $i$ and $i-1$ ,
	and $(i-1)$ th row and column of A was interchanged
	with the <i>m</i> th row and column.
	If $uplo = 'L'$ and $ipiv(i) = ipiv(i+1) = -m < 0$ ,
	then D has a 2-by-2 block in rows/columns $i$ and $i+1$ ,
	and $(i+1)$ th row and column of A was interchanged
	with the <i>m</i> th row and column.
work(1)	If <i>info</i> =0, on exit <i>work</i> (1) contains the minimum
	value of <i>lwork</i> required for optimum performance. Use
	this <i>lwork</i> for subsequent runs.
info	<b>INTEGER</b> . If <i>info</i> =0, the execution is successful.
	If $info = -i$ , the <i>i</i> th parameter had an illegal value.
	If $info = i$ , $d_{ii}$ is 0. The factorization has been
	completed, but $D$ is exactly singular, so the solution
	could not be computed.

### **Application Notes**

For better performance, try using lwork = n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use *lwork* =-1 for the first run. In this case, a workspace query is assumed; the routine only calculates the optimal size of the *work* array, returns this value as the first entry *work(1)* of the *work* array, and no error message related to *lwork* is issued by XERBLA. On exit, examine *work(1)* and use this value for subsequent runs.

# ?spsv

Computes the solution to the system of linear equations with a real or complex symmetric matrix A stored in packed format, and multiple right-hand sides.

> call sspsv (uplo, n, nrhs, ap, ipiv, b, ldb, info) call dspsv (uplo, n, nrhs, ap, ipiv, b, ldb, info) call cspsv (uplo, n, nrhs, ap, ipiv, b, ldb, info) call zspsv (uplo, n, nrhs, ap, ipiv, b, ldb, info)

### **Discussion**

This routine solves for X the real or complex system of linear equations AX = B, where A is an *n*-by-*n* symmetric matrix stored in packed format, the columns of matrix *B* are individual right-hand sides, and the columns of X are the corresponding solutions.

The diagonal pivoting method is used to factor A as  $A = U D U^T$  or  $A = L D L^T$ , where U (or L) is a product of permutation and unit upper (lower) triangular matrices, and D is symmetric and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

The factored form of *A* is then used to solve the system of equations AX = B.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether the upper or lower triangular part of $A$
	is stored and how A is factored:
	If $uplo = 'U'$ , the array $ap$ stores the upper triangular
	part of the matrix A, and A is factored as $UDU^{T}$ .
	If $uplo = 'L'$ , the array $ap$ stores the lower triangular
	part of the matrix A; A is factored as $LDL^{T}$ .
п	<b>INTEGER.</b> The order of matrix $A (n \ge 0)$ .
nrhs	<b>INTEGER.</b> The number of right-hand sides; the number of columns in <i>B</i> ( <i>nrhs</i> $\ge$ 0).

ap, b	REAL for sspsv DOUBLE PRECISION for dspsv COMPLEX for cspsv DOUBLE COMPLEX for zspsv. Arrays: $ap(*)$ , $b(1db, *)$ The dimension of $ap$ must be at least $max(1,n(n+1)/2)$ . The array $ap$ contains the factor $U$ or $L$ , as specified by up1o, in packed storage (see Matrix Storage Schemes). The array $b$ contains the matrix $B$ whose columns are the right-hand sides for the systems of equations. The second dimension of $b$ must be at least
	$\max(1, nrhs)$ .
ldb	<b>INTEGER</b> . The first dimension of <b>b</b> ; $1db \ge max(1, n)$ .
Output Parame	eters
ap	The block-diagonal matrix $D$ and the multipliers used to obtain the factor $U$ (or $L$ ) from the factorization of $A$ as computed by <u>?sptrf</u> , stored as a packed triangular matrix in the same storage format as $A$ .
b	If $info = 0$ , b is overwritten by the solution matrix X.
ipiv	INTEGER. Array, DIMENSION at least max(1, <i>n</i> ). Contains details of the interchanges and the block structure of <i>D</i> , as determined by <u>?sptrf</u> . If $ipiv(i) = k > 0$ , then $d_{ii}$ is a 1-by-1 block, and the <i>i</i> th row and column of <i>A</i> was interchanged with the <i>k</i> th row and column.
	If $uplo = 'U'$ and $ipiv(i) = ipiv(i-1) = -m < 0$ , then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> -1, and ( <i>i</i> -1) th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column.
	If $uplo = 'L'$ and $ipiv(i) = ipiv(i+1) = -m < 0$ , then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> +1, and ( <i>i</i> +1) th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column.

infoINTEGER. If info=0, the execution is successful.If info = -i, the *i*th parameter had an illegal value.If info = i,  $d_{ii}$  is 0. The factorization has been<br/>completed, but D is exactly singular, so the solution<br/>could not be computed.

## ?spsvx

Uses the diagonal pivoting factorization to compute the solution to the system of linear equations with a real or complex symmetric matrix A stored in packed format, and provides error bounds on the solution.

### **Discussion**

This routine uses the diagonal pivoting factorization to compute the solution to a real or complex system of linear equations AX = B, where A is a *n*-by-*n* symmetric matrix stored in packed format, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

Error bounds on the solution and a condition estimate are also provided.

The routine **?spsvx** performs the following steps:

1. If *fact* = 'N', the diagonal pivoting method is used to factor the matrix A. The form of the factorization is  $A = UD U^T$  or  $A = LD L^T$ , where U (or L) is a product of permutation and unit upper (lower) triangular matrices, and D is symmetric and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

2. If some  $d_{i,i} = 0$ , so that *D* is exactly singular, then the routine returns with *info* = i. Otherwise, the factored form of *A* is used to estimate the condition number of the matrix *A*. If the reciprocal of the condition number

is less than machine precision, info = n + 1 is returned as a warning, but the routine still goes on to solve for X and compute error bounds as described below.

3. The system of equations is solved for X using the factored form of A.

4. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

fact	CHARACTER*1. Must be 'F' or 'N'.
	Specifies whether or not the factored form of the matrix <i>A</i> has been supplied on entry.
	If <i>fact</i> = 'F': on entry, <i>afp</i> and <i>ipiv</i> contain the factored form of A. Arrays <i>ap</i> , <i>afp</i> , and <i>ipiv</i> will not be modified.
	If $fact = 'N'$ , the matrix A will be copied to $afp$ and factored.
uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether the upper or lower triangular part of <i>A</i> is stored and how <i>A</i> is factored:
	If $uplo = 'U'$ , the array <i>ap</i> stores the upper triangular part of the symmetric matrix <i>A</i> , and <i>A</i> is factored as $UDU^{T}$ .
	If $uplo = 'L'$ , the array $ap$ stores the lower triangular part of the symmetric matrix A; A is factored as $LDL^T$ .
n	<b>INTEGER.</b> The order of matrix $A (n \ge 0)$ .
nrhs	<b>INTEGER.</b> The number of right-hand sides; the number of columns in <i>B</i> ( <i>nrhs</i> $\ge$ 0).
ap,afp,b,work	REAL for sspsvx DOUBLE PRECISION for dspsvx COMPLEX for cspsvx DOUBLE COMPLEX for zspsvx. Arrays: ap(*), afp(*), b(ldb,*), work (*).

The array *ap* contains the upper or lower triangle of the symmetric matrix A in *packed storage* (see <u>Matrix</u> <u>Storage Schemes</u>).

The array *afp* is an input argument if *fact* = 'F'. It contains the block diagonal matrix *D* and the multipliers used to obtain the factor *U* or *L* from the factorization  $A = UDU^T$  or  $A = LDL^T$  as computed by <u>?sptrf</u>, in the same storage format as *A*.

The array b contains the matrix B whose columns are the right-hand sides for the systems of equations. work (*) is a workspace array.

The dimension of arrays ap and afp must be at least  $\max(1, n(n+1)/2)$ ; the second dimension of b must be at least  $\max(1, nrhs)$ ; the dimension of work must be at least  $\max(1, 3*n)$  for real flavors and  $\max(1, 2*n)$  for complex flavors.

**INTEGER.** The first dimension of *b*;  $ldb \ge max(1, n)$ .

#### INTEGER.

Array, **DIMENSION** at least max(1,*n*).

The array *ipiv* is an input argument if *fact* = 'F'. It contains details of the interchanges and the block structure of *D*, as determined by <u>?sptrf</u>.

If ipiv(i) = k > 0, then  $d_{ii}$  is a 1-by-1 diagonal block, and the *i*th row and column of *A* was interchanged with the *k*th row and column.

If uplo = 'U' and ipiv(i) = ipiv(i-1) = -m < 0, then *D* has a 2-by-2 block in rows/columns *i* and *i*-1, and (*i*-1) th row and column of *A* was interchanged with the *m*th row and column.

If uplo = 'L' and ipiv(i) = ipiv(i+1) = -m < 0, then *D* has a 2-by-2 block in rows/columns *i* and *i*+1, and (*i*+1) th row and column of *A* was interchanged with the *m*th row and column.

**INTEGER.** The leading dimension of the output array x;  $ldx \ge max(1, n)$ .

ldb ipiv

ldx

iwork	INTEGER.
	Workspace array, DIMENSION at least max(1, n); used
	in real flavors only.
rwork	REAL for cspsvx;
	DOUBLE PRECISION for zspsvx.
	Workspace array, DIMENSION at least $max(1, n)$ ; used
	in complex flavors only.

x	REAL for sspsvx DOUBLE PRECISION for dspsvx COMPLEX for cspsvx DOUBLE COMPLEX for zspsvx. Array, DIMENSION (1dx,*).
	If $info = 0$ or $info = n+1$ , the array x contains the solution matrix X to the system of equations. The second dimension of x must be at least max $(1,nrhs)$ .
afp, ipiv	These arrays are output arguments if $fact = 'N'$ . See the description of $afp$ , $ipiv$ in <i>Input Arguments</i> section.
rcond	<b>REAL</b> for single precision flavors. <b>DOUBLE PRECISION</b> for double precision flavors. An estimate of the reciprocal condition number of the matrix A. If <i>rcond</i> is less than the machine precision (in particular, if <i>rcond</i> = 0), the matrix is singular to working precision. This condition is indicated by a return code of <i>info</i> > 0.
ferr, berr	<b>REAL</b> for single precision flavors. <b>DOUBLE PRECISION</b> for double precision flavors. Arrays, <b>DIMENSION</b> at least max(1, <i>nrhs</i> ). Contain the component-wise forward and relative backward errors, respectively, for each solution vector.
info	<b>INTEGER.</b> If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$ , the <i>i</i> th parameter had an illegal value. If <i>info</i> = $i$ , and $i \leq n$ , then $d_{ii}$ is exactly zero. The factorization has been completed, but the block diagonal

matrix *D* is exactly singular, so the solution and error bounds could not be computed; rcond = 0 is returned. If info = i, and i = n + 1, then *D* is nonsingular, but rcond is less than machine precision, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of rcondwould suggest.

# ?hpsvx

Uses the diagonal pivoting factorization to compute the solution to the system of linear equations with a Hermitian matrix A stored in packed format, and provides error bounds on the solution.

### **Discussion**

This routine uses the diagonal pivoting factorization to compute the solution to a complex system of linear equations AX = B, where A is a *n*-by-*n* Hermitian matrix stored in packed format, the columns of matrix *B* are individual right-hand sides, and the columns of *X* are the corresponding solutions.

Error bounds on the solution and a condition estimate are also provided.

The routine **?hpsvx** performs the following steps:

1. If fact = 'N', the diagonal pivoting method is used to factor the matrix A. The form of the factorization is  $A = UDU^H$  or  $A = LDL^H$ , where U (or L) is a product of permutation and unit upper (lower) triangular matrices, and D is Hermitian and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

2. If some  $d_{i,i} = 0$ , so that *D* is exactly singular, then the routine returns with info = i. Otherwise, the factored form of *A* is used to estimate the condition number of the matrix *A*. If the reciprocal of the condition number is less than machine precision, info = n + 1 is returned as a warning, but the routine still goes on to solve for *X* and compute error bounds as described below.

3. The system of equations is solved for *X* using the factored form of *A*.

4. Iterative refinement is applied to improve the computed solution matrix and calculate error bounds and backward error estimates for it.

fact	CHARACTER*1. Must be 'F' or 'N'.
	Specifies whether or not the factored form of the matrix <i>A</i> has been supplied on entry.
	If <i>fact</i> = 'F': on entry, <i>afp</i> and <i>ipiv</i> contain the factored form of <i>A</i> . Arrays <i>ap</i> , <i>afp</i> , and <i>ipiv</i> will not be modified.
	If $fact = 'N'$ , the matrix A will be copied to $afp$ and factored.
uplo	CHARACTER*1. Must be 'U' or 'L'. Indicates whether the upper or lower triangular part of $A$ is stored and how $A$ is factored:
	If $uplo = 'U'$ , the array $ap$ stores the upper triangular part of the Hermitian matrix $A$ , and $A$ is factored as $UDU^{H}$ .
n	If $uplo = 'L'$ , the array $ap$ stores the lower triangular part of the Hermitian matrix $A$ ; $A$ is factored as $LDL^H$ . INTEGER. The order of matrix $A$ $(n \ge 0)$ .
nrhs	<b>INTEGER.</b> The number of right-hand sides; the number of columns in <i>B</i> ( <i>nrhs</i> $\ge$ 0).
ap,afp,b,work	COMPLEX for chpsvx DOUBLE COMPLEX for zhpsvx. Arrays: ap(*), afp(*), b(ldb,*), work (*).
	The array <i>ap</i> contains the upper or lower triangle of the Hermitian matrix A in <i>packed storage</i> (see <u>Matrix</u> <u>Storage Schemes</u> ).
	The array <i>afp</i> is an input argument if <i>fact</i> = 'F'. It contains the block diagonal matrix <i>D</i> and the multipliers used to obtain the factor <i>U</i> or <i>L</i> from the factorization $A = UD U^H$ or $A = LD L^H$ as computed by <u>?hptrf</u> , in the same storage format as <i>A</i> .
	The array <b>b</b> contains the matrix <b>B</b> whose columns are the right-hand sides for the systems of equations. <b>work</b> (*) is a workspace array.

	The dimension of arrays <i>ap</i> and <i>afp</i> must be at least $\max(1, n(n+1)/2)$ ; the second dimension of <i>b</i> must be at least $\max(1, nrhs)$ ; the dimension of <i>work</i> must be at least $\max(1, 2*n)$ .
ldb	<b>INTEGER.</b> The first dimension of <b>b</b> ; $1db \ge max(1, n)$ .
ipiv	INTEGER. Array, DIMENSION at least max(1, <i>n</i> ). The array <i>ipiv</i> is an input argument if <i>fact</i> = 'F'. It contains details of the interchanges and the block structure of <i>D</i> , as determined by <u>?hptrf</u> . If <i>ipiv(i)</i> = $k > 0$ , then $d_{ii}$ is a 1-by-1 diagonal block, and the <i>i</i> th row and column of <i>A</i> was interchanged with the <i>k</i> th row and column.
	If $uplo = 'U'$ and $ipiv(i) = ipiv(i-1) = -m < 0$ , then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> -1, and $(i-1)$ th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column. If $uplo = 'L'$ and $ipiv(i) = ipiv(i+1) = -m < 0$ , then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> +1, and $(i+1)$ th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column.
ldx	<b>INTEGER.</b> The leading dimension of the output array $x$ ; $ldx \ge max(1, n)$ .
rwork	REAL for chpsvx; DOUBLE PRECISION for zhpsvx. Workspace array, DIMENSION at least max(1, n).

x	COMPLEX for chpsvx
	DOUBLE COMPLEX for zhpsvx.
	Array, DIMENSION (1dx, *).
	If $info = 0$ or $info = n+1$ , the array x contains the
	solution matrix X to the system of equations. The
	second dimension of x must be at least $max(1,nrhs)$ .

afp, ipiv	These arrays are output arguments if $fact = 'N'$ . See the description of $afp$ , $ipiv$ in <i>Input Arguments</i> section.
rcond	<b>REAL</b> for chpsvx; <b>DOUBLE PRECISION</b> for zhpsvx. An estimate of the reciprocal condition number of the matrix <i>A</i> . If <i>rcond</i> is less than the machine precision (in particular, if <i>rcond</i> = 0), the matrix is singular to working precision. This condition is indicated by a return code of <i>info</i> > 0.
ferr, berr	REAL for chpsvx; DOUBLE PRECISION for zhpsvx. Arrays, DIMENSION at least max(1, <i>nrhs</i> ). Contain the component-wise forward and relative backward errors, respectively, for each solution vector.
info	<b>INTEGER.</b> If $info=0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , and $i \leq n$ , then $d_{ii}$ is exactly zero. The factorization has been completed, but the block diagonal matrix $D$ is exactly singular, so the solution and error bounds could not be computed; $rcond = 0$ is returned. If $info = i$ , and $i = n + 1$ , then $D$ is nonsingular, but $rcond$ is less than machine precision, meaning that the matrix is singular to working precision. Nevertheless, the solution and error bounds are computed because there are a number of situations where the computed solution can be more accurate than the value of $rcond$ would suggest.

# ?hpsv

Computes the solution to the system of linear equations with a Hermitian matrix A stored in packed format, and multiple right-hand sides.

call chpsv (uplo, n, nrhs, ap, ipiv, b, ldb, info)
call zhpsv (uplo, n, nrhs, ap, ipiv, b, ldb, info)

### **Discussion**

This routine solves for X the system of linear equations AX = B, where A is an *n*-by-*n* Hermitian matrix stored in packed format, the columns of matrix *B* are individual right-hand sides, and the columns of X are the corresponding solutions.

The diagonal pivoting method is used to factor A as  $A = U D U^{H}$  or  $A = L D L^{H}$ , where U (or L) is a product of permutation and unit upper (lower) triangular matrices, and D is Hermitian and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

The factored form of *A* is then used to solve the system of equations AX = B.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Indicates whether the upper or lower triangular part of A
	is stored and how A is factored:
	If $uplo = 'U'$ , the array $ap$ stores the upper triangular
	part of the matrix A, and A is factored as $UDU^{H}$ .
	If $uplo = 'L'$ , the array $ap$ stores the lower triangular
	part of the matrix A; A is factored as $LDL^{H}$ .
п	<b>INTEGER</b> . The order of matrix $A (n \ge 0)$ .
nrhs	<b>INTEGER.</b> The number of right-hand sides; the number
	of columns in $B$ ( <i>nrhs</i> $\geq$ 0).

ap, b	COMPLEX for chpsv
	DOUBLE COMPLEX for zhpsv.
	Arrays: $ap(*), b(ldb, *)$
	The dimension of ap must be at least $\max(1, n(n+1)/2)$ .
	The array $a_p$ contains the factor U or L, as specified by
	uplo, in packed storage (see Matrix Storage Schemes).
	The array $b$ contains the matrix $B$ whose columns are
	the right-hand sides for the systems of equations.
	The second dimension of <i>b</i> must be at least
	max(1, <i>nrhs</i> ).
ldb	<b>INTEGER.</b> The first dimension of <b>b</b> ; $1db \ge max(1, n)$ .

ap	The block-diagonal matrix $D$ and the multipliers used to obtain the factor $U$ (or $L$ ) from the factorization of $A$ as computed by <u>?hptrf</u> , stored as a packed triangular matrix in the same storage format as $A$ .
b	If <i>info</i> = 0, $b$ is overwritten by the solution matrix X.
ipiv	INTEGER. Array, DIMENSION at least max(1, <i>n</i> ). Contains details of the interchanges and the block structure of <i>D</i> , as determined by <u>?hptrf</u> . If $ipiv(i) = k > 0$ , then $d_{ii}$ is a 1-by-1 block, and the <i>i</i> th row and column of <i>A</i> was interchanged with the <i>k</i> th row and column.
	If $uplo = 'U'$ and $ipiv(i) = ipiv(i-1) = -m < 0$ , then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> -1, and ( <i>i</i> -1) th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column.
	If $uplo = 'L'$ and $ipiv(i) = ipiv(i+1) = -m < 0$ , then <i>D</i> has a 2-by-2 block in rows/columns <i>i</i> and <i>i</i> +1, and ( <i>i</i> +1) th row and column of <i>A</i> was interchanged with the <i>m</i> th row and column.

infoINTEGER. If info=0, the execution is successful.If info = -i, the *i*th parameter had an illegal value.If info = i,  $d_{ii}$  is 0. The factorization has been<br/>completed, but D is exactly singular, so the solution<br/>could not be computed.

# LAPACK Routines: Least Squares and Eigenvalue Problems



This chapter describes the Intel[®] Math Kernel Library implementation of routines from the LAPACK package that are used for solving linear least-squares problems, eigenvalue and singular value problems, as well as performing a number of related computational tasks.

Sections in this chapter include descriptions of LAPACK <u>computational</u> <u>routines</u> and <u>driver routines</u>.

For full reference on LAPACK routines and related information see [LUG].

**Least-Squares Problems.** A typical *least-squares problem* is as follows: given a matrix *A* and a vector *b*, find the vector *x* that minimizes the sum of squares  $\Sigma_i ((Ax)_i - b_i)^2$  or, equivalently, find the vector *x* that minimizes the 2-norm  $||Ax - b||_2$ .

In the most usual case, *A* is an *m* by *n* matrix with  $m \ge n$  and rank(*A*) = *n*. This problem is also referred to as finding the *least-squares solution* to an *overdetermined* system of linear equations (here we have more equations than unknowns). To solve this problem, you can use the *QR* factorization of the matrix A (see *QR Factorization* on page 5-6).

If m < n and rank(A) = m, there exist an infinite number of solutions x which exactly satisfy Ax = b, and thus minimize the norm  $||Ax-b||_2$ . In this case it is often useful to find the unique solution that minimizes  $||x||_2$ . This problem is referred to as finding the *minimum-norm solution* to an *underdetermined* system of linear equations (here we have more unknowns than equations). To solve this problem, you can use the LQ factorization of the matrix A (see LQ Factorization on page 5-7).

In the general case you may have a *rank-deficient least-squares problem*, with rank(A) < min(m, n): find the *minimum-norm least-squares solution* that minimizes both  $||x||_2$  and  $||Ax-b||_2$ . In this case (or when the rank of A is in doubt) you can use the *QR* factorization with pivoting or *singular value decomposition* (see page 5-74).

**Eigenvalue Problems** (from German *eigen* "own") are stated as follows: given a matrix *A*, find the *eigenvalues*  $\lambda$  and the corresponding *eigenvectors z* that satisfy the equation

 $Az = \lambda z$  (right eigenvectors z)

or the equation

 $z^{H}A = \lambda z^{H}$  (left eigenvectors z).

If *A* is a real symmetric or complex Hermitian matrix, the above two equations are equivalent, and the problem is called a *symmetric* eigenvalue problem. Routines for solving this type of problems are described in the section *Symmetric Eigenvalue Problems* (see page 5-101).

Routines for solving eigenvalue problems with nonsymmetric or non-Hermitian matrices are described in the section *Nonsymmetric Eigenvalue Problems* (see page 5-174).

The library also includes routines that handle *generalized symmetricdefinite eigenvalue problems*: find the eigenvalues  $\lambda$  and the corresponding eigenvectors *x* that satisfy one of the following equations:

 $Az = \lambda Bz$ ,  $ABz = \lambda z$ , or  $BAz = \lambda z$ 

where *A* is symmetric or Hermitian, and *B* is symmetric positive-definite or Hermitian positive-definite. Routines for reducing these problems to standard symmetric eigenvalue problems are described in the section *Generalized Symmetric-Definite Eigenvalue Problems* (see page 5-157).

* * *

To solve a particular problem, you usually call several computational routines. Sometimes you need to combine the routines of this chapter with other LAPACK routines described in Chapter 4 as well as with BLAS routines (Chapter 2).

For example, to solve a set of least-squares problems minimizing  $||Ax-b||_2$  for all columns *b* of a given matrix *B* (where *A* and *B* are real matrices), you can call **?geqrf** to form the factorization A = QR, then call **?ormqr** to compute  $C = Q^H B$ , and finally call the BLAS routine **?trsm** to solve for *X* the system of equations RX = C.

Another way is to call an appropriate driver routine that performs several tasks in one call. For example, to solve the least-squares problem the driver routine ?gels can be used.

### **Routine Naming Conventions**

s

For each routine in this chapter, you can use the LAPACK name.

**LAPACK names** have the structure **xyyzzz**, which is described below.

The initial letter  $\mathbf{x}$  indicates the data type:

- c complex, single precision
- d real, double precision z complex, double precision

The second and third letters yy indicate the matrix type and storage scheme:

- bd bidiagonal matrix
- ge general matrix
- gb general band matrix
- hs upper Hessenberg matrix

real, single precision

- or (real) orthogonal matrix
- op (real) orthogonal matrix (packed storage)
- un (complex) unitary matrix
- up (complex) unitary matrix (packed storage)
- pt symmetric or Hermitian positive-definite tridiagonal matrix
- sy symmetric matrix
- sp symmetric matrix (packed storage)
- **sb** (real) symmetric band matrix
- st (real) symmetric tridiagonal matrix
- he Hermitian matrix
- hp Hermitian matrix (packed storage)
- hb (complex) Hermitian band matrix
- tr triangular or quasi-triangular matrix.

The last three letters zzz indicate the computation performed, for example:

- **qrf** form the *QR* factorization
- lqf form the *LQ* factorization.

Thus, the routine sgeqrf forms the *QR* factorization of general real matrices in single precision; the corresponding routine for complex matrices is cgeqrf.

### **Matrix Storage Schemes**

LAPACK routines use the following matrix storage schemes:

- *Full storage*: a matrix *A* is stored in a two-dimensional array *a*, with the matrix element *a_{ii}* stored in the array element *a(i, j)*.
- *Packed storage* scheme allows you to store symmetric, Hermitian, or triangular matrices more compactly: the upper or lower triangle of the matrix is packed by columns in a one-dimensional array.
- Band storage: an m by n band matrix with kl sub-diagonals and ku super-diagonals is stored compactly in a two-dimensional array ab with kl+ku+1 rows and n columns. Columns of the matrix are stored in the corresponding columns of the array, and *diagonals* of the matrix are stored in rows of the array.

In Chapters 4 and 5, arrays that hold matrices in packed storage have names ending in *p*; arrays with matrices in band storage have names ending in *b*.

For more information on matrix storage schemes, see <u>Matrix Arguments</u> in Appendix A.

### **Mathematical Notation**

In addition to the mathematical notation used in previous chapters, descriptions of routines in this chapter use the following notation:

$\lambda_i$	<i>Eigenvalues</i> of the matrix <i>A</i> (for the definition of eigenvalues, see <i>Eigenvalue Problems</i> on page 5-2).
₫ _i	Singular values of the matrix A. They are equal to square roots of the eigenvalues of $A^HA$ . (For more information, see <u>Singular Value Decomposition</u> ).
<i>x</i>     ₂	The 2-norm of the vector $x:   x  _2 = (\sum_i  x_i ^2)^{1/2} =   x  _E.$
<i>A</i>    ₂	The 2-norm (or spectral norm) of the matrix A. $  A  _2 = \max_i \sigma_i$ , $  A  _2^2 = \max_{ x =1}(Ax \cdot Ax)$ .
<i>A</i>     _{<i>E</i>}	The <i>Euclidean norm</i> of the matrix $A$ : $  A  _{E}^{2} = \sum_{i} \sum_{j}  a_{ij} ^{2}$ (for vectors, the Euclidean norm and the 2-norm are equal: $  x  _{E} =   x  _{2}$ ).
$\theta(x, y)$	The acute angle between vectors x and y: $\cos \theta(x, y) =  x \cdot y  / (  x  _2   y  _2).$

### **Computational Routines**

In the sections that follow, the descriptions of LAPACK computational routines are given. These routines perform distinct computational tasks that can be used for:

Orthogonal Factorizations Singular Value Decomposition Symmetric Eigenvalue Problems Generalized Symmetric-Definite Eigenvalue Problems Monsymmetric Eigenvalue Problems Generalized Nonsymmetric Eigenvalue Problems Generalized Singular Value Decomposition

See also the respective driver routines.

### **Orthogonal Factorizations**

This section describes the LAPACK routines for the QR(RQ) and LQ(QL) factorization of matrices. Routines for the RZ factorization as well as for generalized QR and RQ factorizations are also included.

**QR Factorization.** Assume that *A* is an *m* by *n* matrix to be factored. If  $m \ge n$ , the *QR* factorization is given by

$$A = \mathcal{Q}\begin{pmatrix} R\\ 0 \end{pmatrix} = (\mathcal{Q}_1, \mathcal{Q}_2)\begin{pmatrix} R\\ 0 \end{pmatrix}$$

where R is an n by n upper triangular matrix with real diagonal elements, and Q is an m by m orthogonal (or unitary) matrix.

You can use the *QR* factorization for solving the following least-squares problem: minimize  $||Ax - b||_2$  where A is a full-rank *m* by *n* matrix  $(m \ge n)$ . After factoring the matrix, compute the solution *x* by solving  $Rx = (Q_1)^T b$ .

If m < n, the *QR* factorization is given by

$$A = QR = Q(R_1R_2)$$

where R is trapezoidal,  $R_1$  is upper triangular and  $R_2$  is rectangular.

The LAPACK routines do not form the matrix Q explicitly. Instead, Q is represented as a product of  $\min(m, n)$  elementary reflectors. Routines are provided to work with Q in this representation.

**LQ Factorization** of an *m* by *n* matrix *A* is as follows. If  $m \leq n$ ,

$$A = (L, 0)Q = (L, 0)\begin{pmatrix} Q_1\\ Q_2 \end{pmatrix} = LQ_1$$

where L is an m by m lower triangular matrix with real diagonal elements, and Q is an n by n orthogonal (or unitary) matrix.

If m > n, the LQ factorization is

$$A = \begin{pmatrix} L_1 \\ L_2 \end{pmatrix} Q$$

where  $L_1$  is an *n* by *n* lower triangular matrix,  $L_2$  is rectangular, and *Q* is an *n* by *n* orthogonal (or unitary) matrix.

You can use the *LQ* factorization to find the minimum-norm solution of an underdetermined system of linear equations Ax = b where *A* is an *m* by *n* matrix of rank *m* (*m* < *n*). After factoring the matrix, compute the solution vector *x* as follows: solve Ly = b for *y*, and then compute  $x = (Q_1)^H y$ .

Table 5-1 lists LAPACK routines that perform orthogonal factorization of matrices.

Matrix type, factorization	Factorize without pivoting	Factorize with pivoting	Generate matrix Q	Apply matrix Q
general matrices, QR factorization	?geqrf	?geqpf ?geqp3	?orgqr ?ungqr	?ormqr ?unmqr
general matrices, RQ factorization	?gerqf		<u>?orgrq</u> ?ungrq	<u>?ormrq</u> ?unmrq
general matrices, LQ factorization	?gelqf		?orglq ?unglq	?ormlq ?unmlq
general matrices, QL factorization	?geqlf		?orgql ?ungql	?ormql ?unmql
trapezoidal matrices, RZ factorization	?tzrzf			?ormrz ?unmrz
pair of matrices, generalized QR factorization	?ggqrf			
pair of matrices, generalized RQ factorization	?ggrqf			

#### Table 5-1 Computational Routines for Orthogonal Factorization

# ?geqrf

Computes the QR factorization of a general m by n matrix.

call sgeqrf ( m, n, a, lda, tau, work, lwork, info )
call dgeqrf ( m, n, a, lda, tau, work, lwork, info )
call cgeqrf ( m, n, a, lda, tau, work, lwork, info )
call zgeqrf ( m, n, a, lda, tau, work, lwork, info )

### **Discussion**

The routine forms the QR factorization of a general m by n matrix A (see *Orthogonal Factorizations* on page 5-6). No pivoting is performed.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of min(m, n) *elementary reflectors*. Routines are provided to work with Q in this representation.

m	<b>INTEGER.</b> The number of rows in the matrix $A (m \ge 0)$ .
п	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgeqrf DOUBLE PRECISION for dgeqrf COMPLEX for cgeqrf DOUBLE COMPLEX for zgeqrf. Arrays: a(lda,*) contains the matrix A. The second dimension of a must be at least max(1, n).
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max(1, $m$ ).
lwork	<b>INTEGER.</b> The size of the <i>work</i> array $(lwork \ge n)$ See <u>Application notes</u> for the suggested value of <i>lwork</i> .

a	Overwritten by the factorization data as follows:
	If $m \ge n$ , the elements below the diagonal are overwritten by the details of the unitary matrix $Q$ , and the upper triangle is overwritten by the corresponding elements of the upper triangular matrix $R$ .
	If $m < n$ , the strictly lower triangular part is overwritten by the details of the unitary matrix $Q$ , and the remaining elements are overwritten by the corresponding elements of the <i>m</i> by <i>n</i> upper trapezoidal matrix <i>R</i> .
tau	REAL for sgeqrf DOUBLE PRECISION for dgeqrf COMPLEX for cgeqrf DOUBLE COMPLEX for zgeqrf. Array, DIMENSION at least max $(1, \min(m, n))$ . Contains additional information on the matrix $Q$ .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER</b> . If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using *lwork* =n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed factorization is the exact factorization of a matrix A + E, where  $||E||_2 = O(\varepsilon) ||A||_2$ .

The approximate number of floating-point operations for real flavors is

(4/3)n ³	if $m = n$ ,
$(2/3)n^2(3m-n)$	if $m > n$ ,
$(2/3)m^2(3n-m)$	if <i>m</i> < <i>n</i> .

The number of operations for complex flavors is 4 times greater.

To solve a set of least-squares problems minimizing  $||Ax - b||_2$  for all columns *b* of a given matrix *B*, you can call the following:

<pre>?geqrf (this routine)</pre>	to factorize $A = QR$ ;	
<u>?ormqr</u>	to compute $C = Q^T B$ (for real matrices);	
<u>?unmqr</u>	to compute $C = Q^H B$ (for complex matrices);	
<u>?trsm</u> (a BLAS routine)	to solve $RX = C$ .	
(The columns of the computed $X$ are the least-squares solution vectors $x$ .)		

To compute the elements of Q explicitly, call

<u>?orgqr</u>	(for real matrices)
<u>?ungqr</u>	(for complex matrices).

# ?geqpf

Computes the QR factorization of a general m by n matrix with pivoting.

```
call sgeqpf ( m, n, a, lda, jpvt, tau, work, info )
call dgeqpf ( m, n, a, lda, jpvt, tau, work, info )
call cgeqpf ( m, n, a, lda, jpvt, tau, work, rwork, info )
call zgeqpf ( m, n, a, lda, jpvt, tau, work, rwork, info )
```

### **Discussion**

This routine is deprecated and has been replaced by routine <u>?geqp3</u>.

The routine ?geqpf forms the QR factorization of a general m by n matrix A with column pivoting: AP = QR (see Orthogonal Factorizations on page 5-6). Here P denotes an n by n permutation matrix.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of min(m, n) *elementary reflectors*. Routines are provided to work with Q in this representation.

m	<b>INTEGER.</b> The number of rows in the matrix $A \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgeqpf DOUBLE PRECISION for dgeqpf COMPLEX for cgeqpf DOUBLE COMPLEX for zgeqpf. Arrays: a (1da,*) contains the matrix A. The second dimension of a must be at least max(1, n).
	work (lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; must be at least $max(1, 3*n)$ .

jpvt	<b>INTEGER.</b> Array, <b>DIMENSION</b> at least $max(1, n)$ .
	On entry, if <i>jpvt(i)</i> >0, the <i>i</i> th column of <i>A</i> is moved to the beginning of <i>AP</i> before the computation, and fixed in place during the computation. If <i>jpvt(i)</i> = 0, the <i>i</i> th column of <i>A</i> is a free column (that is, it may be interchanged during the computation with any other free column).
rwork	REAL for cgeqpf
	DOUBLE PRECISION for zgeqpf.
	A workspace array, DIMENSION at least $max(1, 2*n)$ .
Output Paran	neters
а	Overwritten by the factorization data as follows:
	If $m \ge n$ , the elements below the diagonal are overwritten by the details of the unitary (orthogonal) matrix $Q$ , and the upper triangle is overwritten by the corresponding elements of the upper triangular matrix $R$ .
	If $m < n$ , the strictly lower triangular part is overwritten by the details of the matrix $Q$ , and the remaining elements are overwritten by the corresponding elements of the <i>m</i> by <i>n</i> upper trapezoidal matrix <i>R</i> .
tau	REAL for sgeqpf
	DOUBLE PRECISION for dgeqpf COMPLEX for cgeqpf
	DOUBLE COMPLEX for zgeqpf.
	Array, DIMENSION at least max $(1, \min(m, n))$ .
	Contains additional information on the matrix $Q$ .
jpvt	Overwritten by details of the permutation matrix <i>P</i> in the factorization $AP = QR$ . More precisely, the columns of <i>AP</i> are the columns of <i>A</i> in the following order: $jpvt(1), jpvt(2), \ldots, jpvt(n)$ .
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

The computed factorization is the exact factorization of a matrix A + E, where  $||E||_2 = O(\varepsilon) ||A||_2$ .

The approximate number of floating-point operations for real flavors is

 $\begin{array}{ll} (4/3)n^3 & \mbox{if } m = n, \\ (2/3)n^2(3m-n) & \mbox{if } m > n, \\ (2/3)m^2(3n-m) & \mbox{if } m < n. \end{array}$ 

The number of operations for complex flavors is 4 times greater.

To solve a set of least-squares problems minimizing  $||Ax - b||_2$  for all columns *b* of a given matrix *B*, you can call the following:

<pre>?geqpf (this routine)</pre>	to factorize $AP = QR$ ;
<u>?ormqr</u>	to compute $C = Q^T B$ (for real matrices);
<u>?unmqr</u>	to compute $C = Q^H B$ (for complex matrices);
<u>?trsm</u> (a BLAS routine	) to solve $RX = C$ .

(The columns of the computed *X* are the permuted least-squares solution vectors *x*; the output array *jpvt* specifies the permutation order.)

To compute the elements of Q explicitly, call

<u>?orgqr</u>	(for real matrices)
<u>?ungqr</u>	(for complex matrices)

# ?geqp3

Computes the QR factorization of a general m by n matrix with column pivoting using Level 3 BLAS.

call sgeqp3 ( m, n, a, lda, jpvt, tau, work, lwork, info )
call dgeqp3 ( m, n, a, lda, jpvt, tau, work, lwork, info )
call cgeqp3 ( m, n, a, lda, jpvt, tau, work, lwork, rwork, info )
call zgeqp3 ( m, n, a, lda, jpvt, tau, work, lwork, rwork, info )

### **Discussion**

The routine forms the *QR* factorization of a general *m* by *n* matrix *A* with column pivoting: AP = QR (see *Orthogonal Factorizations* on page 5-6) using Level 3 BLAS. Here *P* denotes an *n* by *n* permutation matrix. Use this routine instead of ?geqpf for better performance.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of min(m, n) *elementary reflectors*. Routines are provided to work with Q in this representation.

m	<b>INTEGER.</b> The number of rows in the matrix $A (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgeqp3 DOUBLE PRECISION for dgeqp3 COMPLEX for cgeqp3 DOUBLE COMPLEX for zgeqp3. Arrays: a (lda,*) contains the matrix A. The second dimension of a must be at least max(1, n).
	work (lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .

a	Overwritten by the factorization data as follows:
	If $m \ge n$ , the elements below the diagonal are overwritten by the details of the unitary (orthogonal) matrix $Q$ , and the upper triangle is overwritten by the corresponding elements of the upper triangular matrix $R$ .
	If $m < n$ , the strictly lower triangular part is overwritten by the details of the matrix $Q$ , and the remaining elements are overwritten by the corresponding elements of the <i>m</i> by <i>n</i> upper trapezoidal matrix <i>R</i> .
tau	REAL for sgeqp3 DOUBLE PRECISION for dgeqp3 COMPLEX for cgeqp3 DOUBLE COMPLEX for zgeqp3. Array, DIMENSION at least max (1, min( <i>m</i> , <i>n</i> )). Contains scalar factors of the elementary reflectors for the matrix <i>Q</i> .

jpvt	Overwritten by details of the permutation matrix $P$ in the factorization $AP = QR$ . More precisely, the columns of $AP$ are the columns of $A$ in the following order: $jpvt(1), jpvt(2), \ldots, jpvt(n)$ .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

To solve a set of least-squares problems minimizing  $||Ax - b||_2$  for all columns *b* of a given matrix *B*, you can call the following:

?geqp3 (this routine)	to factorize $AP = QR$ ;
<u>?ormqr</u>	to compute $C = Q^T B$ (for real matrices);
<u>?unmqr</u>	to compute $C = Q^H B$ (for complex matrices);
<u>?trsm</u> (a BLAS routine)	to solve $RX = C$ .

(The columns of the computed *X* are the permuted least-squares solution vectors *x*; the output array *jpvt* specifies the permutation order.)

To compute the elements of Q explicitly, call

<u>?orgqr</u> (for real matrices)

<u>?ungqr</u> (for complex matrices).

# ?orgqr

Generates the real orthogonal matrix Q of the QR factorization formed by ?geqrf.

call sorgqr ( m, n, k, a, lda, tau, work, lwork, info )
call dorgqr ( m, n, k, a, lda, tau, work, lwork, info )

### **Discussion**

The routine generates the whole or part of *m* by *m* orthogonal matrix *Q* of the *QR* factorization formed by the routines sgeqrf/dgeqrf (see page 5-8) or sgeqpf/dgeqpf (see page 5-11). Use this routine after a call to sgeqrf/dgeqrf or sgeqpf/dgeqpf.

Usually *Q* is determined from the *QR* factorization of an *m* by *p* matrix *A* with  $m \ge p$ . To compute the whole matrix *Q*, use:

call ?orgqr (m, m, p, a, Ida, tau, work, Iwork, info) To compute the leading p columns of Q (which form an orthonormal basis in the space spanned by the columns of A):

call ?orgqr (m, p, p, a, lda, tau, work, lwork, info) To compute the matrix  $Q^k$  of the QR factorization of A's leading k columns: call ?orgqr (m, m, k, a, lda, tau, work, lwork, info) To compute the leading k columns of  $Q^k$  (which form an orthonormal basis in the space spanned by A's leading k columns):

call ?orgqr ( m, k, k, a, lda, tau, work, lwork, info )

m	<b>INTEGER.</b> The order of the orthogonal matrix $Q \ (m \ge 0)$ .
п	<b>INTEGER.</b> The number of columns of $Q$ to be computed $(0 \le n \le m)$ .
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $Q$ ( $0 \leq \leq n$ ).

a, tau, work	REAL for sorgqr
	DOUBLE PRECISION for dorgqr
	Arrays:
	a(lda, *) and $tau(*)$ are the arrays returned by
	sgeqrf/dgeqrf or sgeqpf/dgeqpf.
	The second dimension of a must be at least $max(1, n)$ .
	The dimension of $tau$ must be at least max $(1, k)$ .
	work (lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER</b> . The size of the <i>work</i> array $(lwork \ge n)$
	See Application notes for the suggested value of <i>lwork</i> .

a	Overwritten by $n$ leading columns of the $m$ by $m$ orthogonal matrix $Q$ .
work(1)	If <i>info</i> = 0, on exit <i>work(1)</i> contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using *lwork* =n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed *Q* differs from an exactly orthogonal matrix by a matrix *E* such that  $||E||_2 = O(\varepsilon) ||A||_2$  where  $\varepsilon$  is the machine precision.

The total number of floating-point operations is approximately  $4*m*n*k - 2*(m+n)*k^2 + (4/3)*k^3$ .

If n = k, the number is approximately  $(2/3) * n^2 * (3m - n)$ .

The complex counterpart of this routine is <u>?ungqr</u>.

### ?ormqr

Multiplies a real matrix by the orthogonal matrix Q of the QR factorization formed by ?geqrf or ?geqpf.

call sormqr ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )
call dormqr ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )

### **Discussion**

The routine multiplies a real matrix C by Q or  $Q^T$ , where Q is the orthogonal matrix Q of the QR factorization formed by the routines sgeqrf/dgeqrf (see page 5-8) or sgeqpf/dgeqpf (see page 5-11).

Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^{T}C$ , CQ, or  $CQ^{T}$  (overwriting the result on *C*).

side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^T$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^T$ is applied to $C$ from the right.
trans	CHARACTER*1. Must be either 'N' or 'T'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'T', the routine multiplies C by $Q^{T}$ .
m	<b>INTEGER.</b> The number of rows in the matrix $C \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $C$ $(n \ge 0)$ .
k	<b>INTEGER</b> . The number of elementary reflectors whose product defines the matrix $Q$ . Constraints: $0 \leq k \leq m$ if <i>side</i> = 'L'; $0 \leq k \leq n$ if <i>side</i> = 'R'.
a,work,tau,c	REAL for sgeqrf DOUBLE PRECISION for dgeqrf. Arrays: a(lda,*) and tau(*) are the arrays returned by

	sgeqrf / dgeqrf or sgeqpf / dgeqpf. The second dimension of a must be at least $\max(1, k)$ . The dimension of $tau$ must be at least $\max(1, k)$ .
	c(ldc, *) contains the matrix C. The second dimension of c must be at least max $(1, n)$
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of a. Constraints: $lda \ge max(1, m)$ if $side = 'L'$ ; $lda \ge max(1, n)$ if $side = 'R'$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ . Constraint: $ldc \ge max(1, m)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array. Constraints: $lwork \ge max(1, n)$ if <i>side</i> = 'L'; $lwork \ge max(1, m)$ if <i>side</i> = 'R'. See Application notes for the suggested value of <i>lwork</i> .

С	Overwritten by the product $QC$ , $Q^{T}C$ , $CQ$ , or $CQ^{T}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using lwork = n*blocksize (if side = 'L') or lwork = m*blocksize (if side = 'R') where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The complex counterpart of this routine is <u>?unmqr</u>.

# ?ungqr

Generates the complex unitary matrix Q of the QR factorization formed by ?geqrf.

call cungqr ( m, n, k, a, lda, tau, work, lwork, info )
call zungqr ( m, n, k, a, lda, tau, work, lwork, info )

### **Discussion**

The routine generates the whole or part of m by m unitary matrix Q of the QR factorization formed by the routines cgeqrf/zgeqrf (see page 5-8) or cgeqpf/zgeqpf (see page 5-11). Use this routine after a call to cgeqrf/zgeqrf or cgeqpf/zgeqpf.

Usually *Q* is determined from the *QR* factorization of an *m* by *p* matrix *A* with  $m \ge p$ . To compute the whole matrix *Q*, use:

call ?ungqr (m, m, p, a, Ida, tau, work, Iwork, info) To compute the leading p columns of Q (which form an orthonormal basis in the space spanned by the columns of A):

call ?ungqr (m, p, p, a, lda, tau, work, lwork, info) To compute the matrix  $Q^k$  of the QR factorization of A's leading k columns: call ?ungqr (m, m, k, a, lda, tau, work, lwork, info) To compute the leading k columns of  $Q^k$  (which form an orthonormal basis in the space spanned by A's leading k columns):

call ?ungqr ( m, k, k, a, lda, tau, work, lwork, info )

m	<b>INTEGER.</b> The order of the unitary matrix $Q \ (m \ge 0)$ .
п	<b>INTEGER</b> . The number of columns of $Q$ to be computed $(0 \le n \le m)$ .
k	<b>INTEGER</b> . The number of elementary reflectors whose product defines the matrix $O(0 \le \le n)$ .

a, tau, work	COMPLEX for cungqr
	DOUBLE COMPLEX for zungqr
	Arrays:
	a(lda, *) and tau(*) are the arrays returned by
	cgeqrf/zgeqrf or cgeqpf/zgeqpf.
	The second dimension of $a$ must be at least max $(1, n)$ .
	The dimension of $tau$ must be at least max $(1, k)$ .
	work (lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER.</b> The size of the work array $(lwork \ge n)$
	See Application notes for the suggested value of <i>lwork</i> .

a	Overwritten by <i>n</i> leading columns of the <i>m</i> by <i>m</i> unitary matrix $Q$ .
work(1)	If <i>info</i> = 0, on exit <i>work(1)</i> contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using *lwork* =n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed *Q* differs from an exactly unitary matrix by a matrix *E* such that  $||E||_2 = O(\varepsilon) ||A||_2$  where  $\varepsilon$  is the machine precision.

The total number of floating-point operations is approximately  $16*m*n*k - 8*(m+n)*k^2 + (16/3)*k^3$ .

If n = k, the number is approximately  $(8/3) * n^2 * (3m - n)$ .

The real counterpart of this routine is <u>?orgqr</u>.

### ?unmqr

Multiplies a complex matrix by the unitary matrix Q of the QR factorization formed by ?geqrf.

call cunmqr ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )
call zunmqr ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )

### **Discussion**

The routine multiplies a rectangular complex matrix C by Q or  $Q^H$ , where Q is the unitary matrix Q of the QR factorization formed by the routines cgeqrf/zgeqrf (see page 5-8) or cgeqpf/zgeqpf (see page 5-11).

Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^{H}C$ , CQ, or  $CQ^{H}$  (overwriting the result on *C*).

side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^H$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^H$ is applied to $C$ from the right.
trans	CHARACTER*1. Must be either 'N' or 'C'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'C', the routine multiplies C by $Q^{H}$ .
m	<b>INTEGER</b> . The number of rows in the matrix $C \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $C$ ( $n \ge 0$ ).
k	<b>INTEGER</b> . The number of elementary reflectors whose product defines the matrix $Q$ . Constraints: $0 \leq k \leq m$ if <i>side</i> = 'L'; $0 \leq k \leq n$ if <i>side</i> = 'R'.
a,work,tau,c	COMPLEX for cgeqrf DOUBLE COMPLEX for zgeqrf. Arrays: a(lda,*) and tau(*) are the arrays returned by

	cgeqrf / zgeqrf or cgeqpf / zgeqpf. The second dimension of a must be at least $max(1, k)$ . The dimension of <i>tau</i> must be at least $max(1, k)$ .
	c(ldc, *) contains the matrix C. The second dimension of c must be at least max $(1, n)$
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of <i>a</i> . Constraints: $lda \ge max(1, m)$ if <i>side</i> = 'L'; $lda \ge max(1, n)$ if <i>side</i> = 'R'.
ldc	<b>INTEGER.</b> The first dimension of $c$ . Constraint: $ldc \ge max(1, m)$ .
lwork	<pre>INTEGER. The size of the work array. Constraints: lwork ≥ max(1, n) if side = 'L'; lwork ≥ max(1, m) if side = 'R'. See Application notes for the suggested value of lwork.</pre>

С	Overwritten by the product $QC$ , $Q^{H}C$ , $CQ$ , or $CQ^{H}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using lwork = n*blocksize (if side = 'L') or lwork = m*blocksize (if side = 'R') where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The real counterpart of this routine is <u>?ormqr</u>.

# ?gelqf

Computes the LQ factorization of a general m by n matrix.

call sgelqf ( m, n, a, lda, tau, work, lwork, info )
call dgelqf ( m, n, a, lda, tau, work, lwork, info )
call cgelqf ( m, n, a, lda, tau, work, lwork, info )
call zgelqf ( m, n, a, lda, tau, work, lwork, info )

### **Discussion**

The routine forms the LQ factorization of a general m by n matrix A (see *Orthogonal Factorizations* on page 5-6). No pivoting is performed.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of min(m, n) *elementary reflectors*. Routines are provided to work with Q in this representation.

m	<b>INTEGER.</b> The number of rows in the matrix $A (m \ge 0)$ .
п	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgelqf DOUBLE PRECISION for dgelqf COMPLEX for cgelqf DOUBLE COMPLEX for zgelqf. Arrays: a(lda,*) contains the matrix A. The second dimension of a must be at least max(1, n).
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; at least max(1, <i>m</i> ). See <i>Application notes</i> for the suggested value of <i>lwork</i> .

a	Overwritten by the factorization data as follows:
	If $m \leq n$ , the elements above the diagonal are overwritten by the details of the unitary (orthogonal) matrix $Q$ , and the lower triangle is overwritten by the corresponding elements of the lower triangular matrix $L$ .
	If $m > n$ , the strictly upper triangular part is overwritten by the details of the matrix $Q$ , and the remaining elements are overwritten by the corresponding elements of the <i>m</i> by <i>n</i> lower trapezoidal matrix <i>L</i> .
tau	REAL for sgelqf DOUBLE PRECISION for dgelqf COMPLEX for cgelqf DOUBLE COMPLEX for zgelqf. Array, DIMENSION at least max(1, min( <i>m</i> , <i>n</i> )). Contains additional information on the matrix <i>Q</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using *lwork* =*m***blocksize*, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed factorization is the exact factorization of a matrix A + E, where  $||E||_2 = O(\varepsilon) ||A||_2$ .

The approximate number of floating-point operations for real flavors is

 $\begin{array}{ll} (4/3)n^3 & \text{if } m = n, \\ (2/3)n^2(3m-n) & \text{if } m > n, \\ (2/3)m^2(3n-m) & \text{if } m < n. \end{array}$ 

The number of operations for complex flavors is 4 times greater.

To find the minimum-norm solution of an underdetermined least-squares problem minimizing  $||Ax - b||_2$  for all columns *b* of a given matrix *B*, you can call the following:

<pre>?gelqf (this routine)</pre>	to factorize $A = LQ$ ;
<u>?trsm</u> (a BLAS routine)	to solve $LY = B$ for Y;
<u>?ormlq</u>	to compute $X = (Q_1)^T Y$ (for real matrices);
<u>?unmlq</u>	to compute $X = (Q_1)^H Y$ (for complex matrices).

(The columns of the computed *X* are the minimum-norm solution vectors *x*. Here *A* is an *m* by *n* matrix with m < n;  $Q_1$  denotes the first *m* columns of *Q*).

To compute the elements of Q explicitly, call

<u>?orglq</u>	(for real matrices)
<u>?unglq</u>	(for complex matrices).

# ?orglq

Generates the real orthogonal matrix Q of the LQ factorization formed by ?gelqf.

call sorglq ( m, n, k, a, lda, tau, work, lwork, info )
call dorglq ( m, n, k, a, lda, tau, work, lwork, info )

### **Discussion**

The routine generates the whole or part of *n* by *n* orthogonal matrix *Q* of the LQ factorization formed by the routines sgelqf/dgelqf (see page 5-25). Use this routine after a call to sgelqf/dgelqf.

Usually *Q* is determined from the *LQ* factorization of an *p* by *n* matrix *A* with  $n \ge p$ . To compute the whole matrix *Q*, use:

call ?orglq (n, n, p, a, lda, tau, work, lwork, info) To compute the leading p rows of Q (which form an orthonormal basis in the space spanned by the rows of A):

call ?orglq (p, n, p, a, lda, tau, work, lwork, info) To compute the matrix  $Q^k$  of the LQ factorization of A's leading k rows: call ?orglq (n, n, k, a, lda, tau, work, lwork, info)

To compute the leading k rows of  $Q^k$  (which form an orthonormal basis in the space spanned by A's leading k rows):

call ?orgqr ( k, n, k, a, lda, tau, work, lwork, info )

m	<b>INTEGER.</b> The number of rows of $Q$ to be computed $(0 \le m \le n)$ .
п	<b>INTEGER</b> . The order of the orthogonal matrix $Q$ ( $n \ge m$ ).
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $O(0 \leq k \leq m)$ .

a, tau, work	REAL for sorglq
	DOUBLE PRECISION for dorglq
	Arrays:
	a(lda, *) and tau(*) are the arrays returned by
	sgelqf/dgelqf.
	The second dimension of a must be at least $max(1, n)$ .
	The dimension of $tau$ must be at least max $(1, k)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of <i>a</i> ; at least max(1, <i>m</i> ).
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; at least max(1, <i>m</i> ).
	See <i>Application notes</i> for the suggested value of <i>lwork</i> .

a	Overwritten by <i>m</i> leading rows of the <i>n</i> by <i>n</i> orthogonal matrix $Q$ .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using *lwork* =*m***blocksize*, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed *Q* differs from an exactly orthogonal matrix by a matrix *E* such that  $||E||_2 = O(\varepsilon) ||A||_2$  where  $\varepsilon$  is the machine precision.

The total number of floating-point operations is approximately  $4*m*n*k - 2*(m+n)*k^2 + (4/3)*k^3$ .

If m = k, the number is approximately  $(2/3) * m^2 * (3n - m)$ .

The complex counterpart of this routine is <u>?unglq</u>.

## ?ormlq

Multiplies a real matrix by the orthogonal matrix Q of the LQ factorization formed by ?gelqf.

call sormlq ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )
call dormlq ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )

### **Discussion**

The routine multiplies a real *m*-by-*n* matrix *C* by *Q* or  $Q^T$ , where *Q* is the orthogonal matrix *Q* of the *LQ* factorization formed by the routine sgelqf/dgelqf (see page 5-25).

Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^{T}C$ , CQ, or  $CQ^{T}$  (overwriting the result on *C*).

side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^T$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^T$ is applied to $C$ from the right.
trans	CHARACTER*1. Must be either 'N' or 'T'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'T', the routine multiplies C by $Q^{T}$ .
m	<b>INTEGER</b> . The number of rows in the matrix $C \ (m \ge 0)$ .
п	<b>INTEGER.</b> The number of columns in $C$ $(n \ge 0)$ .
k	INTEGER. The number of elementary reflectors whose product defines the matrix $Q$ . Constraints: $0 \le k \le n$ if <i>side</i> = 'L'; $0 \le k \le n$ if <i>side</i> = 'R'.
a,work,tau,c	REAL for sormlq DOUBLE PRECISION for dormlq. Arrays: a(lda,*) and tau(*) are arrays returned by ?gelqf.

	The second dimension of a must be: at least $max(1, m)$ if <i>side</i> = 'L'; at least $max(1, n)$ if <i>side</i> = 'R'. The dimension of <i>tau</i> must be at least $max(1, k)$ .
	c(ldc,*) contains the matrix C. The second dimension of c must be at least max $(1, n)$
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of <i>a</i> ; $1da \ge max(1, k)$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ ; $ldc \ge max(1, m)$ .
lwork	<b>INTEGER.</b> The size of the work array. Constraints: $lwork \ge max(1, n)$ if $side = 'L';$ $lwork \ge max(1, m)$ if $side = 'R'.$ See Application notes for the suggested value of $lwork$ .

С	Overwritten by the product $QC$ , $Q^{T}C$ , $CQ$ , or $CQ^{T}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using lwork = n*blocksize (if side = 'L') or lwork = m*blocksize (if side = 'R') where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

The complex counterpart of this routine is <u>?unmlq</u>.

# ?unglq

Generates the complex unitary matrix Q of the LQ factorization formed by ?gelqf.

call cunglq ( m, n, k, a, lda, tau, work, lwork, info )
call zunglq ( m, n, k, a, lda, tau, work, lwork, info )

### **Discussion**

The routine generates the whole or part of *n* by *n* unitary matrix *Q* of the *LQ* factorization formed by the routines cgelqf/zgelqf (see page 5-25). Use this routine after a call to cgelqf/zgelqf.

Usually *Q* is determined from the *LQ* factorization of an *p* by *n* matrix *A* with  $n \ge p$ . To compute the whole matrix *Q*, use:

call ?unglq (n, n, p, a, Ida, tau, work, Iwork, info) To compute the leading p rows of Q (which form an orthonormal basis in the space spanned by the rows of A):

call ?unglq (p, n, p, a, lda, tau, work, lwork, info) To compute the matrix  $Q^k$  of the LQ factorization of A's leading k rows:

call ?unglq (n, n, k, a, lda, tau, work, lwork, info) To compute the leading k rows of  $Q^k$  (which form an orthonormal basis in the space spanned by A's leading k rows):

call ?ungqr ( k, n, k, a, lda, tau, work, lwork, info )

m	<b>INTEGER.</b> The number of rows of $Q$ to be computed $(0 \le m \le n)$ .
п	<b>INTEGER.</b> The order of the unitary matrix $Q$ ( $n \ge m$ ).
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $Q$ ( $0 \leq k \leq m$ ).

a, tau, work	COMPLEX for cunglq
	DOUBLE COMPLEX for zunglq
	Arrays:
	a(lda, *) and tau(*) are the arrays returned by
	sgelqf/dgelqf.
	The second dimension of a must be at least $max(1, n)$ .
	The dimension of $tau$ must be at least max $(1, k)$ .
	<i>work</i> ( <i>lwork</i> ) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER</b> . The size of the <i>work</i> array; at least max(1, <i>m</i> ).
	See Application notes for the suggested value of <i>lwork</i> .

a	Overwritten by $m$ leading rows of the $n$ by $n$ unitary matrix $Q$ .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using lwork = m*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed *Q* differs from an exactly unitary matrix by a matrix *E* such that  $||E||_2 = O(\varepsilon) ||A||_2$  where  $\varepsilon$  is the machine precision.

The total number of floating-point operations is approximately  $16*m*n*k - 8*(m+n)*k^2 + (16/3)*k^3$ .

If m = k, the number is approximately  $(8/3) * m^2 * (3n - m)$ .

The real counterpart of this routine is <u>?orglq</u>.

# ?unmlq

Multiplies a complex matrix by the unitary matrix Q of the LQ factorization formed by ?gelqf.

call cunmlq ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )
call zunmlq ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )

### **Discussion**

The routine multiplies a real *m*-by-*n* matrix *C* by *Q* or  $Q^H$ , where *Q* is the unitary matrix *Q* of the *LQ* factorization formed by the routine cgelqf/zgelqf (see page 5-25).

Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^{H}C$ , CQ, or  $CQ^{H}$  (overwriting the result on *C*).

side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^H$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^H$ is applied to $C$ from the right.
trans	CHARACTER*1. Must be either 'N' or 'C'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'C', the routine multiplies C by $Q^{H}$ .
m	<b>INTEGER</b> . The number of rows in the matrix $C \ (m \ge 0)$ .
п	<b>INTEGER</b> . The number of columns in $C$ $(n \ge 0)$ .
k	INTEGER. The number of elementary reflectors whose product defines the matrix $Q$ . Constraints: $0 \le k \le n$ if side = 'L'; $0 \le k \le n$ if side = 'R'.
a,work,tau,c	COMPLEX for cunmlq DOUBLE COMPLEX for zunmlq. Arrays: a(lda,*) and tau(*) are arrays returned by ?gelqf.

	The second dimension of a must be: at least $max(1, m)$ if <i>side</i> = 'L'; at least $max(1, n)$ if <i>side</i> = 'R'. The dimension of <i>tau</i> must be at least $max(1, k)$ .
	c(ldc,*) contains the matrix C. The second dimension of c must be at least max $(1, n)$
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of <i>a</i> ; $1da \ge max(1, k)$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ ; $ldc \ge max(1, m)$ .
lwork	<b>INTEGER.</b> The size of the work array. Constraints: $lwork \ge max(1, n)$ if $side = 'L';$ $lwork \ge max(1, m)$ if $side = 'R'.$ See Application notes for the suggested value of $lwork$ .

С	Overwritten by the product $QC$ , $Q^{H}C$ , $CQ$ , or $CQ^{H}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using lwork = n*blocksize (if side = 'L') or lwork = m*blocksize (if side = 'R') where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

The real counterpart of this routine is <u>?ormlq</u>.

# ?geqlf

Computes the QL factorization of a general m by n matrix.

call sgeqlf ( m, n, a, lda, tau, work, lwork, info )
call dgeqlf ( m, n, a, lda, tau, work, lwork, info )
call cgeqlf ( m, n, a, lda, tau, work, lwork, info )
call zgeqlf ( m, n, a, lda, tau, work, lwork, info )

#### **Discussion**

The routine forms the QL factorization of a general *m*-by-*n* matrix *A*. No pivoting is performed.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of min(m, n) elementary reflectors. Routines are provided to work with Q in this representation.

m	<b>INTEGER.</b> The number of rows in the matrix $A (m \ge 0)$ .
п	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgeqlf DOUBLE PRECISION for dgeqlf COMPLEX for cgeqlf DOUBLE COMPLEX for zgeqlf. Arrays: a(lda,*) contains the matrix A. The second dimension of a must be at least max(1, n).
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; at least max(1, <i>n</i> ). See <i>Application notes</i> for the suggested value of <i>lwork</i> .

a	Overwritten on exit by the factorization data as follows:
	<ul> <li>if m≥ n, the lower triangle of the subarray</li> <li>a(m-n+1:m, 1:n) contains the n-by-n lower triangular matrix L;</li> <li>if m ≤n, the elements on and below the (n-m)th</li> <li>superdiagonal contain the m-by-n lower trapezoidal matrix L;</li> <li>in both cases, the remaining elements, with the array</li> <li>tau, represent the orthogonal/unitary matrix Q as a product of elementary reflectors.</li> </ul>
tau	REAL for sgeqlf DOUBLE PRECISION for dgeqlf COMPLEX for cgeqlf DOUBLE COMPLEX for zgeqlf. Array, DIMENSION at least max(1, min( <i>m</i> , <i>n</i> )). Contains scalar factors of the elementary reflectors for the matrix <i>Q</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

#### **Application Notes**

For better performance, try using *lwork* =n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs. Related routines include:

<u>?orgql</u>	to generate matrix Q (for real matrices);
<u>?ungql</u>	to generate matrix Q (for complex matrices);
<u>?ormql</u>	to apply matrix Q (for real matrices);
<u>?unmql</u>	to apply matrix Q (for complex matrices).

# ?orgql

Generates the real matrix Q of the QL factorization formed by ?geqlf.

call sorgql ( m, n, k, a, lda, tau, work, lwork, info )
call dorgql ( m, n, k, a, lda, tau, work, lwork, info )

### **Discussion**

The routine generates an *m*-by-*n* real matrix *Q* with orthonormal columns, which is defined as the last *n* columns of a product of *k* elementary reflectors  $H_i$  of order  $m: Q = H_k \cdot \cdot \cdot H_2 H_1$  as returned by the routines sgeqlf/dgeqlf. Use this routine after a call to sgeqlf/dgeqlf.

m	<b>INTEGER.</b> The number of rows of the matrix $Q$ ( $m \ge 0$ ).
n	<b>INTEGER</b> . The number of columns of the matrix $Q$ ( $m \ge n \ge 0$ ).
k	<b>INTEGER</b> . The number of elementary reflectors whose product defines the matrix $Q$ ( $n \ge k \ge 0$ ).
a, tau, work	REAL for sorgql DOUBLE PRECISION for dorgql Arrays: a(lda,*), tau(*), work(lwork).
	On entry, the $(n - k + i)$ th column of a must contain the vector which defines the elementary reflector $H_i$ , for $i = 1,2,,k$ , as returned by sgeqlf/dgeqlf in the last k columns of its array argument a; tau(i) must contain the scalar factor of the elementary reflector $H_i$ , as returned by sgeqlf/dgeqlf;
	The second dimension of a must be at least $\max(1, n)$ . The dimension of $tau$ must be at least $\max(1, k)$ .
	work(lwork) is a workspace array.

lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; at least $max(1, n)$ .
	See Application notes for the suggested value of <i>lwork</i> .

a	Overwritten by the $m$ -by- $n$ matrix $Q$ .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using lwork = n*blocksize, where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

The complex counterpart of this routine is <u>?ungql</u>.

# ?ungql

Generates the complex matrix Q of the QL factorization formed by ?geqlf.

call cungql ( m, n, k, a, lda, tau, work, lwork, info )
call zungql ( m, n, k, a, lda, tau, work, lwork, info )

#### **Discussion**

The routine generates an *m*-by-*n* complex matrix Q with orthonormal columns, which is defined as the last *n* columns of a product of *k* elementary reflectors  $H_i$  of order  $m: Q = H_k \cdot \cdot \cdot H_2 H_1$  as returned by the routines <u>cgeqlf/zgeqlf</u>. Use this routine after a call to <u>cgeqlf/zgeqlf</u>.

m	<b>INTEGER</b> . The number of rows of the matrix $Q$ ( $m \ge 0$ ).
п	<b>INTEGER</b> . The number of columns of the matrix $Q$ ( $m \ge n \ge 0$ ).
k	<b>INTEGER</b> . The number of elementary reflectors whose product defines the matrix $Q$ ( $n \ge k \ge 0$ ).
a, tau, work	COMPLEX for cungql DOUBLE COMPLEX for zungql Arrays: a(lda,*), tau(*), work(lwork).
	On entry, the $(n - k + i)$ th column of a must contain the vector which defines the elementary reflector $H_i$ , for $i = 1,2,,k$ , as returned by cgeqlf/zgeqlf in the last k columns of its array argument a; tau(i) must contain the scalar factor of the elementary reflector $H_i$ , as returned by cgeqlf/zgeqlf;
	The second dimension of a must be at least $\max(1, n)$ . The dimension of $tau$ must be at least $\max(1, k)$ .
	work(lwork) is a workspace array.

lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; at least $max(1, n)$ .
	See Application notes for the suggested value of <i>lwork</i> .

a	Overwritten by the $m$ -by- $n$ matrix $Q$ .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using *lwork* =n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The real counterpart of this routine is <u>?orgql</u>.

# ?ormql

Multiplies a real matrix by the orthogonal matrix Q of the QL factorization formed by ?geqlf.

call sormql ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )
call dormql ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )

#### **Discussion**

This routine multiplies a real *m*-by-*n* matrix *C* by *Q* or  $Q^T$ , where *Q* is the orthogonal matrix *Q* of the *QL* factorization formed by the routine  $\underline{sgeqlf}/\underline{dgeqlf}$ .

Depending on the parameters *side* and *trans*, the routine ?ormql can form one of the matrix products QC,  $Q^{T}C$ , CQ, or  $CQ^{T}$  (overwriting the result over C).

side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^T$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^T$ is applied to $C$ from the right.
trans	CHARACTER*1. Must be either 'N' or 'T'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'T', the routine multiplies C by $Q^{T}$ .
m	<b>INTEGER.</b> The number of rows in the matrix $C \ (m \ge 0)$ .
п	<b>INTEGER.</b> The number of columns in $C$ $(n \ge 0)$ .
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $Q$ . Constraints: $0 \leq k \leq m$ if <i>side</i> = 'L'; $0 \leq k \leq n$ if <i>side</i> = 'R'.

a,tau,c,work	REAL for sormal DOUBLE PRECISION for dormal.
	Arrays: a(lda,*), tau(*), c(ldc,*), work(lwork).
	On entry, the <i>i</i> th column of <i>a</i> must contain the vector which defines the elementary reflector $H_i$ , for $i = 1,2,,k$ , as returned by sgeqlf/dgeqlf in the last <i>k</i> columns of its array argument <i>a</i> . The second dimension of <i>a</i> must be at least max $(1, k)$ .
	$tau(i)$ must contain the scalar factor of the elementary reflector $H_i$ , as returned by sgeqlf/dgeqlf. The dimension of $tau$ must be at least max $(1, k)$ .
	c(ldc, *) contains the m-by-n matrix C. The second dimension of c must be at least max $(1, n)$
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of <i>a</i> ;
	if side ='L', $lda \ge max(1, m)$ ; if side ='R', $lda \ge max(1, n)$ .
ldc	<b>INTEGER</b> . The first dimension of $c$ ; $ldc \ge max(1, m)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array. Constraints: $lwork \ge max(1, n)$ if <i>side</i> = 'L'; $lwork \ge max(1, m)$ if <i>side</i> = 'R'. See Application notes for the suggested value of <i>lwork</i> .

С	Overwritten by the product $QC$ , $Q^{T}C$ , $CQ$ , or $CQ^{T}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## **Application Notes**

For better performance, try using lwork = n*blocksize (if side = 'L') or lwork = m*blocksize (if side = 'R') where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

The complex counterpart of this routine is <u>?unmql</u>.

# ?unmql

Multiplies a complex matrix by the unitary matrix Q of the QL factorization formed by ?geqlf.

call cunmql ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )
call zunmql ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )

### **Discussion**

The routine multiplies a complex *m*-by-*n* matrix *C* by *Q* or  $Q^H$ , where *Q* is the unitary matrix *Q* of the *QL* factorization formed by the routine cgeqlf/zgeqlf.

Depending on the parameters *side* and *trans*, the routine ?unmql can form one of the matrix products QC,  $Q^{H}C$ , CQ, or  $CQ^{H}$  (overwriting the result over C).

side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^H$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^H$ is applied to $C$ from the right.
trans	CHARACTER*1. Must be either 'N' or 'C'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'C', the routine multiplies C by $Q^{H}$ .
m	<b>INTEGER</b> . The number of rows in the matrix $C \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $C$ $(n \ge 0)$ .
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $Q$ . Constraints: $0 \le k \le m$ if side = 'L'; $0 \le k \le n$ if side = 'R'.

a,tau,c,work	COMPLEX for cunmql DOUBLE COMPLEX for zunmql.
	<pre>Arrays: a(lda,*), tau(*), c(ldc,*), work(lwork).</pre>
	On entry, the <i>i</i> th column of <i>a</i> must contain the vector which defines the elementary reflector $H_i$ , for $i = 1,2,,k$ , as returned by cgeqlf/zgeqlf in the last <i>k</i> columns of its array argument <i>a</i> . The second dimension of <i>a</i> must be at least max $(1, k)$ .
	$tau(i)$ must contain the scalar factor of the elementary reflector $H_i$ , as returned by cgeqlf/zgeqlf. The dimension of $tau$ must be at least max(1, k).
	c(ldc, *) contains the <i>m</i> -by- <i>n</i> matrix <i>C</i> . The second dimension of <i>c</i> must be at least max $(1, n)$
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of <i>a</i> ;
	if side = 'L', $lda \ge max(1, m)$ ; if side = 'R', $lda \ge max(1, n)$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ ; $ldc \ge max(1, m)$ .
lwork	<pre>INTEGER. The size of the work array. Constraints: lwork ≥ max(1, n) if side = 'L'; lwork ≥ max(1, m) if side = 'R'. See Application notes for the suggested value of lwork.</pre>

С	Overwritten by the product $QC$ , $Q^{H}C$ , $CQ$ , or $CQ^{H}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using *lwork* = n*blocksize (if *side* = 'L') or *lwork* = m*blocksize (if *side* = 'R') where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The real counterpart of this routine is <u>?ormql</u>.

# ?gerqf

Computes the RQ factorization of a general m by n matrix.

call sgerqf ( m, n, a, lda, tau, work, lwork, info )
call dgerqf ( m, n, a, lda, tau, work, lwork, info )
call cgerqf ( m, n, a, lda, tau, work, lwork, info )
call zgerqf ( m, n, a, lda, tau, work, lwork, info )

#### **Discussion**

The routine forms the RQ factorization of a general *m*-by-*n* matrix *A*. No pivoting is performed.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of min(m, n) *elementary reflectors*. Routines are provided to work with Q in this representation.

m	<b>INTEGER.</b> The number of rows in the matrix $A (m \ge 0)$ .
п	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgerqf DOUBLE PRECISION for dgerqf COMPLEX for cgerqf DOUBLE COMPLEX for zgerqf. Arrays: a(lda,*) contains the <i>m</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; $lwork \ge max(1, m)$ . See <u>Application notes</u> for the suggested value of <i>lwork</i> .

a	Overwritten on exit by the factorization data as follows: if $m \le n$ , the upper triangle of the subarray a(1:m, n-m+1:n) contains the <i>m</i> -by- <i>m</i> upper triangular matrix <i>R</i> ; if $m \ge n$ , the elements on and above the $(m-n)$ th subdiagonal contain the <i>m</i> -by- <i>n</i> upper trapezoidal matrix <i>R</i> ; in both cases, the remaining elements, with the array <i>t</i> au, represent the orthogonal/unitary matrix <i>Q</i> as a product of min( <i>m</i> , <i>n</i> ) elementary reflectors.
tau	REAL for sgerqf DOUBLE PRECISION for dgerqf COMPLEX for cgerqf DOUBLE COMPLEX for zgerqf. Array, DIMENSION at least max (1, min( <i>m</i> , <i>n</i> )). Contains scalar factors of the elementary reflectors for the matrix <i>Q</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using *lwork* =*m***blocksize*, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs. Related routines include:

<u>?orgrq</u>	to generate matrix Q (for real matrices);
<u>?ungrq</u>	to generate matrix Q (for complex matrices);
<u>?ormrq</u>	to apply matrix Q (for real matrices);
<u>?unmrq</u>	to apply matrix Q (for complex matrices).

# ?orgrq

Generates the real matrix Q of the RQ factorization formed by ?gerqf.

call sorgrq ( m, n, k, a, lda, tau, work, lwork, info )
call dorgrq ( m, n, k, a, lda, tau, work, lwork, info )

#### **Discussion**

The routine generates an *m*-by-*n* real matrix Q with orthonormal rows, which is defined as the last *m* rows of a product of *k* elementary reflectors  $H_i$  of order  $n: Q = H_1 H_2 \cdots H_k$  as returned by the routines <u>sgerqf/dgerqf</u>. Use this routine after a call to <u>sgerqf/dgerqf</u>.

m	<b>INTEGER</b> . The number of rows of the matrix $Q$ ( $m \ge 0$ ).
n	<b>INTEGER</b> . The number of columns of the matrix $Q$ $(n \ge m)$ .
k	<b>INTEGER</b> . The number of elementary reflectors whose product defines the matrix $Q$ ( $m \ge k \ge 0$ ).
a, tau, work	REAL for sorgrq DOUBLE PRECISION for dorgrq Arrays: a(lda,*), tau(*), work(lwork).
	On entry, the $(m - k + i)$ th row of a must contain the vector which defines the elementary reflector $H_i$ , for $i = 1,2,,k$ , as returned by sgerqf/dgerqf in the last k rows of its array argument a; tau(i) must contain the scalar factor of the elementary reflector $H_i$ , as returned by sgerqf/dgerqf;
	The second dimension of a must be at least $max(1, n)$ . The dimension of $tau$ must be at least $max(1, k)$ .
	work(lwork) is a workspace array.

lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER</b> . The size of the <i>work</i> array; at least $max(1, m)$ .
	See Application notes for the suggested value of <i>lwork</i> .

a	Overwritten by the <i>m</i> -by- <i>n</i> matrix <i>Q</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using lwork = m*blocksize, where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

The complex counterpart of this routine is <u>?ungrq</u>.

# ?ungrq

Generates the complex matrix Q of the RQ factorization formed by ?gerqf.

call cungrq ( m, n, k, a, lda, tau, work, lwork, info )
call zungrq ( m, n, k, a, lda, tau, work, lwork, info )

#### **Discussion**

The routine generates an *m*-by-*n* complex matrix Q with orthonormal rows, which is defined as the last *m* rows of a product of *k* elementary reflectors  $H_i$  of order  $n: Q = H_1^H H_2^H \cdots H_k^H$  as returned by the routines sgerqf/dgerqf. Use this routine after a call to sgerqf/dgerqf.

m	<b>INTEGER.</b> The number of rows of the matrix $Q$ $(m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns of the matrix $Q$ $(n \ge m)$ .
k	<b>INTEGER</b> . The number of elementary reflectors whose product defines the matrix $Q$ ( $m \ge k \ge 0$ ).
a, tau, work	REAL for cungrq DOUBLE PRECISION for zungrq Arrays: a(lda,*), tau(*), work(lwork).
	On entry, the $(m - k + i)$ th row of a must contain the vector which defines the elementary reflector $H_i$ , for $i = 1,2,,k$ , as returned by sgerqf/dgerqf in the last k rows of its array argument a; tau(i) must contain the scalar factor of the elementary reflector $H_i$ , as returned by sgerqf/dgerqf;
	The second dimension of a must be at least $max(1, n)$ . The dimension of $tau$ must be at least $max(1, k)$ .
	work(lwork) is a workspace array.

lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER</b> . The size of the <i>work</i> array; at least $max(1, m)$ .
	See <i>Application notes</i> for the suggested value of <i>lwork</i> .

a	Overwritten by the <i>m</i> -by- <i>n</i> matrix <i>Q</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using *lwork* =m*blocksize, where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the blocked algorithm. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The real counterpart of this routine is <u>?orgrq</u>.

## ?ormrq

Multiplies a real matrix by the orthogonal matrix Q of the RQ factorization formed by ?gerqf.

call sormrq ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )
call dormrq ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )

#### **Discussion**

The routine multiplies a real *m*-by-*n* matrix *C* by *Q* or *Q^T*, where *Q* is the real orthogonal matrix defined as a product of *k* elementary reflectors  $H_i$ :  $Q = H_1 H_2 \cdot \cdot \cdot H_k$  as returned by the *RQ* factorization routine <u>sgergf/dgerqf</u>.

Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^{T}C$ , CQ, or  $CQ^{T}$  (overwriting the result over *C*).

side	<b>CHARACTER*1.</b> Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^T$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^T$ is applied to $C$ from the right.
trans	CHARACTER*1. Must be either 'N' or 'T'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'T', the routine multiplies C by $Q^{T}$ .
m	<b>INTEGER.</b> The number of rows in the matrix $C \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $C$ ( $n \ge 0$ ).
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $Q$ . Constraints: $0 \le k \le m$ , if side = 'L'; $0 \le k \le n$ , if side = 'R'.

a,tau,c,work	<pre>REAL for sormrq DOUBLE PRECISION for dormrq. Arrays: a(lda,*), tau(*), c(ldc,*), work(lwork).</pre>
	On entry, the <i>i</i> th row of <b>a</b> must contain the vector which defines the elementary reflector $H_i$ , for $i = 1, 2,, k$ , as returned by sgerqf/dgerqf in the last <i>k</i> rows of its array argument <b>a</b> . The second dimension of <b>a</b> must be at least max $(1, m)$ if side = 'L', and at least max $(1, n)$ if side = 'R'.
	tau(i) must contain the scalar factor of the elementary reflector $H_i$ , as returned by sgerqf/dgerqf. The dimension of $tau$ must be at least max(1, k).
	c(ldc, *) contains the <i>m</i> -by- <i>n</i> matrix <i>C</i> . The second dimension of <i>c</i> must be at least max(1, <i>n</i> )
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; $1da \ge max(1, k)$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ ; $ldc \ge max(1, m)$ .
lwork	<pre>INTEGER. The size of the work array. Constraints: lwork ≥ max(1, n) if side = 'L'; lwork ≥ max(1, m) if side = 'R'. See Application notes for the suggested value of lwork.</pre>
Output Parame	eters

С	Overwritten by the product $QC$ , $Q^{T}C$ , $CQ$ , or $CQ^{T}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## **Application Notes**

For better performance, try using lwork = n*blocksize (if side = 'L') or lwork = m*blocksize (if side = 'R') where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

The complex counterpart of this routine is <u>?unmrq</u>.

# ?unmrq

Multiplies a complex matrix by the unitary matrix Q of the RQ factorization formed by ?gerqf.

call cunmrq ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )
call zunmrq ( side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info )

### **Discussion**

The routine multiplies a complex *m*-by-*n* matrix *C* by *Q* or *Q^H*, where *Q* is the complex unitary matrix defined as a product of *k* elementary reflectors  $H_i: Q = H_1^H H_2^H \cdots H_k^H$  as returned by the *RQ* factorization routine  $\underline{cgerqf/zgerqf}$ .

Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^{H}C$ , CQ, or  $CQ^{H}$  (overwriting the result over *C*).

side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^H$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^H$ is applied to $C$ from the right.
trans	CHARACTER*1. Must be either 'N' or 'C'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'C', the routine multiplies C by $Q^{H}$ .
m	<b>INTEGER</b> . The number of rows in the matrix $C \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $C$ $(n \ge 0)$ .
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $Q$ . Constraints: $0 \le k \le m$ , if <i>side</i> = 'L'; $0 \le k \le n$ , if <i>side</i> = 'R'.

a,tau,c,work	COMPLEX for cunmrq DOUBLE COMPLEX for zunmrq. Arrays: a(lda,*), tau(*), c(ldc,*), work(lwork).
	On entry, the <i>i</i> th row of <i>a</i> must contain the vector which defines the elementary reflector $H_i$ , for $i = 1, 2,, k$ , as returned by cgerqf/zgerqf in the last <i>k</i> rows of its array argument <i>a</i> . The second dimension of <i>a</i> must be at least max $(1, m)$ if side = 'L', and at least max $(1, n)$ if side = 'R'.
	$tau(i)$ must contain the scalar factor of the elementary reflector $H_i$ , as returned by cgerqf/zgerqf. The dimension of $tau$ must be at least max $(1, k)$ .
	c(ldc, *) contains the m-by-n matrix C. The second dimension of c must be at least max $(1, n)$
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; $lda \ge max(1, k)$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ ; $ldc \ge max(1, m)$ .
lwork	<b>INTEGER.</b> The size of the work array. Constraints: $lwork \ge max(1, n)$ if side = 'L'; $lwork \ge max(1, m)$ if side = 'R'. See Application notes for the suggested value of $lwork$ .
Output Paramo	eters
С	Overwritten by the product $QC$ , $Q^{H}C$ , $CQ$ , or $CQ^{H}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If $info = 0$ , on exit work(1) contains the minimum

value of *lwork* required for optimum performance. Use this *lwork* for subsequent runs.*info* INTEGER.

If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value.

### **Application Notes**

For better performance, try using *lwork* = n*blocksize (if *side* = 'L') or *lwork* = m*blocksize (if *side* = 'R') where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The real counterpart of this routine is <u>?ormrq</u>.

## ?tzrzf

*Reduces the upper trapezoidal matrix A to upper triangular form.* 

call stzrzf ( m, n, a, lda, tau, work, lwork, info )
call dtzrzf ( m, n, a, lda, tau, work, lwork, info )
call ctzrzf ( m, n, a, lda, tau, work, lwork, info )
call ztzrzf ( m, n, a, lda, tau, work, lwork, info )

#### **Discussion**

This routine reduces the *m*-by-*n* ( $m \le n$ ) real/complex upper trapezoidal matrix *A* to upper triangular form by means of orthogonal/unitary transformations. The upper trapezoidal matrix *A* is factored as

 $A = (R \ 0) * Z,$ 

where *Z* is an *n*-by-*n* orthogonal/unitary matrix and R is an *m*-by-*m* upper triangular matrix.

m	<b>INTEGER.</b> The number of rows in the matrix $A (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $A (n \ge m)$ .
a, work	REAL for stzrzf DOUBLE PRECISION for dtzrzf COMPLEX for ctzrzf DOUBLE COMPLEX for ztzrzf. Arrays: a(lda,*), work(lwork). The leading m-by-n upper trapezoidal part of the array a contains the matrix A to be factorized. The second dimension of a must be at least max(1, n).
	work is a workspace array.
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max(1, $m$ ).
lwork	<b>INTEGER</b> . The size of the <i>work</i> array;

 $lwork \ge max(1, m)$ . See Application notes for the suggested value of lwork.

#### **Output Parameters**

а	Overwritten on exit by the factorization data as follows:
	the leading <i>m</i> -by- <i>m</i> upper triangular part of <i>a</i> contains the upper triangular matrix <i>R</i> , and elements $m + 1$ to <i>n</i> of the first <i>m</i> rows of <i>a</i> , with the array <i>tau</i> , represent the orthogonal matrix <i>Z</i> as a product of <i>m</i> elementary reflectors.
tau	REAL for stzrzf
	DOUBLE PRECISION for dtzrzf
	COMPLEX for ctzrzf
	DOUBLE COMPLEX for ztzrzf.
	Array, DIMENSION at least max (1, m).
	Contains scalar factors of the elementary reflectors for the matrix Z.
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using *lwork* =*m***blocksize*, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work(1)* and use this value for subsequent runs.

Related routines include:

<u>?ormrz</u>	to apply matrix Q (for real matrices);
<u>?unmrz</u>	to apply matrix Q (for complex matrices).

## ?ormrz

Multiplies a real matrix by the orthogonal matrix defined from the factorization formed by ?tzrzf.

call sormrz ( side,trans,m,n,k,l,a,lda,tau,c,ldc,work,lwork,info )
call dormrz ( side,trans,m,n,k,l,a,lda,tau,c,ldc,work,lwork,info )

#### **Discussion**

The routine multiplies a real *m*-by-*n* matrix *C* by *Q* or  $Q^T$ , where *Q* is the real orthogonal matrix defined as a product of *k* elementary reflectors  $H_i$ :  $Q=H_1H_2 \cdot \cdot \cdot H_k$  as returned by the factorization routine <u>stzrzf/dtzrzf</u>. Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^TC$ , CQ, or  $CQ^T$  (overwriting the result over *C*).

The matrix Q is of order *m* if *side* = 'L' and of order *n* if *side* = 'R'.

side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^T$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^T$ is applied to $C$ from the right.
trans	CHARACTER*1. Must be either 'N' or 'T'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'T', the routine multiplies C by $Q^{T}$ .
m	<b>INTEGER</b> . The number of rows in the matrix $C \ (m \ge 0)$ .
п	<b>INTEGER.</b> The number of columns in $C$ $(n \ge 0)$ .
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $Q$ . Constraints: $0 \le k \le m$ , if <i>side</i> = 'L'; $0 \le k \le n$ , if <i>side</i> = 'R'.
1	INTEGER.

	The number of columns of the matrix A containing the meaningful part of the Householder reflectors. Constraints: $0 \le 1 \le m$ , if side = 'L'; $0 \le l \le n$ , if side = 'R'.
a,tau,c,work	<pre>REAL for sormrz DOUBLE PRECISION for dormrz. Arrays: a(lda,*), tau(*), c(ldc,*), work(lwork).</pre>
	On entry, the <i>i</i> th row of <i>a</i> must contain the vector which defines the elementary reflector $H_i$ , for $i = 1, 2,, k$ , as returned by stzrzf/dtzrzf in the last <i>k</i> rows of its array argument <i>a</i> . The second dimension of <i>a</i> must be at least max $(1, m)$ if side = 'L', and at least max $(1, n)$ if side = 'R'.
	tau(i) must contain the scalar factor of the elementary reflector $H_i$ , as returned by $stzrzf/dtzrzf$ . The dimension of $tau$ must be at least max $(1, k)$ .
	c(ldc, *) contains the <i>m</i> -by- <i>n</i> matrix <i>C</i> . The second dimension of <i>c</i> must be at least max(1, <i>n</i> )
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; $1 da \ge max(1, k)$ .
ldc	<b>INTEGER</b> . The first dimension of $c$ ; $ldc \ge max(1, m)$ .
lwork	<b>INTEGER.</b> The size of the work array. Constraints: $lwork \ge max(1, n)$ if side = 'L'; $lwork \ge max(1, m)$ if side = 'R'. See Application notes for the suggested value of <i>lwork</i> .

С	Overwritten by the product $QC$ , $Q^{T}C$ , $CQ$ , or $CQ^{T}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.

info

INTEGER. If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value.

### **Application Notes**

For better performance, try using lwork = n*blocksize (if side = 'L') or lwork = m*blocksize (if side = 'R') where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The complex counterpart of this routine is <u>?unmrz</u>.

## ?unmrz

Multiplies a complex matrix by the unitary matrix defined from the factorization formed by ?tzrzf.

call cunmrz ( side,trans,m,n,k,l,a,lda,tau,c,ldc,work,lwork,info )
call zunmrz ( side,trans,m,n,k,l,a,lda,tau,c,ldc,work,lwork,info )

#### **Discussion**

The routine multiplies a complex *m*-by-*n* matrix *C* by *Q* or *Q^H*, where *Q* is the unitary matrix defined as a product of *k* elementary reflectors  $H_i: Q = H_1^H H_2^H \cdots H_k^H$  as returned by the factorization routine <u>ctzrzf/ztzrzf</u>.

Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^{H}C$ , CQ, or  $CQ^{H}$  (overwriting the result over *C*).

The matrix Q is of order m if *side* = 'L' and of order n if *side* = 'R'.

side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^H$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^H$ is applied to $C$ from the right.
trans	CHARACTER*1. Must be either 'N' or 'C'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'C', the routine multiplies C by $Q^{H}$ .
m	<b>INTEGER.</b> The number of rows in the matrix $C \ (m \ge 0)$ .
n	<b>INTEGER</b> . The number of columns in $C$ ( $n \ge 0$ ).
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $Q$ . Constraints: $0 \le k \le m$ , if side = 'L'; $0 \le k \le n$ , if side = 'R'.
1	INTEGER.

	The number of columns of the matrix A containing the meaningful part of the Householder reflectors. Constraints: $0 \le 1 \le m$ , if side = 'L'; $0 \le 1 \le n$ , if side = 'R'.	
a,tau,c,work	COMPLEX for cunmrz DOUBLE COMPLEX for zunmrz. Arrays: a(lda,*), tau(*), c(ldc,*), work(lwork).	
	On entry, the <i>i</i> th row of <i>a</i> must contain the vector which defines the elementary reflector $H_i$ , for $i = 1, 2,, k$ , as returned by ctzrzf/ztzrzf in the last <i>k</i> rows of its array argument <i>a</i> . The second dimension of <i>a</i> must be at least max $(1, m)$ if side = 'L', and at least max $(1, n)$ if side = 'R'.	
	tau(i) must contain the scalar factor of the elementary reflector $H_i$ , as returned by $ctzrzf/ztzrzf$ . The dimension of $tau$ must be at least max $(1, k)$ .	
	c(ldc, *) contains the <i>m</i> -by- <i>n</i> matrix <i>C</i> . The second dimension of <i>c</i> must be at least max(1, <i>n</i> )	
	work(lwork) is a workspace array.	
lda	<b>INTEGER.</b> The first dimension of $a$ ; $lda \ge max(1, k)$ .	
ldc	<b>INTEGER</b> . The first dimension of $c$ ; $1dc \ge max(1, m)$ .	
lwork	<pre>INTEGER. The size of the work array. Constraints: lwork ≥ max(1, n) if side = 'L'; lwork ≥ max(1, m) if side = 'R'. See Application notes for the suggested value of lwork.</pre>	
Output Parameters		

С	Overwritten by the product $QC$ , $Q^{H}C$ , $CQ$ , or $CQ^{H}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.

infoINTEGER.If info = 0, the execution is successful.If info = -i, the ith parameter had an illegal value.

## **Application Notes**

For better performance, try using lwork = n*blocksize (if side = 'L') or lwork = m*blocksize (if side = 'R') where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The real counterpart of this routine is <u>?ormrz</u>.

# ?ggqrf

*Computes the generalized QR factorization of two matrices.* 

call sggqrf (n, m, p, a, lda, taua, b, ldb, taub, work, lwork, info) call dggqrf (n, m, p, a, lda, taua, b, ldb, taub, work, lwork, info) call cggqrf (n, m, p, a, lda, taua, b, ldb, taub, work, lwork, info) call zggqrf (n, m, p, a, lda, taua, b, ldb, taub, work, lwork, info)

#### **Discussion**

The routine forms the generalized QR factorization of an *n*-by-*m* matrix *A* and an *n*-by-*p* matrix *B* as A = QR, B = QTZ, where *Q* is an *n*-by-*n* orthogonal/unitary matrix, *Z* is a *p*-by-*p* orthogonal/unitary matrix, and *R* and *T* assume one of the forms:

$$R = m \begin{pmatrix} R \\ n - m \end{pmatrix}, \text{ if } n \ge m$$

or

$$n \quad m-n$$
  
 $R = n \quad (R_{11} \quad R_{12}) \quad , \text{ if } n < m ,$ 

where  $R_{11}$  is upper triangular, and

 $\begin{array}{rrr} p-n & n \\ T = n & \left( \begin{array}{cc} 0 & T_{12} \end{array} \right) \ , \ \ \mbox{if} \ \underline{n} \leq p \ , \ \mbox{or} \end{array}$ 

$$T = \begin{array}{c} p \\ T = n - p \\ p \end{array} \begin{pmatrix} T_{11} \\ T_{21} \end{pmatrix} , \text{ if } n > p$$

where  $T_{12}$  or  $T_{21}$  is a *p*-by-*p* upper triangular matrix.

In particular, if *B* is square and nonsingular, the *GQR* factorization of *A* and *B* implicitly gives the *QR* factorization of  $B^{-1}A$  as:

 $B^{-1}A = \mathbf{Z}^H(T^{-1}R)$ 

## **Input Parameters**

n	<b>INTEGER.</b> The number of rows of the matrices <i>A</i> and <i>B</i> $(n \ge 0)$ .
m	<b>INTEGER.</b> The number of columns in $A (m \ge 0)$ .
р	<b>INTEGER.</b> The number of columns in $B \ (p \ge 0)$ .
a, b, work	REAL for sggqrf DOUBLE PRECISION for dggqrf COMPLEX for cggqrf DOUBLE COMPLEX for zggqrf. Arrays: a(lda,*) contains the matrix A. The second dimension of a must be at least max(1, m).
	b(1db, *) contains the matrix <i>B</i> . The second dimension of <i>b</i> must be at least max $(1, p)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .
lwork	<b>INTEGER</b> . The size of the <i>work</i> array; must be at least max(1, <i>n</i> , <i>m</i> , <i>p</i> ) See Application notes for the suggested value of <i>lwork</i> .

### **Output Parameters**

a,	b	Overwritten by the factorization data as follows:
		on exit, the elements on and above the diagonal of the array a contain the $\min(n,m)$ -by- <i>m</i> upper trapezoidal matrix $R$ ( $R$ is upper triangular if $n \ge m$ ); the elements below the diagonal, with the array <i>taua</i> , represent the orthogonal/unitary matrix $Q$ as a product of $\min(n,m)$ elementary reflectors;

	if $n \leq p$ , the upper triangle of the subarray b(1:n, p-n+1:p) contains the <i>n</i> -by- <i>n</i> upper triangular matrix <i>T</i> ; if $n > p$ , the elements on and above the $(n-p)$ th subdiagonal contain the <i>n</i> -by- <i>p</i> upper trapezoidal matrix <i>T</i> ; the remaining elements, with the array <i>taub</i> , represent the orthogonal/unitary matrix <i>Z</i> as a product of elementary reflectors.
taua, taub	REAL for sggqrf DOUBLE PRECISION for dggqrf COMPLEX for cggqrf DOUBLE COMPLEX for zggqrf. Arrays, DIMENSION at least max $(1, \min(n, m))$ for taua and at least max $(1, \min(n, p))$ for taub. The array taua contains the scalar factors of the elementary reflectors which represent the orthogonal/unitary matrix $Q$ .
	The array <i>taub</i> contains the scalar factors of the elementary reflectors which represent the orthogonal/unitary matrix <i>Z</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using

*lwork*  $\geq \max(n,m,p) * \max(nb1,nb2,nb3),$ 

where *nb1* is the optimal blocksize for the *QR* factorization of an *n*-by-*m* matrix, *nb2* is the optimal blocksize for the *RQ* factorization of an *n*-by-*p* matrix, and *nb3* is the optimal blocksize for a call of ?ormgr/?unmgr.

# ?ggrqf

Computes the generalized RQ factorization of two matrices.

call sggrqf (m, p, n, a, lda, taua, b, ldb, taub, work, lwork, info) call dggrqf (m, p, n, a, lda, taua, b, ldb, taub, work, lwork, info) call cggrqf (m, p, n, a, lda, taua, b, ldb, taub, work, lwork, info) call zggrqf (m, p, n, a, lda, taua, b, ldb, taub, work, lwork, info)

#### Discussion

The routine forms the generalized RQ factorization of an *m*-by-*n* matrix A and an *p*-by-*n* matrix B as A = RQ, B = Z TQ, where Q is an *n*-by-*n* orthogonal/unitary matrix, Z is a *p*-by-*p* orthogonal/unitary matrix, and R and T assume one of the forms:

$$\begin{array}{ccc} n-m & m \\ R &= m & (0 & R_{12}) \ , \ \ \mathrm{if} \ m \leq n \ , \end{array}$$

or

$$R = m - n \begin{pmatrix} n \\ R_{11} \\ n \end{pmatrix} , \text{ if } m > n$$

where  $R_{11}$  or  $R_{21}$  is upper triangular, and

$$T = n \begin{pmatrix} n \\ T_{11} \\ p - n \begin{pmatrix} T_{11} \\ 0 \end{pmatrix} , \text{ if } p \ge n$$

or

$$\begin{array}{ccc} p & n-p \\ T = p & (T_{11} & T_{12}) & , & \text{if } p < n \end{array}$$

where  $T_{11}$  is upper triangular.

In particular, if *B* is square and nonsingular, the *GRQ* factorization of *A* and *B* implicitly gives the *RQ* factorization of  $AB^{-1}$  as:

 $AB^{-1} = (R \ T^{-1}) Z^{H}$ 

#### **Input Parameters**

m	<b>INTEGER</b> . The number of rows of the matrix $A \ (m \ge 0)$ .
р	<b>INTEGER</b> . The number of rows in $B \ (p \ge 0)$ .
n	<b>INTEGER.</b> The number of columns of the matrices <i>A</i> and <i>B</i> $(n \ge 0)$ .
a, b, work	REAL for sggrqf DOUBLE PRECISION for dggrqf COMPLEX for cggrqf DOUBLE COMPLEX for zggrqf. Arrays: a(lda,*) contains the m-by-n matrix A. The second dimension of a must be at least max(1, n).
	b(ldb, *) contains the p-by-n matrix B. The second dimension of b must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, m)$ .
ldb	<b>INTEGER</b> . The first dimension of $b$ ; at least max $(1, p)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; must be at least $max(1, n, m, p)$ See Application notes for the suggested value of <i>lwork</i> .

### **Output Parameters**

a,

b	Overwritten by the factorization data as follows:
	on exit, if $m \leq n$ , the upper triangle of the subarray a(1:m, n-m+1:n) contains the <i>m</i> -by- <i>m</i> upper triangular matrix <i>R</i> ; if $m > n$ , the elements on and above the ( <i>m</i> - <i>n</i> )th
	subdiagonal contain the <i>m</i> -by- <i>n</i> upper trapezoidal

	matrix <i>R</i> ; the remaining elements, with the array <i>taua</i> , represent the orthogonal/unitary matrix <i>Q</i> as a product of elementary reflectors; the elements on and above the diagonal of the array <i>b</i> contain the min( <i>p</i> , <i>n</i> )-by- <i>n</i> upper trapezoidal matrix <i>T</i> ( <i>T</i> is upper triangular if $p \ge n$ ); the elements below the diagonal, with the array <i>taub</i> , represent the orthogonal/unitary matrix <i>Z</i> as a product of elementary reflectors.
taua, taub	REAL for sggrqf DOUBLE PRECISION for dggrqf COMPLEX for cggrqf DOUBLE COMPLEX for zggrqf. Arrays, DIMENSION at least max $(1, \min(m, n))$ for taua and at least max $(1, \min(p, n))$ for taub. The array taua contains the scalar factors of the elementary reflectors which represent the orthogonal/unitary matrix $Q$ .
	The array <i>taub</i> contains the scalar factors of the elementary reflectors which represent the orthogonal/unitary matrix <i>Z</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

For better performance, try using  $lwork \ge max(n,m,p)*max(nb1,nb2,nb3),$ 

where nb1 is the optimal blocksize for the RQ factorization of an *m*-by-*n* matrix, nb2 is the optimal blocksize for the QR factorization of an *p*-by-*n* matrix, and nb3 is the optimal blocksize for a call of ?ormrq/?unmrq. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

#### **Singular Value Decomposition**

This section describes LAPACK routines for computing the *singular value decomposition* (SVD) of a general *m* by *n* matrix *A*:

 $A = U\Sigma V^{H}.$ 

In this decomposition, *U* and *V* are unitary (for complex *A*) or orthogonal (for real *A*);  $\Sigma$  is an *m* by *n* diagonal matrix with real diagonal elements  $\sigma_i$ :

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{\min(m, n)} \geq 0.$$

The diagonal elements  $\sigma_i$  are *singular values* of *A*. The first min(*m*, *n*) columns of the matrices *U* and *V* are, respectively, *left* and *right singular vectors* of *A*. The singular values and singular vectors satisfy

$$Av_i = \sigma_i u_i$$
 and  $A^H u_i = \sigma_i v_i$ 

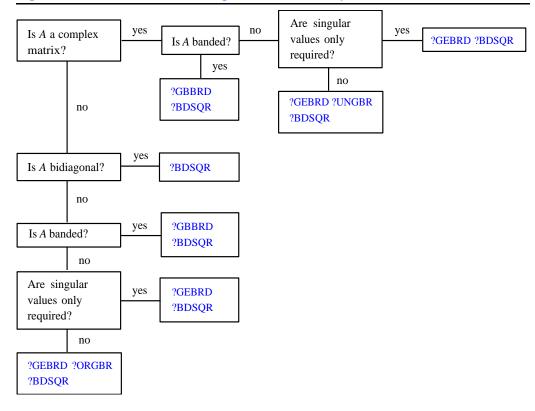
where  $u_i$  and  $v_i$  are the *i*th columns of U and V, respectively.

To find the SVD of a general matrix *A*, call the LAPACK routine **?gebrd** or **?gbbrd** for reducing *A* to a bidiagonal matrix *B* by a unitary (orthogonal) transformation:  $A = QBP^{H}$ . Then call **?bdsqr**, which forms the SVD of a bidiagonal matrix:  $B = U_1 \Sigma V_1^{H}$ .

Thus, the sought-for SVD of A is given by  $A = U\Sigma V^{H} = (QU_{1}) \Sigma (V_{1}^{H}P^{H})$ .

#### Table 5-2Computational Routines for Singular Value Decomposition (SVD)

Operation	Real matrices	Complex matrices
Reduce A to a bidiagonal matrix B: $A = QBP^{H}$ (full storage)	?gebrd	?gebrd
Reduce A to a bidiagonal matrix B: $A = QBP^{H}$ (band storage)	?gbbrd	?gbbrd
Generate the orthogonal (unitary) matrix Q or P	?orgbr	?ungbr
Apply the orthogonal (unitary) matrix Q or <i>P</i>	?ormbr	?unmbr
Form singular value decomposition of the bidiagonal matrix <i>B</i> : $B = U \Sigma V^{H}$	<u>?bdsqr</u> ?bdsdc	<u>?bdsqr</u>



#### Figure 5-1 Decision Tree: Singular Value Decomposition

Figure 5-1 presents a decision tree that helps you choose the right sequence of routines for SVD, depending on whether you need singular values only or singular vectors as well, whether *A* is real or complex, and so on.

You can use the SVD to find a minimum-norm solution to a (possibly) rank-deficient least-squares problem of minimizing  $||Ax-b||_2$ . The effective rank *k* of the matrix *A* can be determined as the number of singular values which exceed a suitable threshold. The minimum-norm solution is

$$x = V_k(\Sigma_k)^{-1}c$$

where  $\Sigma_k$  is the leading *k* by *k* submatrix of  $\Sigma$ , the matrix  $V_k$  consists of the first *k* columns of  $V = PV_1$ , and the vector *c* consists of the first *k* elements of  $U^H b = U_1^H Q^H b$ .

### ?gebrd

*Reduces a general matrix to bidiagonal form.* 

call sgebrd ( m, n, a, lda, d, e, tauq, taup, work, lwork, info )
call dgebrd ( m, n, a, lda, d, e, tauq, taup, work, lwork, info )
call cgebrd ( m, n, a, lda, d, e, tauq, taup, work, lwork, info )
call zgebrd ( m, n, a, lda, d, e, tauq, taup, work, lwork, info )

#### **Discussion**

The routine reduces a general m by n matrix A to a bidiagonal matrix B by an orthogonal (unitary) transformation.

If  $m \ge n$ , the reduction is given by

$$A = QBP^{H} = Q\binom{B_{1}}{0}P^{H} = Q_{1}B_{1}P^{H},$$

where  $B_1$  is an *n* by *n* upper diagonal matrix, *Q* and *P* are orthogonal or, for a complex *A*, unitary matrices;  $Q_1$  consists of the first *n* columns of *Q*.

If m < n, the reduction is given by

$$A = QBP^{H} = Q(B_{1}0)P^{H} = Q_{1}B_{1}P_{1}^{H},$$

where  $B_1$  is an *m* by *m* lower diagonal matrix, *Q* and *P* are orthogonal or, for a complex *A*, unitary matrices;  $P_1$  consists of the first *m* rows of *P*.

The routine does not form the matrices Q and P explicitly, but represents them as products of elementary reflectors. Routines are provided to work with the matrices Q and P in this representation:

If the matrix A is real,

- to compute *Q* and *P* explicitly, call <u>?orgbr</u>.
- to multiply a general matrix by *Q* or *P*, call <u>?ormbr</u>.

If the matrix A is complex,

- to compute *Q* and *P* explicitly, call <u>?ungbr</u>.
- to multiply a general matrix by *Q* or *P*, call <u>?unmbr</u>.

#### **Input Parameters**

m	<b>INTEGER.</b> The number of rows in the matrix $A (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgebrd DOUBLE PRECISION for dgebrd COMPLEX for cgebrd DOUBLE COMPLEX for zgebrd.
	Arrays: a(lda,*) contains the matrix A. The second dimension of a must be at least max(1, n). work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
lwork	<b>INTEGER.</b> The dimension of <i>work</i> ; at least $max(1, m, n)$ . See Application notes for the suggested value of <i>lwork</i> .

#### **Output Parameters**

a	If $m \ge n$ , the diagonal and first super-diagonal of <i>a</i> are overwritten by the upper bidiagonal matrix <i>B</i> . Elements below the diagonal are overwritten by details of <i>Q</i> , and the remaining elements are overwritten by details of <i>P</i> .
	If $m < n$ , the diagonal and first sub-diagonal of a are overwritten by the lower bidiagonal matrix <i>B</i> . Elements above the diagonal are overwritten by details of <i>P</i> , and the remaining elements are overwritten by details of <i>Q</i> .
d	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. Array, <b>DIMENSION</b> at least $max(1, min(m, n))$ . Contains the diagonal elements of <i>B</i> .
е	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. Array, <b>DIMENSION</b> at least $max(1, min(m, n) - 1)$ . Contains the off-diagonal elements of <i>B</i> .

tauq,taup	REAL for sgebrd
	DOUBLE PRECISION for dgebrd COMPLEX for cgebrd
	DOUBLE COMPLEX for zgebrd.
	Arrays, <b>DIMENSION</b> at least max $(1, \min(m, n))$ . Contain further details of the matrices $Q$ and $P$ .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

For better performance, try using lwork = (m + n)*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed matrices Q, B, and P satisfy  $QBP^{H} = A + E$ , where  $||E||_{2} = c(n)\varepsilon ||A||_{2}$ , c(n) is a modestly increasing function of n, and  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations for real flavors is  $(4/3)*n^2*(3*m-n)$  for  $m \ge n$ ,

 $(4/3)*m^2*(3*n-m)$  for m < n.

The number of operations for complex flavors is four times greater.

If *n* is much less than *m*, it can be more efficient to first form the *QR* factorization of *A* by calling <u>?geqrf</u> and then reduce the factor *R* to bidiagonal form. This requires approximately  $2*n^2*(m+n)$  floating-point operations.

If *m* is much less than *n*, it can be more efficient to first form the *LQ* factorization of *A* by calling <u>?gelqf</u> and then reduce the factor *L* to bidiagonal form. This requires approximately  $2*m^2*(m+n)$  floating-point operations.

## ?gbbrd

*Reduces a general band matrix to bidiagonal form.* 

#### **Discussion**

This routine reduces an *m* by *n* band matrix *A* to upper bidiagonal matrix *B*:  $A = QBP^{H}$ . Here the matrices *Q* and *P* are orthogonal (for real *A*) or unitary (for complex *A*). They are determined as products of Givens rotation matrices, and may be formed explicitly by the routine if required. The routine can also update a matrix *C* as follows:  $C = Q^{H}C$ .

#### **Input Parameters**

vect	CHARACTER*1. Must be 'N' or 'Q' or 'P' or 'B'. If $vect = 'N'$ , neither $Q$ nor $P^H$ is generated. If $vect = 'Q'$ , the routine generates the matrix $Q$ . If $vect = 'P'$ , the routine generates the matrix $P^H$ . If $vect = 'B'$ , the routine generates both $Q$ and $P^H$ .
m	<b>INTEGER.</b> The number of rows in the matrix $A \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
ncc	<b>INTEGER.</b> The number of columns in $C$ ( <i>ncc</i> $\ge$ 0).
kl	INTEGER. The number of sub-diagonals within the
	band of $A$ (kl $\geq 0$ ).
ku	INTEGER. The number of super-diagonals within the
	band of $A$ ( $ku \ge 0$ ).

ab,c,work	REAL for sgbbrd DOUBLE PRECISION for dgbbrd
	COMPLEX for cgbbrd
	DOUBLE COMPLEX for zgbbrd. Arrays:
	ab(1dab, *) contains the matrix A in band storage (see <u>Matrix Storage Schemes</u> ). The second dimension of a must be at least max(1, n).
	c(1dc, *) contains an <i>m</i> by <i>ncc</i> matrix <i>C</i> . If <i>ncc</i> = 0, the array <i>c</i> is not referenced. The second dimension of <i>c</i> must be at least max(1, <i>ncc</i> ).
	<pre>work(*) is a workspace array. The dimension of work must be at least $2*\max(m, n)$ for real flavors, or $\max(m, n)$ for complex flavors.</pre>
ldab	<b>INTEGER.</b> The first dimension of the array <i>ab</i> $(1dab \ge kl + ku + 1)$ .
ldq	<b>INTEGER.</b> The first dimension of the output array $q$ . $ldq \ge max(1, m)$ if $vect = 'Q'$ or 'B', $ldq \ge 1$ otherwise.
ldpt	<b>INTEGER.</b> The first dimension of the output array $pt$ . $ldpt \ge max(1, n)$ if $vect = 'P'$ or 'B', $ldpt \ge 1$ otherwise.
ldc	<b>INTEGER.</b> The first dimension of the array $c$ . $ldc \ge max(1, m)$ if $ncc > 0$ ; $ldc \ge 1$ if $ncc = 0$ .
rwork	REAL for cgbbrd DOUBLE PRECISION for zgbbrd. A workspace array, DIMENSION at least max(m, n).
Output Parameters	

ab	Overwritten by values generated during the reduction.
d	<b>REAL</b> for single-precision flavors
	DOUBLE PRECISION for double-precision flavors.
	Array, DIMENSION at least max(1, min( <i>m</i> , <i>n</i> )).
	Contains the diagonal elements of the matrix <i>B</i> .

e	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. Array, <b>DIMENSION</b> at least $max(1, min(m, n) - 1)$ . Contains the off-diagonal elements of <i>B</i> .
g, pt	REAL for sgebrd DOUBLE PRECISION for dgebrd COMPLEX for cgebrd DOUBLE COMPLEX for zgebrd. Arrays:
	q(ldq, *) contains the output <i>m</i> by <i>m</i> matrix <i>Q</i> . The second dimension of <i>q</i> must be at least max(1, <i>m</i> ).
	$p(ldpt, *)$ contains the output <i>n</i> by <i>n</i> matrix $P^{H}$ . The second dimension of <i>pt</i> must be at least max $(1, n)$ .
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

The computed matrices *Q*, *B*, and *P* satisfy  $QBP^H = A + E$ , where  $||E||_2 = c(n)\varepsilon ||A||_2$ , c(n) is a modestly increasing function of *n*, and  $\varepsilon$  is the machine precision.

If m = n, the total number of floating-point operations for real flavors is approximately the sum of:

if $vect = 'N'$ and $ncc = 0$ ,
if <i>C</i> is updated, and
if either $Q$ or $P^H$ is generated (double this if both).

To estimate the number of operations for complex flavors, use the same formulas with the coefficients 20 and 10 (instead of 6 and 3).

### ?orgbr

Generates the real orthogonal matrix Q or  $P^T$  determined by ?gebrd.

call sorgbr ( vect, m, n, k, a, lda, tau, work, lwork, info )
call dorgbr ( vect, m, n, k, a, lda, tau, work, lwork, info )

#### **Discussion**

The routine generates the whole or part of the orthogonal matrices Q and  $P^T$  formed by the routines sgebrd/dgebrd (see <u>page 5-76</u>). Use this routine after a call to sgebrd/dgebrd. All valid combinations of arguments are described in *Input parameters*. In most cases you'll need the following:

To compute the whole *m* by *m* matrix *Q*: call ?orgbr ( 'Q', m, m, n, a ... ) (note that the array *a* must have at least *m* columns). To form the *n* leading columns of *Q* if m > n: call ?orgbr ( 'Q', m, n, n, a ... ) To compute the whole *n* by *n* matrix  $P^T$ : call ?orgbr ( 'P', n, n, m, a ... ) (note that the array *a* must have at least *n* rows).

To form the *m* leading rows of  $P^T$  if m < n: call ?orgbr ( 'P', m, n, m, a ... )

#### **Input Parameters**

vect	CHARACTER*1. Must be 'Q' or 'P'. If vect = 'Q', the routine generates the matrix $Q$ . If vect = 'P', the routine generates the matrix $P^T$ .
m	<b>INTEGER</b> . The number of required rows of $Q$ or $P^T$ .
n	<b>INTEGER</b> . The number of required columns of $Q$ or $P^T$ .
k	<b>INTEGER.</b> One of the dimensions of A in <b>?gebrd</b> : If $vect = 'Q'$ , the number of columns in A; If $vect = 'P'$ , the number of rows in A.

	Constraints: $m \ge 0$ , $n \ge 0$ , $k \ge 0$ . For vect = 'Q': $k \le n \le m$ if $m > k$ , or $m = n$ if $m \le k$ . For vect = 'P': $k \le m \le n$ if $n > k$ , or $m = n$ if $n \le k$ .
a, work	<pre>REAL for sorgbr DOUBLE PRECISION for dorgbr. Arrays: a(lda,*) is the array a as returned by ?gebrd. The second dimension of a must be at least max(1, n).</pre>
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, m)$ .
tau	<b>REAL</b> for sorgbr <b>DOUBLE PRECISION</b> for dorgbr. For vect = 'Q', the array tauq as returned by ?gebrd. For vect = 'P', the array taup as returned by ?gebrd. The dimension of tau must be at least max(1, min( $m,k$ )) for vect = 'Q', or max(1, min( $m, k$ )) for vect = 'P'.
lwork	<b>INTEGER</b> . The size of the <i>work</i> array. See <i>Application notes</i> for the suggested value of <i>lwork</i> .

#### **Output Parameters**

a	Overwritten by the orthogonal matrix $Q$ or $P^T$ (or the leading rows or columns thereof) as specified by <i>vect</i> , <i>m</i> , and <i>n</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

#### **Application Notes**

For better performance, try using *lwork* = min(m, n)*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work(1)* and use this value for subsequent runs.

The computed matrix *Q* differs from an exactly orthogonal matrix by a matrix *E* such that  $||E||_2 = O(\varepsilon)$ .

The approximate numbers of floating-point operations for the cases listed in *Discussion* are as follows:

To form the whole of *Q*:

$(4/3)n(3m^2 - 3m*n + n^2)$	if $m > n$ ;
$(4/3)m^3$	if <u>m ≤n</u> .

To form the *n* leading columns of *Q* when m > n:

To form the whole of  $P^T$ :

(4/3) ^{n³}	if $m \ge n$ ;
$(4/3)m(3n^2 - 3m*n + m^2)$	if <i>m</i> < <i>n</i> .

To form the *m* leading columns of  $P^T$  when m < n:

$(2/3)n^{-}(3m - n^{-})$ II $m > n$ .	$(2/3)n^2(3m - n^2)$	if <u>m</u> > <u>n</u> .
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The complex counterpart of this routine is <u>?ungbr</u>.

### ?ormbr

Multiplies an arbitrary real matrix by the real orthogonal matrix Q or  $P^T$ determined by ?gebrd.

call sormbr (vect, side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info) call dormbr (vect, side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

#### Discussion

Given an arbitrary real matrix *C*, this routine forms one of the matrix products  $QC, Q^TC, CQ, CQ^T, PC, P^TC, CP$ , or  $CP^T$ , where Q and P are orthogonal matrices computed by a call to sgebrd/dgebrd (see page 5-76). The routine overwrites the product on *C*.

#### **Input Parameters**

In the descriptions below, $r$ denotes the order of $Q$ or $P^T$ : If <i>side</i> = 'L', $r = m$ ; if <i>side</i> = 'R', $r = n$ .	
vect	CHARACTER*1. Must be 'Q' or 'P'. If $vect = 'Q'$ , then Q or $Q^T$ is applied to C. If $vect = 'P'$ , then P or $P^T$ is applied to C.
side	CHARACTER*1. Must be 'L' or 'R'. If <i>side</i> = 'L', multipliers are applied to <i>C</i> from the left. If <i>side</i> = 'R', they are applied to <i>C</i> from the right.
trans	CHARACTER*1. Must be 'N' or 'T'. If $trans =$ 'N', then $Q$ or $P$ is applied to $C$ . If $trans =$ 'T', then $Q^T$ or $P^T$ is applied to $C$ .
m	<b>INTEGER</b> . The number of rows in <i>C</i> .
п	<b>INTEGER</b> . The number of columns in <i>C</i> .
k	<b>INTEGER.</b> One of the dimensions of A in ?gebrd: If $vect = 'Q'$ , the number of columns in A; If $vect = 'P'$ , the number of rows in A.
	Constraints: $m \ge 0, n \ge 0, k \ge 0$ .

a, c, work	REAL for sormbr DOUBLE PRECISION for dormbr. Arrays: a(lda,*) is the array a as returned by ?gebrd. Its second dimension must be at least max(1, min(r,k))
	for $vect = 'Q'$ , or $max(1, r)$ ) for $vect = 'P'$ . c(ldc, *) holds the matrix C.
	Its second dimension must be at least $max(1, n)$ .
	work(lwork) is a workspace array.
lda	INTEGER. The first dimension of a. Constraints: $lda \ge max(1, r)$ if $vect = 'Q'$ ; $lda \ge max(1, min(r,k))$ if $vect = 'P'$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ ; $ldc \ge max(1, m)$ .
tau	REAL for sormbr DOUBLE PRECISION for dormbr. Array, DIMENSION at least max (1, min( <i>r</i> , <i>k</i> )). For <i>vect</i> = 'Q', the array <i>tauq</i> as returned by ?gebrd. For <i>vect</i> = 'P', the array <i>taup</i> as returned by ?gebrd.
lwork	<pre>INTEGER. The size of the work array. Constraints: lwork ≥ max(1, n) if side = 'L'; lwork ≥ max(1, m) if side = 'R'. See Application notes for the suggested value of lwork.</pre>
Output Parame	ters

#### Output Parameters

С	Overwritten by the product $QC$ , $Q^TC$ , $CQ$ , $CQ^T$ , $PC$ , $P^TC$ , $CP$ , or $CP^T$ , as specified by <i>vect</i> , <i>side</i> , and
	trans.
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

For better performance, try using

lwork = n*blocksize for side = 'L', or lwork = m*blocksize for side = 'R',

where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work(1)* and use this value for subsequent runs.

The computed product differs from the exact product by a matrix *E* such that  $||E||_2 = O(\varepsilon) ||C||_2$ .

The total number of floating-point operations is approximately

2*n*k(2*m-k)	if <i>side</i> = 'L' and $m \ge k$ ;
2*m*k(2*n-k)	if <i>side</i> = 'R' and $n \ge k$ ;
2*m ² *n	if <i>side</i> = 'L' and $m < k$ ;
$2*n^2*m$	if <i>side</i> = 'R' and $n < k$ .

The complex counterpart of this routine is <u>?unmbr</u>.

### ?ungbr

Generates the complex unitary matrix Q or  $P^H$  determined by ?gebrd.

call cungbr ( vect, m, n, k, a, lda, tau, work, lwork, info )
call zungbr ( vect, m, n, k, a, lda, tau, work, lwork, info )

#### **Discussion**

The routine generates the whole or part of the unitary matrices Q and  $P^H$  formed by the routines cgebrd/zgebrd (see page 5-76). Use this routine after a call to cgebrd/zgebrd. All valid combinations of arguments are described in *Input Parameters*; in most cases you'll need the following:

To compute the whole *m* by *m* matrix *Q*: call ?ungbr ( 'Q', m, m, n, a ... ) (note that the array *a* must have at least *m* columns). To form the *n* leading columns of *Q* if m > n: call ?ungbr ( 'Q', m, n, n, a ... ) To compute the whole *n* by *n* matrix  $P^{H}$ : call ?ungbr ( 'P', n, n, m, a ... ) (note that the array *a* must have at least *n* rows).

To form the *m* leading rows of  $P^H$  if m < n: call ?ungbr ( 'P', m, n, m, a ... )

#### **Input Parameters**

vect	CHARACTER*1. Must be 'Q' or 'P'. If $vect = 'Q'$ , the routine generates the matrix $Q$ . If $vect = 'P'$ , the routine generates the matrix $P^{H}$ .
m	<b>INTEGER</b> . The number of required rows of $Q$ or $P^H$ .
n	<b>INTEGER</b> . The number of required columns of $Q$ or $P^H$ .
k	<b>INTEGER.</b> One of the dimensions of A in <b>?gebrd</b> : If $vect = 'Q'$ , the number of columns in A; If $vect = 'P'$ , the number of rows in A.

	Constraints: $m \ge 0$ , $n \ge 0$ , $k \ge 0$ . For vect = 'Q': $k \le n \le m$ if $m > k$ , or $m = n$ if $m \le k$ . For vect = 'P': $k \le m \le n$ if $n > k$ , or $m = n$ if $n \le k$ .
a, work	COMPLEX for cungbr DOUBLE COMPLEX for zungbr. Arrays: a(lda,*) is the array a as returned by ?gebrd. The second dimension of a must be at least max(1, n).
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
tau	COMPLEX for cungbr DOUBLE COMPLEX for zungbr. For $vect = 'Q'$ , the array <i>tauq</i> as returned by ?gebrd. For $vect = 'P'$ , the array <i>taup</i> as returned by ?gebrd. The dimension of <i>tau</i> must be at least max(1, min( <i>m</i> , <i>k</i> )) for $vect = 'Q'$ , or max(1, min( <i>m</i> , <i>k</i> )) for $vect = 'P'$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array. Constraint: $lwork \ge max(1, min(m, n))$ . See <i>Application notes</i> for the suggested value of <i>lwork</i> .

### **Output Parameters**

a	Overwritten by the orthogonal matrix $Q$ or $P^T$ (or the leading rows or columns thereof) as specified by <i>vect</i> , <i>m</i> , and <i>n</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

For better performance, try using lwork = min(m, n)*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed matrix *Q* differs from an exactly orthogonal matrix by a matrix *E* such that  $||E||_2 = O(\varepsilon)$ .

The approximate numbers of floating-point operations for the cases listed in *Discussion* are as follows:

To form the whole of *Q*:

$(16/3)n(3m^2 - 3m*n + n^2)$	if $m > n$ ;
$(16/3)m^3$	if <u>m ≤n</u> .

To form the *n* leading columns of *Q* when m > n:

To form the whole of  $P^T$ :

(16/3	) <mark>n</mark> 3				if <mark>r</mark>	n≥n;
(16/3	) <mark>m</mark> (3	n ² ·	- 3 <u>m</u> *	$(n + m^2)$	if <mark>r</mark>	<i>n</i> < <i>n</i> .
					a = T	

To form the *m* leading columns of  $P^T$  when m < n:

$$(8/3)n^2(3m - n^2)$$
 if  $m > n$ .

The real counterpart of this routine is <u>?orgbr</u>.

### ?unmbr

Multiplies an arbitrary complex matrix by the unitary matrix Q or P determined by ?gebrd.

call cunmbr (vect,side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info)
call zunmbr (vect,side,trans,m,n,k,a,lda,tau,c,ldc,work,lwork,info)

#### **Discussion**

Given an arbitrary complex matrix C, this routine forms one of the matrix products QC,  $Q^{H}C$ , CQ,  $CQ^{H}$ , PC,  $P^{H}C$ , CP, or  $CP^{H}$ , where Q and P are orthogonal matrices computed by a call to cgebrd/zgebrd (see page 5-76). The routine overwrites the product on C.

#### **Input Parameters**

In the descriptions below,  $\mathbf{r}$  denotes the order of Q or  $P^H$ : If side = 'L', r = m; if side = 'R', r = n. vect CHARACTER*1. Must be 'Q' or 'P'. If **vect** = 'Q', then Q or  $Q^H$  is applied to C. If vect = P', then P or  $P^H$  is applied to C. CHARACTER*1. Must be 'L' or 'R'. side If *side* = 'L', multipliers are applied to C from the left. If side = 'R', they are applied to C from the right. CHARACTER*1. Must be 'N' or 'C'. trans If trans = 'N', then Q or P is applied to C. If *trans* = 'C', then  $Q^H$  or  $P^H$  is applied to C. INTEGER. The number of rows in *C*. т INTEGER. The number of columns in C. n **INTEGER**. One of the dimensions of *A* in ?gebrd: k If *vect* = 'Q', the number of columns in A; If vect = 'P', the number of rows in A. Constraints:  $m \ge 0, n \ge 0, k \ge 0$ .

a, c, work	COMPLEX for cunmbr DOUBLE COMPLEX for zunmbr. Arrays:
	a(1da, *) is the array $a$ as returned by ?gebrd. Its second dimension must be at least max(1, min( $r,k$ )) for $vect = 'Q'$ , or max(1, $r$ )) for $vect = 'P'$ .
	c(ldc, *) holds the matrix C. Its second dimension must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of <i>a</i> . Constraints: $lda \ge max(1, r)$ if $vect = 'Q'$ ; $lda \ge max(1, min(r,k))$ if $vect = 'P'$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ ; $ldc \ge max(1, m)$ .
tau	COMPLEX for cummbr DOUBLE COMPLEX for zummbr. Array, DIMENSION at least max $(1, \min(r, k))$ . For vect = 'Q', the array tauq as returned by ?gebrd. For vect = 'P', the array taup as returned by ?gebrd.
lwork	<pre>INTEGER. The size of the work array. Constraints: lwork ≥ max(1, n) if side = 'L'; lwork ≥ max(1, m) if side = 'R'. See Application notes for the suggested value of lwork.</pre>
Output Deremo	toro

#### **Output Parameters**

С	Overwritten by the product $QC$ , $Q^{H}C$ , $CQ$ , $CQ^{H}$ , $PC$ , $P^{H}C$ , $CP$ , or $CP^{H}$ , as specified by <u>vect</u> , <u>side</u> , and
	trans.
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

For better performance, try using

lwork = n*blocksize for side = 'L', or lwork = m*blocksize for side = 'R',

where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work(1)* and use this value for subsequent runs.

The computed product differs from the exact product by a matrix *E* such that  $||E||_2 = O(\varepsilon) ||C||_2$ .

The total number of floating-point operations is approximately

8*n*k(2*m-k)	if side = 'L' and $m \ge k$ ;
8*m*k(2*n-k)	if <i>side</i> = 'R' and $n \ge k$ ;
8*m ² *n	if <i>side</i> = 'L' and $m < k$ ;
$8*n^2*m$	if <i>side</i> = 'R' and $n < k$ .

The real counterpart of this routine is <u>?ormbr</u>.

### ?bdsqr

Computes the singular value decomposition of a general matrix that has been reduced to bidiagonal form.

```
call sbdsqr ( uplo, n, ncvt, nru, ncc, d, e, vt, ldvt, u, ldu,
        c, ldc, work, info )
call dbdsqr ( uplo, n, ncvt, nru, ncc, d, e, vt, ldvt, u, ldu,
        c, ldc, work, info )
call cbdsqr ( uplo, n, ncvt, nru, ncc, d, e, vt, ldvt, u, ldu,
        c, ldc, work, info )
call zbdsqr ( uplo, n, ncvt, nru, ncc, d, e, vt, ldvt, u, ldu,
        c, ldc, work, info )
```

#### Discussion

This routine computes the singular values and, optionally, the right and/or left singular vectors from the <u>Singular Value Decomposition</u> (SVD) of a real *n*-by-*n* (upper or lower) bidiagonal matrix *B* using the implicit zero-shift *QR* algorithm. The SVD of *B* has the form  $B = Q * S * P^H$  where *S* is the diagonal matrix of singular values, *Q* is an orthogonal matrix of left singular vectors, and *P* is an orthogonal matrix of right singular vectors. If left singular vectors are requested, this subroutine actually returns U * Q instead of *Q*, and, if right singular vectors are requested, this subroutine returns  $P^H * VT$  instead of  $P^H$ , for given real/complex input matrices *U* and *VT*. When *U* and *VT* are the orthogonal/unitary matrices that reduce a general matrix *A* to bidiagonal form: A = U * B * VT, as computed by ?gebrd, then  $A = (U * Q) * S * (P^H * VT)$ 

is the SVD of A. Optionally, the subroutine may also compute  $Q^H * C$  for a given real/complex input matrix C.

#### **Input Parameters**

```
uploCHARACTER*1. Must be 'U' or 'L'.If uplo = 'U', B is an upper bidiagonal matrix.If uplo = 'L', B is a lower bidiagonal matrix.
```

n	<b>INTEGER.</b> The order of the matrix $B$ ( $n \ge 0$ ).
ncvt	<b>INTEGER.</b> The number of columns of the matrix <i>VT</i> , that is, the number of right singular vectors ( $ncvt \ge 0$ ). Set $ncvt = 0$ if no right singular vectors are required.
nru	<b>INTEGER.</b> The number of rows in <i>U</i> , that is, the number of left singular vectors ( $nru \ge 0$ ). Set $nru = 0$ if no left singular vectors are required.
ncc	<b>INTEGER.</b> The number of columns in the matrix <i>C</i> used for computing the product $Q^H C$ ( <i>ncc</i> $\ge 0$ ). Set <i>ncc</i> = 0 if no matrix <i>C</i> is supplied.
d, e, work	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. Arrays: d(*) contains the diagonal elements of <i>B</i> . The dimension of <i>d</i> must be at least max $(1, n)$ .
	e(*) contains the $(n-1)$ off-diagonal elements of $B$ . The dimension of $e$ must be at least max $(1, n)$ . e(n) is used for workspace.
	work(*) is a workspace array. The dimension of work must be at least max(1, 2*n) if $ncvt = nru = ncc = 0$ ; max(1, 4*(n-1)) otherwise.
vt, u, c	<pre>REAL for sbdsqr DOUBLE PRECISION for dbdsqr COMPLEX for cbdsqr DOUBLE COMPLEX for zbdsqr. Arrays: vt(ldvt,*) contains an n by ncvt matrix VT. The second dimension of vt must be at least max(1, ncvt). vt is not referenced if ncvt = 0. u(ldu,*) contains an nru by n unit matrix U. The second dimension of u must be at least max(1, n).</pre>
	<b>u</b> is not referenced if $nru = 0$ .

	$c(ldc, *)$ contains the matrix C for computing the product $Q^{H} * C$ . The second dimension of c must be at least max $(1,ncc)$ . The array is not referenced if $ncc = 0$ .
ldvt	<b>INTEGER.</b> The first dimension of vt. Constraints: $ldvt \ge max(1, n)$ if $ncvt > 0$ ; $ldvt \ge 1$ if $ncvt = 0$ .
ldu	<b>INTEGER.</b> The first dimension of <i>u</i> . Constraint: $ldu \ge max(1, nru)$ .
ldc	<b>INTEGER.</b> The first dimension of <i>c</i> . Constraints: $ldc \ge max(1, n)$ if $ncc > 0$ ; $ldc \ge 1$ otherwise.

#### **Output Parameters**

d	On exit, if $info = 0$ , overwritten by the singular values in decreasing order (see <i>info</i> ).
е	On exit, if $info = 0$ , $e$ is destroyed. See also $info$ below.
С	Overwritten by the product $Q^H * C$ .
vt	On exit, this array is overwritten by $P^H * VT$ .
u	On exit, this array is overwritten by $U * Q$ .
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = i, the algorithm failed to converge; i specifies how many off-diagonals did not converge. In this case, d and e contain on exit the diagonal and off-diagonal elements, respectively, of a bidiagonal matrix orthogonally equivalent to B.</pre>

#### **Application Notes**

Each singular value and singular vector is computed to high relative accuracy. However, the reduction to bidiagonal form (prior to calling the routine) may decrease the relative accuracy in the small singular values of the original matrix if its singular values vary widely in magnitude. If  $\sigma_i$  is an exact singular value of *B*, and  $s_i$  is the corresponding computed value, then

 $|s_i - \sigma_i| \leq p(m, n) \varepsilon \sigma_i$ 

where p(m, n) is a modestly increasing function of *m* and *n*, and  $\varepsilon$  is the machine precision. If only singular values are computed, they are computed more accurately than when some singular vectors are also computed (that is, the function p(m, n) is smaller).

If  $u_i$  is the corresponding exact left singular vector of *B*, and  $w_i$  is the corresponding computed left singular vector, then the angle  $\theta(u_i, w_i)$  between them is bounded as follows:

 $\theta(u_i, w_i) \leq p(m, n) \varepsilon / \min_{i \neq j} (|\sigma_i - \sigma_j| / |\sigma_i + \sigma_j|).$ 

Here  $\min_{i \neq j} (|\sigma_i - \sigma_j| / |\sigma_i + \sigma_j|)$  is the *relative gap* between  $\sigma_i$  and the other singular values. A similar error bound holds for the right singular vectors.

The total number of real floating-point operations is roughly proportional to  $n^2$  if only the singular values are computed. About  $6n^2 * nru$  additional operations  $(12n^2 * nru$  for complex flavors) are required to compute the left singular vectors and about  $6n^2 * ncvt$  operations  $(12n^2 * ncvt$  for complex flavors) to compute the right singular vectors.

### ?bdsdc

Computes the singular value decomposition of a real bidiagonal matrix using a divide and conquer method.

#### **Discussion**

This routine computes the <u>Singular Value Decomposition</u> (SVD) of a real *n*-by-*n* (upper or lower) bidiagonal matrix *B*:  $B = U \Sigma V^{T}$ , using a divide and conquer method, where  $\Sigma$  is a diagonal matrix with non-negative diagonal elements (the singular values of *B*), and *U* and *V* are orthogonal matrices of left and right singular vectors, respectively. ?bdsdc can be used to compute all singular values, and optionally, singular vectors or singular vectors in compact form.

#### **Input Parameters**

CHARACTER*1. Must be 'U' or 'L'.
If $uplo = 'U'$ , B is an upper bidiagonal matrix.
If $uplo = 'L'$ , B is a lower bidiagonal matrix.
CHARACTER*1. Must be 'N', 'P', or 'I'.
If $compq = 'N'$ , compute singular values only.
If <i>compq</i> = 'P', compute singular values and compute
singular vectors in compact form.
If <i>compq</i> = 'I', compute singular values and singular
vectors.
<b>INTEGER.</b> The order of the matrix $B$ $(n \ge 0)$ .
REAL for sbdsdc
DOUBLE PRECISION for sbdsdc.
Arrays:

	d(*) contains the <i>n</i> diagonal elements of the bidiagonal matrix <i>B</i> . The dimension of <i>d</i> must be at least max(1, <i>n</i> ). e(*) contains the off-diagonal elements of the bidiagonal matrix <i>B</i> . The dimension of <i>e</i> must be at least max(1, <i>n</i> ).
	<pre>work(*) is a workspace array. The dimension of work must be at least: $max(1, 4*n)$, if $compq = 'N';$ $max(1, 6*n)$, if $compq = 'P';$ $max(1, 3*n^2+4*n)$, if $compq = 'I'.$</pre>
ldu	<b>INTEGER.</b> The first dimension of the output array $u$ ; $ldu \ge 1$ . If singular vectors are desired, then $ldu \ge max(1, n)$ .
ldvt	<b>INTEGER.</b> The first dimension of the output array $vt$ ; $ldvt \ge 1$ . If singular vectors are desired, then $ldvt \ge max(1, n)$ .
iwork	<b>INTEGER.</b> Workspace array, dimension at least max(1, 8*n).

### **Output Parameters**

d	If $info = 0$ , overwritten by the singular values of <i>B</i> .
е	On exit, e is overwritten.
u, vt, q	REAL for sbdsdc DOUBLE PRECISION for sbdsdc. Arrays: $u(ldu, *)$ , $vt(ldvt, *)$ , $q(*)$ . If $compq = 'I'$ , then on exit $u$ contains the left singular vectors of the bidiagonal matrix $B$ , unless $info \neq 0$ (see info). For other values of $compq$ , $u$ is not referenced. The second dimension of $u$ must be at least max(1, $n$ ).
	If $compq = 'I'$ , then on exit $vt$ contains the right singular vectors of the bidiagonal matrix <i>B</i> , unless $info \neq 0$ (see info). For other values of compq, $vt$ is not referenced. The second dimension of $vt$ must be at least max $(1,n)$ .

iq

info

If compq = 'P', then on exit, if info = 0, q and iq contain the left and right singular vectors in a compact form. Specifically, q contains all the REAL (for sbdsdc) or DOUBLE PRECISION (for dbdsdc) data for singular vectors. For other values of compq, q is not referenced. See Application notes for details.

#### INTEGER.

#### Array: iq(*).

If *compq* = 'P', then on exit, if *info* = 0, *q* and *iq* contain the left and right singular vectors in a compact form. Specifically, *iq* contains all the INTEGER data for singular vectors. For other values of *compq*, *iq* is not referenced. See Application notes for details.

#### INTEGER.

If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value. If info = i, the algorithm failed to compute a singular value. The update process of divide and conquer failed.

#### Symmetric Eigenvalue Problems

*Symmetric eigenvalue problems* are posed as follows: given an *n* by *n* real symmetric or complex Hermitian matrix *A*, find the *eigenvalues*  $\lambda$  and the corresponding *eigenvectors z* that satisfy the equation

 $Az = \lambda z$ . (or, equivalently,  $z^H A = \lambda z^H$ ).

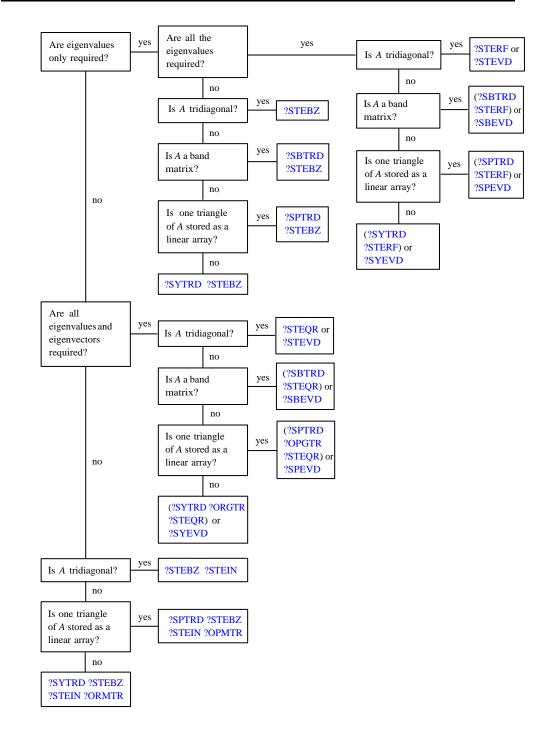
In such eigenvalue problems, all n eigenvalues are real not only for real symmetric but also for complex Hermitian matrices A, and there exists an orthonormal system of n eigenvectors. If A is a symmetric or Hermitian positive-definite matrix, all eigenvalues are positive.

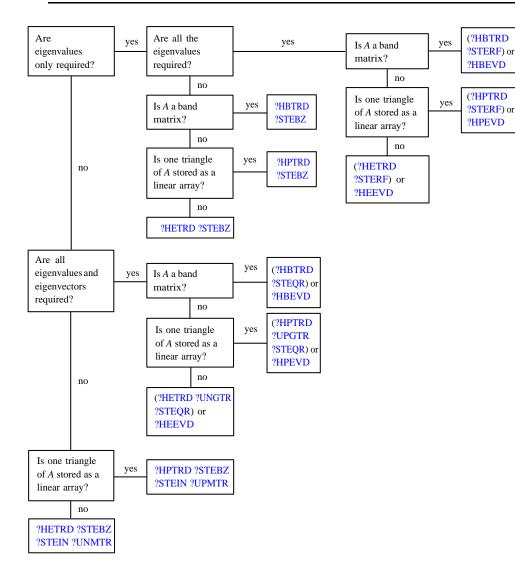
To solve a symmetric eigenvalue problem with LAPACK, you usually need to reduce the matrix to tridiagonal form and then solve the eigenvalue problem with the tridiagonal matrix obtained. LAPACK includes routines for reducing the matrix to a tridiagonal form by an orthogonal (or unitary) similarity transformation  $A = QTQ^H$  as well as for solving tridiagonal symmetric eigenvalue problems. These routines are listed in <u>Table 5-3</u>.

There are different routines for symmetric eigenvalue problems, depending on whether you need all eigenvectors or only some of them or eigenvalues only, whether the matrix *A* is positive-definite or not, and so on. These routines are based on three primary algorithms for computing eigenvalues and eigenvectors of symmetric problems: the divide and conquer algorithm, the QR algorithm, and bisection followed by inverse iteration. The divide and conquer algorithm is generally more efficient and is recommended for computing all eigenvalues and eigenvectors. Furthermore, to solve an eigenvalue problem using the divide and conquer algorithm, you need to call only one routine. In general, more than one routine has to be called if the QR algorithm or bisection followed by inverse iteration is used.

Decision tree in <u>Figure 5-2</u> will help you choose the right routine or sequence of routines for eigenvalue problems with real symmetric matrices. A similar decision tree for complex Hermitian matrices is presented in <u>Figure 5-3</u>.







#### Figure 5-3 Decision Tree: Complex Hermitian Eigenvalue Problems

Operation	Real symmetric matrices	Complex Hermitian matrices
Reduce to tridiagonal form $A = QTQ^{H}$ (full storage)	?sytrd	?hetrd
Reduce to tridiagonal form $A = QTQ^{H}$ (packed storage)	?sptrd	?hptrd
Reduce to tridiagonal form $A = QTQ^H$ (band storage).	?sbtrd	?hbtrd
Generate matrix Q (full storage)	?orgtr	?ungtr
Generate matrix Q (packed storage)	?opgtr	?upgtr
Apply matrix Q (full storage)	<u>?ormtr</u>	<u>?unmtr</u>
Apply matrix Q (packed storage)	?opmtr	?upmtr
Find all eigenvalues of a tridiagonal matrix $T$	<u>?sterf</u>	
Find all eigenvalues and eigenvectors of a tridiagonal matrix $T$	<u>?steqr</u> <u>?stedc</u>	<u>?steqr</u> <u>?stedc</u>
Find all eigenvalues and eigenvectors of a tridiagonal positive-definite matrix <i>T</i> .	?pteqr	?pteqr
Find selected eigenvalues of a tridiagonal matrix <i>T</i>	<u>?stebz</u> ?stegr	?stegr
Find selected eigenvectors of a tridiagonal matrix <i>T</i>	?stein ?stegr	<u>?stein</u> ?stegr
Compute the reciprocal condition numbers for the eigenvectors	?disna	?disna

# Table 5-3Computational Routines for Solving Symmetric Eigenvalue<br/>Problems

### ?sytrd

*Reduces a real symmetric matrix to tridiagonal form.* 

```
call ssytrd ( uplo,n,a,lda,d,e,tau,work,lwork,info )
call dsytrd ( uplo,n,a,lda,d,e,tau,work,lwork,info )
```

#### **Discussion**

This routine reduces a real symmetric matrix A to symmetric tridiagonal form T by an orthogonal similarity transformation:  $A = QTQ^{T}$ . The orthogonal matrix Q is not formed explicitly but is represented as a product of n-1 elementary reflectors. Routines are provided for working with Q in this representation. (They are described later in this section.)

#### **Input Parameters**

uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , a stores the upper triangular part of A. If $uplo = 'L'$ , a stores the lower triangular part of A.
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
a, work	REAL for ssytrd DOUBLE PRECISION for dsytrd. a(lda,*) is an array containing either upper or lower triangular part of the matrix A, as specified by uplo. The second dimension of a must be at least max(1, n).
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, n)$ .
lwork	<b>INTEGER.</b> The size of the work array $(lwork \ge n)$ See Application notes for the suggested value of $lwork$ .

#### **Output Parameters**

- а
- Overwritten by the tridiagonal matrix T and details of the orthogonal matrix Q, as specified by <u>uplo</u>.

d, e, tau	REAL for ssytrd
	DOUBLE PRECISION for dsytrd.
	Arrays:
	d(*) contains the diagonal elements of the matrix <i>T</i> . The dimension of <i>d</i> must be at least max $(1, n)$ .
	e(*) contains the off-diagonal elements of <i>T</i> . The dimension of $e$ must be at least max $(1, n-1)$ .
	tau(*) stores further details of the orthogonal matrix $Q$ . The dimension of $tau$ must be at least max $(1, n-1)$ .
work(1)	If <i>info</i> =0, on exit <i>work(1)</i> contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

For better performance, try using *lwork* =n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed matrix *T* is exactly similar to a matrix A + E, where  $||E||_2 = c(n)\varepsilon ||A||_2$ , c(n) is a modestly increasing function of *n*, and  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations is  $(4/3)n^3$ .

After calling this routine, you can call the following:

<u>?orgtr</u>	to form the computed matrix $Q$ explicitly;
<u>?ormtr</u>	to multiply a real matrix by $Q$ .

The complex counterpart of this routine is <u>?hetrd</u>.

### ?orgtr

Generates the real orthogonal matrix Q determined by ?sytrd.

call sorgtr ( uplo, n, a, lda, tau, work, lwork, info )
call dorgtr ( uplo, n, a, lda, tau, work, lwork, info )

#### **Discussion**

The routine explicitly generates the *n* by *n* orthogonal matrix *Q* formed by **?sytrd** (see <u>page 5-105</u>) when reducing a real symmetric matrix *A* to tridiagonal form:  $A = QTQ^{T}$ . Use this routine after a call to **?sytrd**.

#### **Input Parameters**

uplo	CHARACTER*1. Must be 'U' or 'L'. Use the same uplo as supplied to ?sytrd.
п	<b>INTEGER.</b> The order of the matrix $Q$ $(n \ge 0)$ .
a, tau, work	<pre>REAL for sorgtr DOUBLE PRECISION for dorgtr. Arrays: a(lda,*) is the array a as returned by ?sytrd. The second dimension of a must be at least max(1, n).</pre>
	tau(*) is the array $tau$ as returned by ?sytrd. The dimension of $tau$ must be at least max $(1, n-1)$ .
7.7.	work (lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
lwork	<b>INTEGER.</b> The size of the work array $(lwork \ge n)$ See Application notes for the suggested value of $lwork$ .

#### **Output Parameters**

а

Overwritten by the orthogonal matrix Q.

work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

#### **Application Notes**

For better performance, try using lwork = (n-1)*blocksize, where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed matrix *Q* differs from an exactly orthogonal matrix by a matrix *E* such that  $||E||_2 = O(\varepsilon)$ , where  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations is  $(4/3)n^3$ .

The complex counterpart of this routine is <u>?ungtr</u>.

## ?ormtr

Multiplies a real matrix by the real orthogonal matrix Q determined by ?sytrd.

call sormtr ( side,uplo,trans,m,n,a,lda,tau,c,ldc,work,lwork,info )
call dormtr ( side,uplo,trans,m,n,a,lda,tau,c,ldc,work,lwork,info )

### **Discussion**

The routine multiplies a real matrix *C* by *Q* or  $Q^T$ , where *Q* is the orthogonal matrix *Q* formed by **?sytrd** (see <u>page 5-105</u>) when reducing a real symmetric matrix *A* to tridiagonal form:  $A = QTQ^T$ . Use this routine after a call to **?sytrd**.

Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^{T}C$ , CQ, or  $CQ^{T}$  (overwriting the result on *C*).

#### **Input Parameters**

In the descriptions below, r denotes the order of Q: If *side* = 'L', r = m; if *side* = 'R', r = n.

side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^T$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^T$ is applied to $C$ from the right.
uplo	CHARACTER*1. Must be 'U' or 'L'. Use the same <i>uplo</i> as supplied to ?sytrd.
trans	CHARACTER*1. Must be either 'N' or 'T'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'T', the routine multiplies C by $Q^{T}$ .
m	<b>INTEGER</b> . The number of rows in the matrix $C (m \ge 0)$ .
n	<b>INTEGER</b> . The number of columns in $C$ ( $n \ge 0$ ).
a,work,tau,c	REAL for sormtr DOUBLE PRECISION for dormtr. a( <i>lda</i> ,*) and <i>tau</i> are the arrays returned by ?sytrd.

	The second dimension of $a$ must be at least max $(1, r)$ . The dimension of $tau$ must be at least max $(1, r-1)$ .
	c(ldc, *) contains the matrix C. The second dimension of c must be at least max $(1, n)$
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of <i>a</i> ; $1da \ge max(1, r)$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ ; $ldc \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The size of the work array. Constraints: $lwork \ge max(1, n)$ if side = 'L'; $lwork \ge max(1, m)$ if side = 'R'. See Application notes for the suggested value of $lwork$ .

С	Overwritten by the product $QC$ , $Q^{T}C$ , $CQ$ , or $CQ^{T}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

#### **Application Notes**

For better performance, try using *lwork* = n*blocksize for *side* = 'L', or *lwork* = m*blocksize for *side* = 'R', where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed product differs from the exact product by a matrix *E* such that  $||E||_2 = O(\varepsilon) ||C||_2$ .

The total number of floating-point operations is approximately  $2*m^2*n$  if side ='L' or  $2*n^2*m$  if side ='R'.

The complex counterpart of this routine is <u>?unmtr</u>.

# ?hetrd

*Reduces a complex Hermitian matrix to tridiagonal form.* 

call chetrd ( uplo,n,a,lda,d,e,tau,work,lwork,info )
call zhetrd ( uplo,n,a,lda,d,e,tau,work,lwork,info )

### **Discussion**

This routine reduces a complex Hermitian matrix A to symmetric tridiagonal form T by a unitary similarity transformation:  $A = QTQ^{H}$ . The unitary matrix Q is not formed explicitly but is represented as a product of n-1 elementary reflectors. Routines are provided to work with Q in this representation. (They are described later in this section.)

### **Input Parameters**

uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , a stores the upper triangular part of A. If $uplo = 'L'$ , a stores the lower triangular part of A.
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
a, work	COMPLEX for chetrd DOUBLE COMPLEX for zhetrd. a(1da, *) is an array containing either upper or lower triangular part of the matrix A, as specified by uplo. The second dimension of a must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
lwork	<b>INTEGER.</b> The size of the work array $(lwork \ge n)$ See Application notes for the suggested value of $lwork$ .

- а
- Overwritten by the tridiagonal matrix T and details of the unitary matrix Q, as specified by <u>uplo</u>.

d, e	REAL for chetrd
	DOUBLE PRECISION for zhetrd.
	Arrays:
	d(*) contains the diagonal elements of the matrix <i>T</i> . The dimension of <i>d</i> must be at least max $(1, n)$ .
	e(*) contains the off-diagonal elements of T.
	The dimension of $e$ must be at least max $(1, n-1)$ .
tau	COMPLEX for chetrd DOUBLE COMPLEX for zhetrd. Array, DIMENSION at least $max(1, n-1)$ .
	Stores further details of the unitary matrix $Q$ .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER</b> . If <i>info</i> = 0, the execution is successful. If <i>info</i> = $-i$ , the <i>i</i> th parameter had an illegal value.

#### **Application Notes**

For better performance, try using *lwork* =n*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed matrix *T* is exactly similar to a matrix A + E, where  $||E||_2 = c(n)\varepsilon ||A||_2$ , c(n) is a modestly increasing function of *n*, and  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations is  $(16/3)n^3$ .

After calling this routine, you can call the following:

<u>?ungtr</u> to form the computed matrix *Q* explicitly;

<u>?unmtr</u> to multiply a complex matrix by *Q*.

The real counterpart of this routine is <u>?sytrd</u>.

# ?ungtr

Generates the complex unitary matrix Q determined by ?hetrd.

call cungtr ( uplo, n, a, lda, tau, work, lwork, info )
call zungtr ( uplo, n, a, lda, tau, work, lwork, info )

#### **Discussion**

The routine explicitly generates the *n* by *n* unitary matrix *Q* formed by ?hetrd (see page 5-111) when reducing a complex Hermitian matrix *A* to tridiagonal form:  $A = QTQ^{H}$ . Use this routine after a call to ?hetrd.

#### **Input Parameters**

uplo	CHARACTER*1. Must be 'U' or 'L'. Use the same <i>uplo</i> as supplied to ?hetrd.
п	<b>INTEGER.</b> The order of the matrix $Q$ ( $n \ge 0$ ).
a, tau, work	COMPLEX for cungtr DOUBLE COMPLEX for zungtr. Arrays: a(lda,*) is the array a as returned by ?hetrd. The second dimension of a must be at least max(1, n).
	tau(*) is the array $tau$ as returned by ?hetrd. The dimension of $tau$ must be at least max $(1, n-1)$ .
	work (lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array ( $lwork \ge n$ ) See Application notes for the suggested value of $lwork$ .

#### **Output Parameters**

a Overwritten by the unitary matrix Q.

work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

#### **Application Notes**

For better performance, try using lwork = (n-1)*blocksize, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed matrix Q differs from an exactly unitary matrix by a matrix E such that  $||E||_2 = O(\varepsilon)$ , where  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations is  $(16/3)n^3$ .

The real counterpart of this routine is <u>?orgtr</u>.

# ?unmtr

Multiplies a complex matrix by the complex unitary matrix Q determined by ?hetrd.

call cunmtr ( side,uplo,trans,m,n,a,lda,tau,c,ldc,work,lwork,info )
call zunmtr ( side,uplo,trans,m,n,a,lda,tau,c,ldc,work,lwork,info )

### **Discussion**

The routine multiplies a complex matrix C by Q or  $Q^H$ , where Q is the unitary matrix Q formed by ?hetrd (see page 5-111) when reducing a complex Hermitian matrix A to tridiagonal form:  $A = QTQ^H$ . Use this routine after a call to ?hetrd.

Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^{H}C$ , CQ, or  $CQ^{H}$  (overwriting the result on *C*).

### **Input Parameters**

In the descriptions below, r denotes the order of Q: If side = 'L', r = m; if side = 'R', r = n.

side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^H$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^H$ is applied to $C$ from the right.
uplo	CHARACTER*1. Must be 'U' or 'L'. Use the same uplo as supplied to ?hetrd.
trans	CHARACTER*1. Must be either 'N' or 'T'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'T', the routine multiplies C by $Q^{H}$ .
m	<b>INTEGER.</b> The number of rows in the matrix $C \ (m \ge 0)$ .
n	<b>INTEGER</b> . The number of columns in $C$ ( $n \ge 0$ ).
a,work,tau,c	COMPLEX for cunmtr DOUBLE COMPLEX for zunmtr. a(lda,*) and tau are the arrays returned by ?hetrd.

	The second dimension of $a$ must be at least max $(1, r)$ . The dimension of $tau$ must be at least max $(1, r-1)$ .
	c(ldc,*) contains the matrix C. The second dimension of c must be at least max $(1, n)$
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of $a$ ; $1da \ge max(1, r)$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ ; $ldc \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array. Constraints: $lwork \ge max(1, n)$ if <i>side</i> = 'L'; $lwork \ge max(1, m)$ if <i>side</i> = 'R'. See Application notes for the suggested value of <i>lwork</i> .

С	Overwritten by the product $QC$ , $Q^{H}C$ , $CQ$ , or $CQ^{H}$ (as specified by <i>side</i> and <i>trans</i> ).
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

#### **Application Notes**

For better performance, try using lwork = n*blocksize (for side = 'L') or lwork = m*blocksize (for side = 'R') where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

The computed product differs from the exact product by a matrix *E* such that  $||E||_2 = O(\varepsilon) ||C||_2$ , where  $\varepsilon$  is the machine precision.

The total number of floating-point operations is approximately  $8*m^2*n$  if side ='L' or  $8*n^2*m$  if side ='R'.

The real counterpart of this routine is <u>?ormtr</u>.

# ?sptrd

Reduces a real symmetric matrix to tridiagonal form using packed storage.

```
call ssptrd ( uplo,n,ap,d,e,tau,info )
call dsptrd ( uplo,n,ap,d,e,tau,info )
```

### **Discussion**

This routine reduces a packed real symmetric matrix A to symmetric tridiagonal form T by an orthogonal similarity transformation:  $A = QTQ^{T}$ . The orthogonal matrix Q is not formed explicitly but is represented as a product of n-1 elementary reflectors. Routines are provided for working with Q in this representation. (They are described later in this section.)

### **Input Parameters**

uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , <i>ap</i> stores the packed upper triangle of <i>A</i> . If $uplo = 'L'$ , <i>ap</i> stores the packed lower triangle of <i>A</i> .
п	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
ap	REAL for ssptrd DOUBLE PRECISION for dsptrd. Array, DIMENSION at least $\max(1, n(n+1)/2)$ . Contains either upper or lower triangle of A (as specified by uplo) in packed form.

ap	Overwritten by the tridiagonal matrix $T$ and details of the orthogonal matrix $Q$ , as specified by uplo.
d, e, tau	REAL for ssptrd DOUBLE PRECISION for dsptrd. Arrays: d(*) contains the diagonal elements of the matrix T. The dimension of d must be at least max $(1, n)$ .

	e(*) contains the off-diagonal elements of $T$ . The dimension of $e$ must be at least max $(1, n-1)$ .
	tau(*) stores further details of the matrix $Q$ . The dimension of $tau$ must be at least max $(1, n-1)$ .
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

#### **Application Notes**

The computed matrix *T* is exactly similar to a matrix A + E, where  $||E||_2 = c(n)\varepsilon ||A||_2$ , c(n) is a modestly increasing function of *n*, and  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations is  $(4/3)n^3$ .

After calling this routine, you can call the following:

<u>?opgtr</u> to form the computed matrix $Q$ explicitly;
-----------------------------------------------------------

<u>?opmtr</u> to multiply a real matrix by Q	' Q.
----------------------------------------------	------

The complex counterpart of this routine is <u>?hptrd</u>.

# ?opgtr

Generates the real orthogonal matrix Q determined by ?sptrd.

call sopgtr ( uplo, n, ap, tau, q, ldq, work, info )
call dopgtr ( uplo, n, ap, tau, q, ldq, work, info )

#### **Discussion**

The routine explicitly generates the *n* by *n* orthogonal matrix *Q* formed by **?sptrd** (see <u>page 5-117</u>) when reducing a packed real symmetric matrix *A* to tridiagonal form:  $A = QTQ^{T}$ . Use this routine after a call to **?sptrd**.

#### **Input Parameters**

uplo	CHARACTER*1. Must be 'U' or 'L'. Use the same uplo as supplied to ?sptrd.
п	<b>INTEGER.</b> The order of the matrix $Q$ $(n \ge 0)$ .
ap, tau	REAL for sopgtr DOUBLE PRECISION for dopgtr. Arrays <i>ap</i> and <i>tau</i> , as returned by ?sptrd. The dimension of <i>ap</i> must be at least $max(1, n(n+1)/2)$ . The dimension of <i>tau</i> must be at least $max(1, n-1)$ .
ldq	<b>INTEGER.</b> The first dimension of the output array $q$ ; at least max $(1, n)$ .
work	REAL for sopgtr DOUBLE PRECISION for dopgtr. Workspace array, DIMENSION at least $max(1, n-1)$ .

q	REAL for sopgtr
	DOUBLE PRECISION for dopgtr.
	Array, DIMENSION (1dq,*).
	Contains the computed matrix $Q$ .
	The second dimension of $q$ must be at least max(1, $n$ ).

info

**INTEGER.** If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value.

#### **Application Notes**

The computed matrix *Q* differs from an exactly orthogonal matrix by a matrix *E* such that  $||E||_2 = O(\varepsilon)$ , where  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations is  $(4/3)n^3$ .

The complex counterpart of this routine is <u>?upgtr</u>.

## ?opmtr

Multiplies a real matrix by the real orthogonal matrix Q determined by ?sptrd.

call sopmtr (side,uplo,trans,m,n,ap,tau,c,ldc,work,info)
call dopmtr (side,uplo,trans,m,n,ap,tau,c,ldc,work,info)

#### **Discussion**

The routine multiplies a real matrix *C* by *Q* or  $Q^T$ , where *Q* is the orthogonal matrix *Q* formed by **?sptrd** (see <u>page 5-117</u>) when reducing a packed real symmetric matrix *A* to tridiagonal form:  $A = QTQ^T$ . Use this routine after a call to **?sptrd**.

Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^{T}C$ , CQ, or  $CQ^{T}$  (overwriting the result on *C*).

#### **Input Parameters**

In the descriptions below, r denotes the order of Q: If side = 'L', r = m; if side = 'R', r = n. side CHARACTER*1. Must be either 'L' or 'R'. If side = 'L', Q or  $Q^T$  is applied to C from the left. If side = 'R', Q or  $Q^T$  is applied to C from the right.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	Use the same uplo as supplied to ?sptrd.
trans	CHARACTER*1. Must be either 'N' or 'T'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'T', the routine multiplies C by $Q^{T}$ .
m	<b>INTEGER.</b> The number of rows in the matrix $C \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $C$ ( $n \ge 0$ ).
ap,work,tau,c	REAL for sopmtr DOUBLE PRECISION for dopmtr. ap and tau are the arrays returned by ?sptrd. The dimension of ap must be at least max $(1, r(r+1)/2)$ . The dimension of tau must be at least max $(1, r-1)$ .
	c(ldc, *) contains the matrix C. The second dimension of c must be at least max $(1, n)$
	<pre>work(*) is a workspace array. The dimension of work must be at least max(1, n) if side = 'L'; max(1, m) if side = 'R'.</pre>
ldc	<b>INTEGER.</b> The first dimension of $c$ ; $ldc \ge max(1, n)$ .

С	Overwritten by the product $QC$ , $Q^{T}C$ , $CQ$ , or $CQ^{T}$ (as specified by <i>side</i> and <i>trans</i> ).
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

The computed product differs from the exact product by a matrix E such that  $||E||_2 = O(\varepsilon) ||C||_2$ , where  $\varepsilon$  is the machine precision. The total number of floating-point operations is approximately  $2*m^2*n$  if side = 'L' or  $2*n^2*m$  if side = 'R'.

The complex counterpart of this routine is <u>?upmtr</u>.

# ?hptrd

*Reduces a complex Hermitian matrix to tridiagonal form using packed storage.* 

```
call chptrd ( uplo,n,ap,d,e,tau,info )
call zhptrd ( uplo,n,ap,d,e,tau,info )
```

#### **Discussion**

This routine reduces a packed complex Hermitian matrix A to symmetric tridiagonal form T by a unitary similarity transformation:  $A = QTQ^{H}$ . The unitary matrix Q is not formed explicitly but is represented as a product of n-1 elementary reflectors. Routines are provided for working with Q in this representation. (They are described later in this section.)

### **Input Parameters**

uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , $ap$ stores the packed upper triangle of A. If $uplo = 'L'$ , $ap$ stores the packed lower triangle of A.
n	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .
ap	COMPLEX for chptrd DOUBLE COMPLEX for zhptrd. Array, DIMENSION at least $\max(1, n(n+1)/2)$ . Contains either upper or lower triangle of A (as specified by uplo) in packed form.

ap	Overwritten by the tridiagonal matrix $T$ and details of the orthogonal matrix $Q$ , as specified by <i>uplo</i> .
d, e	REAL for chptrd DOUBLE PRECISION for zhptrd. Arrays: d(*) contains the diagonal elements of the matrix T. The dimension of d must be at least max $(1, n)$ .

	e(*) contains the off-diagonal elements of <i>T</i> . The dimension of $e$ must be at least max $(1, n-1)$ .
tau	COMPLEX for chptrd DOUBLE COMPLEX for zhptrd. Arrays, DIMENSION at least $max(1, n-1)$ . Contains further details of the orthogonal matrix $Q$ .
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th parameter had an illegal value.

#### **Application Notes**

The computed matrix *T* is exactly similar to a matrix A + E, where  $||E||_2 = c(n)\varepsilon ||A||_2$ , c(n) is a modestly increasing function of *n*, and  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations is  $(16/3)n^3$ .

After calling this routine, you can call the following:

 $\frac{2 \text{upgtr}}{2 \text{ to form the computed matrix } Q \text{ explicitly;}}$ 

 $\frac{2upmtr}{2}$  to multiply a complex matrix by Q.

The real counterpart of this routine is <u>?sptrd</u>.

# ?upgtr

Generates the complex unitary matrix Q determined by ?hptrd.

call cupgtr ( uplo, n, ap, tau, q, ldq, work, info )
call zupgtr ( uplo, n, ap, tau, q, ldq, work, info )

#### **Discussion**

The routine explicitly generates the *n* by *n* unitary matrix *Q* formed by ?hptrd (see page 5-122) when reducing a packed complex Hermitian matrix *A* to tridiagonal form:  $A = QTQ^{H}$ . Use this routine after a call to ?hptrd.

#### **Input Parameters**

uplo	CHARACTER*1. Must be 'U' or 'L'. Use the same <i>uplo</i> as supplied to ?sptrd.
п	<b>INTEGER.</b> The order of the matrix $Q$ $(n \ge 0)$ .
ap, tau	COMPLEX for cupgtr DOUBLE COMPLEX for zupgtr. Arrays <i>ap</i> and <i>tau</i> , as returned by ?hptrd. The dimension of <i>ap</i> must be at least $\max(1, n(n+1)/2)$ . The dimension of <i>tau</i> must be at least $\max(1, n-1)$ .
ldq	<b>INTEGER.</b> The first dimension of the output array $q$ ; at least max $(1, n)$ .
work	COMPLEX for cupgtr DOUBLE COMPLEX for zupgtr. Workspace array, DIMENSION at least $max(1, n-1)$ .

đ	COMPLEX for cupgtr DOUBLE COMPLEX for zupgtr. Array, DIMENSION $(ldq, *)$ . Contains the computed matrix $Q$ . The second dimension of $q$ must be at least max $(1, n)$ .
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

The computed matrix *Q* differs from an exactly orthogonal matrix by a matrix *E* such that  $||E||_2 = O(\varepsilon)$ , where  $\varepsilon$  is the machine precision. The approximate number of floating-point operations is  $(16/3)n^3$ . The real counterpart of this routine is <u>?opgtr</u>.

# ?upmtr

Multiplies a complex matrix by the unitary matrix Q determined by ?hptrd.

call cupmtr (side,uplo,trans,m,n,ap,tau,c,ldc,work,info)
call zupmtr (side,uplo,trans,m,n,ap,tau,c,ldc,work,info)

### **Discussion**

The routine multiplies a complex matrix C by Q or  $Q^H$ , where Q is the unitary matrix Q formed by ?hptrd (see page 5-122) when reducing a packed complex Hermitian matrix A to tridiagonal form:  $A = QTQ^H$ . Use this routine after a call to ?hptrd.

Depending on the parameters *side* and *trans*, the routine can form one of the matrix products QC,  $Q^{H}C$ , CQ, or  $CQ^{H}$  (overwriting the result on C).

## **Input Parameters**

In the descriptions below, $r$ denotes the order of $Q$ : If <i>side</i> = 'L', $r = m$ ; if <i>side</i> = 'R', $r = n$ .		
side	CHARACTER*1. Must be either 'L' or 'R'. If <i>side</i> = 'L', $Q$ or $Q^H$ is applied to $C$ from the left. If <i>side</i> = 'R', $Q$ or $Q^H$ is applied to $C$ from the right.	
uplo	CHARACTER*1. Must be 'U' or 'L'. Use the same <i>uplo</i> as supplied to ?hptrd.	
trans	CHARACTER*1. Must be either 'N' or 'T'. If $trans =$ 'N', the routine multiplies C by Q. If $trans =$ 'T', the routine multiplies C by $Q^{H}$ .	
m	<b>INTEGER</b> . The number of rows in the matrix $C \ (m \ge 0)$ .	
п	<b>INTEGER.</b> The number of columns in $C$ $(n \ge 0)$ .	
ap,tau,c,work	COMPLEX for cupmtr DOUBLE COMPLEX for zupmtr. <i>ap</i> and <i>tau</i> are the arrays returned by ?hptrd.	
	The dimension of $a_p$ must be at least max $(1, r(r+1)/2)$ . The dimension of $tau$ must be at least max $(1, r-1)$ .	
	c(ldc, *) contains the matrix C. The second dimension of c must be at least max $(1, n)$	
	<pre>work(*) is a workspace array. The dimension of work must be at least max(1, n) if side = 'L'; max(1, m) if side = 'R'.</pre>	
ldc	<b>INTEGER</b> . The first dimension of $c$ ; $1dc \ge max(1, n)$ .	

С	Overwritten by the product $QC$ , $Q^{H}C$ , $CQ$ , or $CQ^{H}$ (as specified by <i>side</i> and <i>trans</i> ).
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

The computed product differs from the exact product by a matrix *E* such that  $||E||_2 = O(\varepsilon) ||C||_2$ , where  $\varepsilon$  is the machine precision.

The total number of floating-point operations is approximately  $8*m^2*n$  if side = 'L' or  $8*n^2*m$  if side = 'R'.

The real counterpart of this routine is <u>?opmtr</u>.

# ?sbtrd

*Reduces a real symmetric band matrix to tridiagonal form.* 

call ssbtrd (vect,uplo,n,kd,ab,ldab,d,e,q,ldq,work,info)
call dsbtrd (vect,uplo,n,kd,ab,ldab,d,e,q,ldq,work,info)

#### **Discussion**

This routine reduces a real symmetric band matrix A to symmetric tridiagonal form T by an orthogonal similarity transformation:  $A = QTQ^{T}$ . The orthogonal matrix Q is determined as a product of Givens rotations. If required, the routine can also form the matrix Q explicitly.

#### **Input Parameters**

vect	CHARACTER*1. Must be 'V' or 'N'.
	If $vect = V'$ , the routine returns the explicit matrix $Q$ .
	If $vect = 'N'$ , the routine does not return $Q$ .
uplo	CHARACTER*1. Must be 'U' or 'L'.
	If $uplo = 'U'$ , <i>ab</i> stores the upper triangular part of A.
	If $uplo = 'L'$ , <i>ab</i> stores the lower triangular part of A.
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
kd	<b>INTEGER</b> . The number of super- or sub-diagonals in A
	$(kd \ge 0).$
ab, work	REAL for ssbtrd
	DOUBLE PRECISION for dsbtrd.
	ab (ldab, *) is an array containing either upper or
	lower triangular part of the matrix A (as specified by
	uplo) in band storage format.
	The second dimension of $ab$ must be at least max $(1, n)$ .
	work (*) is a workspace array.
	The dimension of <i>work</i> must be at least $max(1, n)$ .
ldab	

ldqINTEGER. The first dimension of q. Constraints: $ldq \ge max(1, n)$  if vect = 'V'; $ldq \ge 1$  if vect = 'N'.

#### **Output Parameters**

ab On exit, the array *ab* is overwritten. d, e, q REAL for ssbtrd DOUBLE PRECISION for dsbtrd. Arrays: d(*) contains the diagonal elements of the matrix T. The dimension of *d* must be at least  $\max(1, n)$ . e(*) contains the off-diagonal elements of T. The dimension of *e* must be at least  $\max(1, n-1)$ .  $q(ldq, \star)$  is not referenced if vect = 'N'. If vect = V', q contains the n by n matrix Q. The second dimension of q must be: at least max(1, n) if vect = 'V'; at least 1 if vect = 'N'. info INTEGER. If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value.

#### **Application Notes**

The computed matrix *T* is exactly similar to a matrix A + E, where  $||E||_2 = c(n)\varepsilon ||A||_2$ , c(n) is a modestly increasing function of *n*, and  $\varepsilon$  is the machine precision. The computed matrix *Q* differs from an exactly orthogonal matrix by a matrix *E* such that  $||E||_2 = O(\varepsilon)$ .

The total number of floating-point operations is approximately  $6n^2 * kd$  if vect = N', with  $3n^3 * (kd-1)/kd$  additional operations if vect = V'.

The complex counterpart of this routine is <u>?hbtrd</u>.

# ?hbtrd

*Reduces a complex Hermitian band matrix to tridiagonal form.* 

call chbtrd (vect,uplo,n,kd,ab,ldab,d,e,q,ldq,work,info)
call zhbtrd (vect,uplo,n,kd,ab,ldab,d,e,q,ldq,work,info)

#### **Discussion**

This routine reduces a complex Hermitian band matrix A to symmetric tridiagonal form T by a unitary similarity transformation:  $A = QTQ^{H}$ . The unitary matrix Q is determined as a product of Givens rotations. If required, the routine can also form the matrix Q explicitly.

#### **Input Parameters**

vect	CHARACTER*1. Must be 'V' or 'N'.
	If $vect = V'$ , the routine returns the explicit matrix $Q$ .
	If $vect = 'N'$ , the routine does not return $Q$ .
uplo	CHARACTER*1. Must be 'U' or 'L'.
	If $uplo = 'U'$ , <i>ab</i> stores the upper triangular part of A.
	If $uplo = 'L'$ , <i>ab</i> stores the lower triangular part of A.
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
kd	<b>INTEGER</b> . The number of super- or sub-diagonals in A
	$(kd \ge 0).$
ab, work	COMPLEX for chbtrd
	DOUBLE COMPLEX for zhbtrd.
	ab (ldab, *) is an array containing either upper or
	lower triangular part of the matrix A (as specified by
	uplo) in band storage format.
	The second dimension of $ab$ must be at least max $(1, n)$ .
	work (*) is a workspace array.
	The dimension of <i>work</i> must be at least max(1, <i>n</i> ).
	The dimension of work must be at least max(1, 1).

ldq	<b>INTEGER</b> . The first dimension of <i>q</i> . Constraints:
	$ldq \geq max(1, n)$ if $vect = V'$ ;
	$ldq \ge 1$ if $vect = 'N'$ .

ab	On exit, the array <i>ab</i> is overwritten.
d, e	REAL for chbtrd DOUBLE PRECISION for zhbtrd. Arrays: d(*) contains the diagonal elements of the matrix <i>T</i> . The dimension of <i>d</i> must be at least max $(1, n)$ .
	e(*) contains the off-diagonal elements of <i>T</i> . The dimension of $e$ must be at least max $(1, n-1)$ .
đ	COMPLEX for chbtrd DOUBLE COMPLEX for zhbtrd. Array, DIMENSION $(ldq,*)$ . If $vect = 'N'$ , $q$ is not referenced. If $vect = 'V'$ , $q$ contains the $n$ by $n$ matrix $Q$ . The second dimension of $q$ must be: at least max $(1, n)$ if $vect = 'V'$ ; at least 1 if $vect = 'N'$ .
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th parameter had an illegal value.

#### **Application Notes**

The computed matrix *T* is exactly similar to a matrix A + E, where  $||E||_2 = c(n)\varepsilon ||A||_2$ , c(n) is a modestly increasing function of *n*, and  $\varepsilon$  is the machine precision. The computed matrix *Q* differs from an exactly unitary matrix by a matrix *E* such that  $||E||_2 = O(\varepsilon)$ .

The total number of floating-point operations is approximately  $20n^{2*}kd$  if vect = N', with  $10n^{3*}(kd-1)/kd$  additional operations if vect = V'.

The real counterpart of this routine is <u>?sbtrd</u>.

# ?sterf

Computes all eigenvalues of a real symmetric tridiagonal matrix using QR algorithm.

```
call ssterf ( n, d, e, info )
call dsterf ( n, d, e, info )
```

#### **Discussion**

This routine computes all the eigenvalues of a real symmetric tridiagonal matrix T (which can be obtained by reducing a symmetric or Hermitian matrix to tridiagonal form). The routine uses a square-root-free variant of the QR algorithm.

If you need not only the eigenvalues but also the eigenvectors, call ?steqr (page 5-134).

#### **Input Parameters**

n	<b>INTEGER.</b> The order of the matrix $T (n \ge 0)$ .
d, e	REAL for ssterf DOUBLE PRECISION for dsterf. Arrays: d(*) contains the diagonal elements of <i>T</i> . The dimension of <i>d</i> must be at least max $(1, n)$ .
	e(*) contains the off-diagonal elements of <i>T</i> . The dimension of $e$ must be at least max $(1, n-1)$ .

d	The <i>n</i> eigenvalues in ascending order, unless <i>info</i> > 0. See also <i>info</i> .
е	On exit, the array is overwritten; see <i>info</i> .

infoINTEGER.If info = 0, the execution is successful.If info = i, the algorithm failed to find all theeigenvalues after 30n iterations: i off-diagonal elementshave not converged to zero. On exit, d and e contain,respectively, the diagonal and off-diagonal elements of atridiagonal matrix orthogonally similar to T.If info = -i, the ith parameter had an illegal value.

### **Application Notes**

The computed eigenvalues and eigenvectors are exact for a matrix T + E such that  $||E||_2 = O(\varepsilon) ||T||_2$ , where  $\varepsilon$  is the machine precision.

If  $\lambda_i$  is an exact eigenvalue, and  $\mu_i$  is the corresponding computed value, then

 $|\mu_i - \lambda_i| \leq (n)\varepsilon ||T||_2$ 

where c(n) is a modestly increasing function of n.

The total number of floating-point operations depends on how rapidly the algorithm converges. Typically, it is about  $14n^2$ .

# ?steqr

Computes all eigenvalues and eigenvectors of a symmetric or Hermitian matrix reduced to tridiagonal form (QR algorithm).

call ssteqr ( compz, n, d, e, z, ldz, work, info )
call dsteqr ( compz, n, d, e, z, ldz, work, info )
call csteqr ( compz, n, d, e, z, ldz, work, info )
call zsteqr ( compz, n, d, e, z, ldz, work, info )

#### **Discussion**

This routine computes all the eigenvalues and (optionally) all the eigenvectors of a real symmetric tridiagonal matrix *T*. In other words, the routine can compute the spectral factorization:  $T = Z\Lambda Z^T$ . Here  $\Lambda$  is a diagonal matrix whose diagonal elements are the eigenvalues  $\lambda_i$ ; *Z* is an orthogonal matrix whose columns are eigenvectors. Thus,

 $Tz_i = \lambda_i z_i$  for i = 1, 2, ..., n.

(The routine normalizes the eigenvectors so that  $||z_i||_2 = 1$ .)

You can also use the routine for computing the eigenvalues and eigenvectors of an arbitrary real symmetric (or complex Hermitian) matrix *A* reduced to tridiagonal form  $T: A = QTQ^{H}$ . In this case, the spectral factorization is as follows:  $A = QTQ^{H} = (QZ)\Lambda (QZ)^{H}$ . Before calling ?stegr, you must reduce *A* to tridiagonal form and generate the explicit matrix *Q* by calling the following routines:

	for real matrices:	for complex matrices:
full storage	?sytrd,?orgtr	?hetrd,?ungtr
packed storage	?sptrd,?opgtr	<pre>?hptrd,?upgtr</pre>
band storage	<pre>?sbtrd (vect='V')</pre>	<pre>?hbtrd (vect='V')</pre>

If you need eigenvalues only, it's more efficient to call ?sterf (page 5-132). If *T* is positive-definite, ?pteqr (page 5-146) can compute small eigenvalues more accurately than ?steqr.

To solve the problem by a single call, use one of the divide and conquer routines ?stevd, ?syevd, or ?sbevd for real symmetric matrices or ?heevd, ?hpevd, or ?hbevd for complex Hermitian matrices.

## **Input Parameters**

Compz	CHARACTER*1. Must be 'N' or 'I' or 'V'. If $compz =$ 'N', the routine computes eigenvalues only. If $compz =$ 'I', the routine computes the eigenvalues and eigenvectors of the tridiagonal matrix <i>T</i> . If $compz =$ 'V', the routine computes the eigenvalues and eigenvectors of <i>A</i> (and the array <i>z</i> must contain the matrix <i>Q</i> on entry).
n	<b>INTEGER.</b> The order of the matrix $T$ ( $n \ge 0$ ).
d,e,work	REAL for single-precision flavors DOUBLE PRECISION for double-precision flavors. Arrays: d(*) contains the diagonal elements of <i>T</i> . The dimension of <i>d</i> must be at least max(1, <i>n</i> ).
	e(*) contains the off-diagonal elements of $T$ . The dimension of $e$ must be at least max $(1, n-1)$ .
	<pre>work(*) is a workspace array. The dimension of work must be: at least 1 if compz = 'N'; at least max(1, 2*n-2) if compz = 'V' or 'I'.</pre>
Ζ	REAL for ssteqr DOUBLE PRECISION for dsteqr COMPLEX for csteqr DOUBLE COMPLEX for zsteqr. Array, DIMENSION $(ldz, *)$ If $compz = 'N'$ or 'I', z need not be set. If $vect = 'V'$ , z must contain the n by n matrix Q. The second dimension of z must be: at least 1 if $compz = 'N'$ ; at least max $(1, n)$ if $compz = 'V'$ or 'I'.
	work (lwork) is a workspace array.
ldz	<b>INTEGER.</b> The first dimension of z. Constraints: $ldz \ge 1$ if $compz = 'N'$ ; $ldz \ge max(1, n)$ if $compz = 'V'$ or 'I'.

d	The <i>n</i> eigenvalues in ascending order, unless $info > 0$ . See also <i>info</i> .
е	On exit, the array is overwritten; see <i>info</i> .
Ζ	If <i>info</i> = 0, contains the <i>n</i> orthonormal eigenvectors, stored by columns. (The <i>i</i> th column corresponds to the <i>i</i> th eigenvalue.)
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = i$ , the algorithm failed to find all the eigenvalues after $30n$ iterations: <i>i</i> off-diagonal elements have not converged to zero. On exit, <i>d</i> and <i>e</i> contain, respectively, the diagonal and off-diagonal elements of a tridiagonal matrix orthogonally similar to <i>T</i> . If <i>info</i> = <i>-i</i> , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

The computed eigenvalues and eigenvectors are exact for a matrix T + Esuch that  $||E||_2 = O(\varepsilon) ||T||_2$ , where  $\varepsilon$  is the machine precision.

If  $\lambda_i$  is an exact eigenvalue, and  $\mu_i$  is the corresponding computed value, then

 $|\mu_i - \lambda_i| \leq c(n)\varepsilon ||T||_2$ 

where c(n) is a modestly increasing function of n.

If  $z_i$  is the corresponding exact eigenvector, and  $w_i$  is the corresponding computed vector, then the angle  $\theta(z_i, w_i)$  between them is bounded as follows:

 $\theta(z_i, w_i) \leq c(n) \varepsilon \mid \mid T \mid \mid_2 / \min_{i \neq j} \mid \lambda_i - \lambda_j \mid .$ 

The total number of floating-point operations depends on how rapidly the algorithm converges. Typically, it is about

 $24n^2$  if compz = 'N';  $7n^3$  (for complex flavors,  $14n^3$ ) if compz = 'V' or 'I'.

## ?stedc

Computes all eigenvalues and eigenvectors of a symmetric tridiagonal matrix using the divide and conquer method.

#### **Discussion**

This routine computes all the eigenvalues and (optionally) all the eigenvectors of a symmetric tridiagonal matrix using the divide and conquer method.

The eigenvectors of a full or band real symmetric or complex Hermitian matrix can also be found if ?sytrd/?hetrd or ?sptrd/?hptrd or ?sbtrd/?hbtrd has been used to reduce this matrix to tridiagonal form.

#### **Input Parameters**

-	CHARACTER*1. Must be 'N' or 'I' or 'V'. If $compz = 'N'$ , the routine computes eigenvalues only. If $compz = 'I'$ , the routine computes the eigenvalues and eigenvectors of the tridiagonal matrix. If $compz = 'V'$ , the routine computes the eigenvalues and eigenvectors of original symmetric/Hermitian matrix. On entry, the array z must contain the orthogonal/unitary matrix used to reduce the original matrix to tridiagonal form.
п	<b>INTEGER.</b> The order of the symmetric tridiagonal matrix $(n \ge 0)$ .

d, e, rwork	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. Arrays: d(*) contains the diagonal elements of the tridiagonal matrix. The dimension of <i>d</i> must be at least max(1, <i>n</i> ). e(*) contains the subdiagonal elements of the tridiagonal matrix. The dimension of <i>e</i> must be at least max(1, <i>n</i> -1).
	<i>rwork</i> ( <i>lrwork</i> ) is a workspace array used in complex flavors only.
z, work	REAL for sstedc DOUBLE PRECISION for dstedc COMPLEX for cstedc DOUBLE COMPLEX for zstedc. Arrays: $z(ldz, *)$ , work(*). If compz = 'V', then, on entry, z must contain the orthogonal/unitary matrix used to reduce the original matrix to tridiagonal form. The second dimension of z must be at least max(1, n).
ldz	work (lwork) is a workspace array. INTEGER. The first dimension of z. Constraints: $ldz \ge 1$ if $compz = 'N'$ ; $ldz \ge max(1, n)$ if $compz = 'V'$ or 'I'.
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> . See <i>Application Notes</i> for the required value of <i>lwork</i> .
lrwork	<b>INTEGER.</b> The dimension of the array <i>rwork</i> (used for complex flavors only). See <i>Application Notes</i> for the required value of <i>lrwork</i> .
iwork	INTEGER. Workspace array, DIMENSION (liwork).
liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . See <i>Application Notes</i> for the required value of <i>liwork</i> .

d	The <i>n</i> eigenvalues in ascending order, unless $info \neq 0$ . See also <i>info</i> .
е	On exit, the array is overwritten; see <i>info</i> .
Ζ	If <i>info</i> = 0, then if <i>compz</i> = 'V', <i>z</i> contains the orthonormal eigenvectors of the original symmetric/Hermitian matrix, and if <i>compz</i> = 'I', <i>z</i> contains the orthonormal eigenvectors of the symmetric tridiagonal matrix. If <i>compz</i> = 'N', <i>z</i> is not referenced.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the optimal <i>lwork</i> .
rwork(1)	On exit, if <i>info</i> = 0, then <i>rwork(1)</i> returns the optimal <i>lrwork</i> (for complex flavors only).
iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the optimal <i>liwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If info = i, the algorithm failed to compute an eigenvalue while working on the submatrix lying in rows and columns $i/(n+1)$ through $mod(i, n+1)$ .

#### **Application Notes**

The required size of workspace arrays must be as follows.

For sstedc/dstedc:

If compz = 'N' or  $n \le 1$  then *lwork* must be at least 1. If compz = 'V' and n > 1 then *lwork* must be at least  $(1 + 3n + 2n \cdot lgn + 3n^2)$ , where lg(n) = smallest integer k such that  $2^k \ge n$ . If compz = 'I' and n > 1 then *lwork* must be at least  $(1 + 4n + n^2)$ . If compz = 'N' or  $n \le 1$  then *liwork* must be at least 1. If compz = 'V' and n > 1 then *liwork* must be at least  $(6 + 6n + 5n \cdot lgn)$ . If compz = 'I' and n > 1 then *liwork* must be at least (3 + 5n). For cstedc/zstedc: If compz = 'N' or 'I', or  $n \le 1$ , *lwork* must be at least 1. If compz = 'V' and n > 1, *lwork* must be at least  $n^2$ . If compz = 'N' or  $n \le 1$ , *lrwork* must be at least 1. If compz = 'V' and n > 1, *lrwork* must be at least  $(1 + 3n + 2n \cdot lgn + 3n^2)$ , where lg(n) = smallest integer k such that  $2^k \ge n$ . If compz = 'I' and n > 1, *lrwork* must be at least $(1 + 4n + 2n^2)$ .

The required value of *liwork* for complex flavors is the same as for real

flavors.

# ?stegr

Computes selected eigenvalues and eigenvectors of a real symmetric tridiagonal matrix.

#### **Discussion**

This routine computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix T. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues. The eigenvalues are computed by the *dqds* algorithm, while orthogonal eigenvectors are computed from various "good"  $LDL^T$  representations (also known as Relatively Robust Representations). Gram-Schmidt orthogonalization is avoided as far as possible. More specifically, the various steps of the algorithm are as follows. For the i-th unreduced block of T,

(a) Compute  $T - \mathbf{q} = L_i D_i L_i^T$ , such that  $L_i D_i L_i^T$  is a relatively robust representation;

(b) Compute the eigenvalues,  $\lambda_j$ , of  $L_i D_i L_i^T$  to high relative accuracy by the *dqds* algorithm;

(c) If there is a cluster of close eigenvalues, "choose"  $\sigma_i$  close to the cluster, and go to step (a);

(d) Given the approximate eigenvalue  $\lambda_j$  of  $L_i D_i L_i^T$ , compute the corresponding eigenvector by forming a rank-revealing twisted factorization.

The desired accuracy of the output can be specified by the input parameter *abstol*.

## **Input Parameters**

input i aramot	
jobz	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'. If <i>range</i> = 'A', the routine computes all eigenvalues. If <i>range</i> = 'V', the routine computes eigenvalues $\lambda_i$ in the half-open interval: $vl < \lambda_i \leq vu$ . If <i>range</i> = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
n	<b>INTEGER</b> . The order of the matrix $T$ ( $n \ge 0$ ).
d, e, work	<b>REAL</b> for single precision flavors <b>DOUBLE PRECISION</b> for double precision flavors. Arrays: d(*) contains the diagonal elements of <i>T</i> . The dimension of <i>d</i> must be at least max(1, <i>n</i> ).
	e(*) contains the subdiagonal elements of $T$ in elements 1 to $n-1$ ; $e(n)$ need not be set. The dimension of $e$ must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
vl, vu	REAL for single precision flavors DOUBLE PRECISION for double precision flavors. If range = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: v1 < vu.
	If <i>range</i> = 'A' or 'I', <i>vl</i> and <i>vu</i> are not referenced.
il, iu	INTEGER. If <i>range</i> = 'I', the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le il \le iu \le n$ , if $n > 0$ ; $il = 1$ and $iu = 0$ if $n = 0$ .

	If <i>range</i> = 'A' or 'V', <i>il</i> and <i>iu</i> are not referenced.
abstol	<b>REAL</b> for single precision flavors <b>DOUBLE PRECISION</b> for double precision flavors. The absolute tolerance to which each eigenvalue/eigenvector is required. If $jobz = 'V'$ , the eigenvalues and eigenvectors output have residual norms bounded by <i>abstol</i> , and the dot products between different eigenvectors are bounded by <i>abstol</i> .If <i>abstol</i> < <i>n</i> $\varepsilon$    <i>T</i>    ₁ , then <i>n</i> $\varepsilon$    <i>T</i>    ₁ willbeused in its place, where $\varepsilon$ is the machine precision. The eigenvalues are computed to an accuracy of $\varepsilon$    <i>T</i>    ₁ irrespective of <i>abstol</i> . If high relative accuracy is important, set <i>abstol</i> to ?lamch ('Safe minimum').
ldz	INTEGER. The leading dimension of the output array z. Constraints: $ldz \ge 1$ if $jobz = 'N'$ ; $ldz \ge max(1, n)$ if $jobz = 'V'$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> , <i>lwork</i> $\geq \max(1, 18n)$ .
iwork	INTEGER. Workspace array, DIMENSION (liwork).
liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> , <i>lwork</i> $\ge \max(1, 10n)$ .

d, e	On exit, $d$ and $e$ are overwritten.
m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If $range = 'A', m = n$ , and if $range = 'I'$ , m = iu - il + 1.
W	<b>REAL</b> for single precision flavors <b>DOUBLE PRECISION</b> for double precision flavors. Array, <b>DIMENSION</b> at least $max(1, n)$ . The selected eigenvalues in ascending order, stored in w(1) to $w(m)$ .

Z	REAL for sstegr
	DOUBLE PRECISION for dstegr
	COMPLEX for cstegr
	DOUBLE COMPLEX for zstegr.
	Array $z(ldz, *)$ , the second dimension of z must be at
	least $\max(1, m)$ .
	If $jobz = 'V'$ , then if $info = 0$ , the first <i>m</i> columns of <i>z</i> contain the orthonormal eigenvectors of the matrix <i>T</i> corresponding to the selected eigenvalues, with the <i>i</i> -th column of <i>z</i> holding the eigenvector associated with $w(i)$ . If $jobz = 'N'$ , then <i>z</i> is not referenced. Note: you must ensure that at least max $(1,m)$ columns are supplied in the array <i>z</i> ; if <i>range</i> = 'V', the exact value of <i>m</i> is not known in advance and an upper bound must be used.
isuppz	INTEGER. Array, DIMENSION at least 2*max(1, m).
	The support of the eigenvectors in z, i.e., the indices indicating the nonzero elements in z. The <i>i</i> -th eigenvector is nonzero only in elements <i>isuppz</i> (2 <i>i</i> -1) through <i>isuppz</i> (2 <i>i</i> ).
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.
	If <i>info</i> = 1, internal error in <i>slarre</i> occurred, If <i>info</i> = 2, internal error in <i>?larry</i> occurred.

# **Application Notes**

Currently ?stegr is only set up to find *all* the *n* eigenvalues and eigenvectors of T in  $O(n^2)$  time, that is, only *range* = 'A' is supported.

Currently the routine ?stein is called when an appropriate  $\mathfrak{F}_i$  cannot be chosen in step (c) above. ?stein invokes modified Gram-Schmidt when eigenvalues are close.

**?stegr** works only on machines which follow IEEE-754 floating-point standard in their handling of infinities and NaNs. Normal execution of **?stegr** may create NaNs and infinities and hence may abort due to a floating point exception in environments which do not conform to the IEEE-754 standard.

# ?pteqr

Computes all eigenvalues and (optionally) all eigenvectors of a real symmetric positive-definite tridiagonal matrix.

call	spteqr	(	compz,	n,	d,	e,	z ,	ldz,	work,	info	)
call	dpteqr	(	compz,	n,	d,	e,	z,	ldz,	work,	info	)
call	cpteqr	(	compz,	n,	d,	e,	z,	ldz,	work,	info	)
call	zpteqr	(	compz,	n,	d,	e,	z,	ldz,	work,	info	)

### **Discussion**

This routine computes all the eigenvalues and (optionally) all the eigenvectors of a real symmetric positive-definite tridiagonal matrix *T*. In other words, the routine can compute the spectral factorization:  $T = Z\Lambda Z^T$ . Here  $\Lambda$  is a diagonal matrix whose diagonal elements are the eigenvalues  $\lambda_i$ ; *Z* is an orthogonal matrix whose columns are eigenvectors. Thus,

 $Tz_i = \lambda_i z_i$  for i = 1, 2, ..., n.

(The routine normalizes the eigenvectors so that  $||z_i||_2 = 1$ .)

You can also use the routine for computing the eigenvalues and eigenvectors of real symmetric (or complex Hermitian) positive-definite matrices A reduced to tridiagonal form  $T: A = QTQ^{H}$ . In this case, the spectral factorization is as follows:  $A = QTQ^{H} = (QZ)\Lambda (QZ)^{H}$ . Before calling **?pteqr**, you must reduce A to tridiagonal form and generate the explicit matrix Q by calling the following routines:

	for real matrices:	for complex matrices:
full storage	?sytrd,?orgtr	?hetrd,?ungtr
packed storage	<pre>?sptrd,?opgtr</pre>	?hptrd,?upgtr
band storage	<pre>?sbtrd (vect='V')</pre>	<pre>?hbtrd (vect='V')</pre>

The routine first factorizes T as  $LDL^H$  where L is a unit lower bidiagonal matrix, and D is a diagonal matrix. Then it forms the bidiagonal matrix  $B = LD^{1/2}$  and calls ?bdsqr to compute the singular values of B, which are the same as the eigenvalues of T.

COMPZ	CHARACTER*1. Must be 'N' or 'I' or 'V'. If $compz = 'N'$ , the routine computes eigenvalues only. If $compz = 'I'$ , the routine computes the eigenvalues and eigenvectors of the tridiagonal matrix <i>T</i> . If $compz = 'V'$ , the routine computes the eigenvalues and eigenvectors of <i>A</i> (and the array <i>z</i> must contain the matrix <i>Q</i> on entry).
n	<b>INTEGER.</b> The order of the matrix $T$ ( $n \ge 0$ ).
d,e,work	REAL for single-precision flavors DOUBLE PRECISION for double-precision flavors. Arrays: d(*) contains the diagonal elements of <i>T</i> .
	The dimension of $d$ must be at least max $(1, n)$ .
	e(*) contains the off-diagonal elements of $T$ . The dimension of $e$ must be at least max $(1, n-1)$ .
	<pre>work(*) is a workspace array. The dimension of work must be: at least 1 if compz = 'N'; at least max(1, 4*n-4) if compz = 'V' or 'I'.</pre>
Ζ	REAL for spteqr DOUBLE PRECISION for dpteqr COMPLEX for cpteqr DOUBLE COMPLEX for zpteqr. Array, DIMENSION ( <i>ldz</i> ,*) If <i>compz</i> = 'N' or 'I', <i>z</i> need not be set. If <i>vect</i> = 'V', <i>z</i> must contains the <i>n</i> by <i>n</i> matrix <i>Q</i> . The second dimension of <i>z</i> must be: at least 1 if <i>compz</i> = 'N'; at least max(1, <i>n</i> ) if <i>compz</i> = 'V' or 'I'.
ldz	<b>INTEGER.</b> The first dimension of z. Constraints: $ldz \ge 1$ if $compz = 'N'$ ; $ldz \ge max(1, n)$ if $compz = 'V'$ or 'I'.

d	The <i>n</i> eigenvalues in descending order, unless <i>info</i> > 0. See also <i>info</i> .
е	On exit, the array is overwritten.
Ζ	If <i>info</i> = 0, contains the <i>n</i> orthonormal eigenvectors, stored by columns. (The <i>i</i> th column corresponds to the <i>i</i> th eigenvalue.)
info	INTEGER. If $info = 0$ , the execution is successful. If $info = i$ , the leading minor of order <i>i</i> (and hence <i>T</i> itself) is not positive-definite. If $info = n + i$ , the algorithm for computing singular values failed to converge; <i>i</i> off-diagonal elements have not converged to zero. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

If  $\lambda_i$  is an exact eigenvalue, and  $\mu_i$  is the corresponding computed value, then

 $|\mu_i - \lambda_i| \leq c(n) \epsilon K \lambda_i$ 

where c(n) is a modestly increasing function of n,  $\varepsilon$  is the machine precision, and  $K = ||DTD||_2 ||(DTD)^{-1}||_2$ , D is diagonal with  $d_{ii} = t_{ii}^{-1/2}$ .

If  $z_i$  is the corresponding exact eigenvector, and  $w_i$  is the corresponding computed vector, then the angle  $\theta(z_i, w_i)$  between them is bounded as follows:

 $\theta(u_i, w_i) \leq c(n) \varepsilon K / \min_{i \neq j} (|\lambda_i - \lambda_j| / |\lambda_i + \lambda_j|).$ 

Here  $\min_{i \neq j} (|\lambda_i - \lambda_j| / |\lambda_i + \lambda_j|)$  is the *relative gap* between  $\lambda_i$  and the other eigenvalues.

The total number of floating-point operations depends on how rapidly the algorithm converges. Typically, it is about

 $30n^2$  if compz = 'N';  $6n^3$  (for complex flavors,  $12n^3$ ) if compz = 'V' or 'I'.

# ?stebz

Computes selected eigenvalues of a real symmetric tridiagonal matrix by bisection.

> call sstebz (range, order, n, vl, vu, il, iu, abstol, d, e, m, nsplit, w, iblock, isplit, work, iwork, info) call dstebz (range, order, n, vl, vu, il, iu, abstol, d, e, m, nsplit, w, iblock, isplit, work, iwork, info)

#### **Discussion**

This routine computes some (or all) of the eigenvalues of a real symmetric tridiagonal matrix T by bisection. The routine searches for zero or negligible off-diagonal elements to see if T splits into block-diagonal form  $T = \text{diag}(T_1, T_2, ...)$ . Then it performs bisection on each of the blocks  $T_i$  and returns the block index of each computed eigenvalue, so that a subsequent call to ?stein can also take advantage of the block structure.

range	CHARACTER*1. Must be 'A' or 'V' or 'I'.
	If $range = 'A'$ , the routine computes all eigenvalues.
	If <b>range</b> = $V'$ , the routine computes eigenvalues $\lambda_i$ in
	the half-open interval: $v_1 < \lambda_i \leq v_u$ .
	If <i>range</i> = 'I', the routine computes eigenvalues with
	indices <i>i1</i> to <i>iu</i> .
order	CHARACTER*1. Must be 'B' or 'E'.
	If order = 'B', the eigenvalues are to be ordered from
	smallest to largest within each split-off block.
	If order = 'E', the eigenvalues for the entire matrix are
	to be ordered from smallest to largest.
n	<b>INTEGER.</b> The order of the matrix T $(n \ge 0)$ .

vl, vu	REAL for sstebz DOUBLE PRECISION for dstebz. If range = 'V', the routine computes eigenvalues $\lambda_i$ in the half-open interval: $vl < \lambda_i \leq vu$ .
	If $range = 'A'$ or 'I', $vI$ and $vu$ are not referenced.
il, iu	<b>INTEGER.</b> Constraint: $1 \le i \le i \le i \le n$ . If <i>range</i> = 'I', the routine computes eigenvalues $\lambda_i$ such that $i \le i $
	If <i>range</i> = 'A' or 'V', <i>il</i> and <i>iu</i> are not referenced.
abstol	<b>REAL</b> for sstebz <b>DOUBLE PRECISION</b> for dstebz. The absolute tolerance to which each eigenvalue is required. An eigenvalue (or cluster) is considered to have converged if it lies in an interval of width <i>abstol</i> . If <i>abstol</i> $\leq 0.0$ , then the tolerance is taken as $\varepsilon   T  _1$ , where $\varepsilon$ is the machine precision.
d, e	<pre>REAL for sstebz DOUBLE PRECISION for dstebz. Arrays: d(*) contains the diagonal elements of T. The dimension of d must be at least max(1, n). e(*) contains the off-diagonal elements of T.</pre>
iwork	The dimension of $e$ must be at least max $(1, n-1)$ . INTEGER. Workspace. Array, DIMENSION at least max $(1, 3n)$ .
Output Parame	eters
m	<b>INTEGER.</b> The actual number of eigenvalues found.
nsplit	<b>INTEGER</b> . The number of diagonal blocks detected in <i>T</i> .
W	REAL for sstebz

DOUBLE PRECISION for dstebz. Array, DIMENSION at least max(1, *n*).

The computed eigenvalues, stored in w(1) to w(m).

#### *iblock, isplit* INTEGER.

info

Arrays, DIMENSION at least max(1, n). A positive value *iblock(i)* is the block number of the eigenvalue stored in w(i) (see also info). The leading *nsplit* elements of *isplit* contain points at which T splits into blocks  $T_i$  as follows: the block  $T_1$  contains rows/columns 1 to *isplit(1)*; the block  $T_2$  contains rows/columns *isplit*(1)+1 to *isplit*(2), and so on. INTEGER. If info = 0, the execution is successful. If info = 1, for range = 'A' or 'V', the algorithm failed to compute some of the required eigenvalues to the desired accuracy; *iblock(i)* < 0 indicates that the eigenvalue stored in w(i) failed to converge. If *info* = 2, for *range* = 'I', the algorithm failed to compute some of the required eigenvalues. Try calling the routine again with range = 'A'. If *info* = 3:

for range = 'A' or 'V', same as info = 1; for range = 'I', same as info = 2.

If *info* = 4, no eigenvalues have been computed. The floating-point arithmetic on the computer is not behaving as expected.

If info = -i, the *i*th parameter had an illegal value.

#### **Application Notes**

The eigenvalues of T are computed to high relative accuracy which means that if they vary widely in magnitude, then any small eigenvalues will be computed more accurately than, for example, with the standard QR method. However, the reduction to tridiagonal form (prior to calling the routine) may exclude the possibility of obtaining high relative accuracy in the small eigenvalues of the original matrix if its eigenvalues vary widely in magnitude.

# ?stein

Computes the eigenvectors corresponding to specified eigenvalues of a real symmetric tridiagonal matrix.

```
call sstein ( n, d, e, m, w, iblock, isplit, z, ldz,
  work, iwork, ifailv, info )
call dstein ( n, d, e, m, w, iblock, isplit, z, ldz,
  work, iwork, ifailv, info )
call cstein ( n, d, e, m, w, iblock, isplit, z, ldz,
  work, iwork, ifailv, info )
call zstein ( n, d, e, m, w, iblock, isplit, z, ldz,
  work, iwork, ifailv, info )
```

### Discussion

This routine computes the eigenvectors of a real symmetric tridiagonal matrix T corresponding to specified eigenvalues, by inverse iteration. It is designed to be used in particular after the specified eigenvalues have been computed by ?stebz with *order* = 'B', but may also be used when the eigenvalues have been computed by other routines. If you use this routine after ?stebz, it can take advantage of the block structure by performing inverse iteration on each block  $T_i$  separately, which is more efficient than using the whole matrix T.

If T has been formed by reduction of a full symmetric or Hermitian matrix A to tridiagonal form, you can transform eigenvectors of T to eigenvectors of A by calling ?ormtr or ?opmtr (for real flavors) or by calling ?unmtr or ?upmtr (for complex flavors).

#### **Input Parameters**

п

- **INTEGER**. The order of the matrix T ( $n \ge 0$ ).
- *m* **INTEGER.** The number of eigenvectors to be returned.

d, e, w	REAL for single-precision flavors DOUBLE PRECISION for double-precision flavors.
	Arrays: d(*) contains the diagonal elements of <i>T</i> . The dimension of <i>d</i> must be at least max $(1, n)$ .
	e(*) contains the off-diagonal elements of <i>T</i> . The dimension of $e$ must be at least max $(1, n-1)$ .
	w(*) contains the eigenvalues of <i>T</i> , stored in $w(1)$ to $w(m)$ (as returned by ?stebz, see page 5-149). Eigenvalues of $T_1$ must be supplied first, in non-decreasing order; then those of $T_2$ , again in non-decreasing order, and so on. Constraint: if $iblock(i) = iblock(i+1), w(i) \leq w(i+1)$ .
	The dimension of w must be at least $max(1, n)$ .
iblock,isplit	INTEGER. Arrays, DIMENSION at least max(1, n). The arrays <i>iblock</i> and <i>isplit</i> , as returned by ?stebz with <i>order</i> = 'B'.
	If you did not call <b>?stebz</b> with <i>order</i> = 'B', set all elements of <i>iblock</i> to 1, and <i>isplit</i> (1) to <i>n</i> .)
ldz	<b>INTEGER.</b> The first dimension of the output array $z$ ; $ldz \ge max(1, n)$ .
work	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. Workspace array, <b>DIMENSION</b> at least max(1, 5 <i>n</i> ).
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least max(1, <i>n</i> ).

z REAL for sstein DOUBLE PRECISION for dstein COMPLEX for cstein DOUBLE COMPLEX for zstein. Array, DIMENSION (*ldz*, *).

	If <i>info</i> = 0, <i>z</i> contains the <i>m</i> orthonormal eigenvectors, stored by columns. (The <i>i</i> th column corresponds to the <i>i</i> th specified eigenvalue.)
ifailv	<b>INTEGER.</b> Array, <b>DIMENSION</b> at least $max(1, m)$ . If <i>info</i> = <i>i</i> > 0, the first <i>i</i> elements of <i>ifailv</i> contain the indices of any eigenvectors that failed to converge.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = i$ , then <i>i</i> eigenvectors (as indicated by the parameter $ifailv$ ) each failed to converge in 5 iterations. The current iterates are stored in the corresponding columns of the array <i>z</i> . If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

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Each computed eigenvector  $z_i$  is an exact eigenvector of a matrix  $T + E_i$ , where  $||E_i||_2 = O(\varepsilon)||T||_2$ . However, a set of eigenvectors computed by this routine may not be orthogonal to so high a degree of accuracy as those computed by ?steqr.

# ?disna

Computes the reciprocal condition numbers for the eigenvectors of a symmetric/ Hermitian matrix or for the left or right singular vectors of a general matrix.

call sdisna (job, m, n, d, sep, info)
call ddisna (job, m, n, d, sep, info)

#### **Discussion**

This routine computes the reciprocal condition numbers for the eigenvectors of a real symmetric or complex Hermitian matrix or for the left or right singular vectors of a general *m*-by-*n* matrix.

The reciprocal condition number is the 'gap' between the corresponding eigenvalue or singular value and the nearest other one.

The bound on the error, measured by angle in radians, in the *i*-th computed vector is given by

```
slamch('E') * ( anorm / sep(i) )
```

where  $anorm = ||A||_2 = max(|d(j)|)$ . sep(i) is not allowed to be smaller than slamch('E')*anorm in order to limit the size of the error bound.

?disna may also be used to compute error bounds for eigenvectors of the generalized symmetric definite eigenproblem.

job	CHARACTER*1. Must be 'E', 'L', or 'R'. Specifies for which problem the reciprocal condition numbers should be computed: <i>job</i> = 'E': for the eigenvectors of a symmetric/Hermitian matrix; <i>job</i> = 'L': for the left singular vectors of a general matrix; <i>job</i> = 'R': for the right singular vectors of a general matrix.
m	<b>INTEGER.</b> The number of rows of the matrix $(m \ge 0)$ .
п	<b>INTEGER.</b> If $job = 'L'$ , or 'R', the number of columns of the matrix $(n \ge 0)$ . Ignored if $job = 'E'$ .
d	<b>REAL</b> for sdisna <b>DOUBLE PRECISION</b> for ddisna. Array, dimension at least max(1,m) if $job = 'E'$ , and at least max(1, min(m, n)) if $job = 'L'$ or 'R'. This array must contain the eigenvalues (if $job = 'E'$ ) or singular values (if $job = 'L'$ or 'R') of the matrix, in either increasing or decreasing order. If singular values, they must be non-negative.

sep	<b>REAL</b> for sdisna <b>DOUBLE PRECISION</b> for ddisna. Array, dimension at least $max(1,m)$ if $job = 'E'$ , and at least $max(1, min(m, n))$ if $job = 'L'or 'R'$ . The reciprocal condition numbers of the vectors.
info	<b>INTEGER</b> . If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

# **Generalized Symmetric-Definite Eigenvalue Problems**

Generalized symmetric-definite eigenvalue problems are as follows: find the eigenvalues  $\lambda$  and the corresponding eigenvectors *z* that satisfy one of these equations:

 $Az = \lambda Bz$ ,  $ABz = \lambda z$ , or  $BAz = \lambda z$ 

where A is an n by n symmetric or Hermitian matrix, and B is an n by n symmetric positive-definite or Hermitian positive-definite matrix.

In these problems, there exist n real eigenvectors corresponding to real eigenvalues (even for complex Hermitian matrices A and B).

Routines described in this section allow you to reduce the above generalized problems to standard symmetric eigenvalue problem  $Cy = \lambda y$ , which you can calve by calling LAPACK routines described earlier in this

which you can solve by calling LAPACK routines described earlier in this chapter (see <u>page 5-101</u>).

Different routines allow the matrices to be stored either conventionally or in packed storage. Prior to reduction, the positive-definite matrix *B* must first be factorized using either ?potrf or ?pptrf.

The reduction routine for the banded matrices A and B uses a split Cholesky factorization for which a specific routine <u>?pbstf</u> is provided. This refinement halves the amount of work required to form matrix C.

# Table 5-4Computational Routines for Reducing Generalized Eigenproblemsto Standard Problems

Matrix type	Reduce to standard problems (full storage)	Reduce to standard problems (packed storage)	Reduce to standard problems (band matrices)	Factorize band matrix
real symmetric matrices	?sygst	?spgst	?sbgst	?pbstf
complex Hermitian matrices	?hegst/	?hpgst	?hbgst	?pbstf

# ?sygst

*Reduces a real symmetric-definite generalized eigenvalue problem to the standard form.* 

```
call ssygst ( itype, uplo, n, a, lda, b, ldb, info )
call dsygst ( itype, uplo, n, a, lda, b, ldb, info )
```

#### **Discussion**

This routine reduces real symmetric-definite generalized eigenproblems

 $Az = \lambda Bz$ ,  $ABz = \lambda z$ , or  $BAz = \lambda z$ 

to the standard form  $Cy = \lambda y$ . Here *A* is a real symmetric matrix, and *B* is a real symmetric positive-definite matrix. Before calling this routine, call **?potrf** to compute the Cholesky factorization:  $B = U^T U$  or  $B = LL^T$  (see page 4-14).

itype	INTEGER. Must be 1 or 2 or 3. If <i>itype</i> = 1, the generalized eigenproblem is $Az = \lambda Bz$ ; for <i>uplo</i> = 'U': $C = U^{-T}AU^{-1}$ , $z = U^{-1}y$ ; for <i>uplo</i> = 'L': $C = L^{-1}AL^{-T}$ , $z = L^{-T}y$ . If <i>itype</i> = 2, the generalized eigenproblem is $ABz = \lambda z$ ; for <i>uplo</i> = 'U': $C = UAU^{T}$ , $z = U^{-1}y$ ; for <i>uplo</i> = 'L': $C = L^{T}AL$ , $z = L^{-T}y$ . If <i>itype</i> = 3, the generalized eigenproblem is $BAz = \lambda z$ ; for <i>uplo</i> = 'U': $C = UAU^{T}$ , $z = U^{T}y$ . If <i>itype</i> = 3, the generalized eigenproblem is $BAz = \lambda z$ ; for <i>uplo</i> = 'U': $C = UAU^{T}$ , $z = U^{T}y$ ; for <i>uplo</i> = 'U': $C = UAU^{T}$ , $z = U^{T}y$ ; for <i>uplo</i> = 'L': $C = L^{T}AL$ , $z = Ly$ .
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , the array <i>a</i> stores the upper triangle of <i>A</i> ; you must supply <i>B</i> in the factored form $B = U^T U$ . If $uplo = 'L'$ , the array <i>a</i> stores the lower triangle of <i>A</i> ; you must supply <i>B</i> in the factored form $B = LL^T$ .
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).

a, b	REAL for ssygst
	DOUBLE PRECISION for dsygst.
	Arrays:
	a(1da, *) contains the upper or lower triangle of A.
	The second dimension of $a$ must be at least max $(1, n)$ .
	b(1db, *) contains the Cholesky-factored matrix B:
	$B = U^T U$ or $B = LL^T$ (as returned by <b>?potrf</b> ).
	The second dimension of $b$ must be at least max $(1, n)$ .
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .

а	The upper or lower triangle of $A$ is overwritten by the upper or lower triangle of $C$ , as specified by the arguments <i>itype</i> and <i>uplo</i> .
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th parameter had an illegal value.

# **Application Notes**

Forming the reduced matrix *C* is a stable procedure. However, it involves implicit multiplication by  $B^{-1}$  (if *itype* = 1) or *B* (if *itype* = 2 or 3). When the routine is used as a step in the computation of eigenvalues and eigenvectors of the original problem, there may be a significant loss of accuracy if *B* is ill-conditioned with respect to inversion.

The approximate number of floating-point operations is  $n^3$ .

# ?hegst

Reduces a complex Hermitian-definite generalized eigenvalue problem to the standard form.

```
call chegst ( itype, uplo, n, a, lda, b, ldb, info )
call zhegst ( itype, uplo, n, a, lda, b, ldb, info )
```

#### **Discussion**

This routine reduces complex Hermitian-definite generalized eigenvalue problems

$$Az = \lambda Bz$$
,  $ABz = \lambda z$ , or  $BAz = \lambda z$ 

to the standard form  $Cy = \lambda y$ . Here the matrix *A* is complex Hermitian, and *B* is complex Hermitian positive-definite. Before calling this routine, you must call **?potrf** to compute the Cholesky factorization:  $B = U^H U$  or  $B = LL^H$  (see page 4-14).

```
INTEGER. Must be 1 or 2 or 3.
itype
                    If itype = 1, the generalized eigenproblem is Az = \lambda Bz;
                          for uplo = 'U': C = U^{-H}AU^{-1}, z = U^{-1}v;
                          for uplo = 'L': C = L^{-1}AL^{-H}, z = L^{-H}y.
                    If itype = 2, the generalized eigenproblem is ABz = \lambda z;
                          for uplo = U' : C = UAU^{H}, z = U^{-1}y;
                          for uplo = 'L': C = L^H A L, z = L^{-H} y.
                    If itype = 3, the generalized eigenproblem is BAz = \lambda z;
                          for uplo = U' : C = UAU^H, z = U^H y;
                          for uplo = 'L': C = L^H AL, z = Ly.
                    CHARACTER*1. Must be 'U' or 'L'.
uplo
                    If uplo = 'U', the array a stores the upper triangle of A;
                    you must supply B in the factored form B = U^H U.
                    If uplo = 'L', the array a stores the lower triangle of A;
                    you must supply B in the factored form B = LL^{H}.
```

n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).	
a, b	COMPLEX for chegst DOUBLE COMPLEX for zhegst. Arrays: a(1da, *) contains the upper or lower triangle of A. The second dimension of a must be at least max $(1, n)$ .	
	b(ldb, *) contains the Cholesky-factored matrix <i>B</i> : $B = U^{H}U$ or $B = LL^{H}$ (as returned by ?potrf). The second dimension of <i>b</i> must be at least max(1, <i>n</i> ).	
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .	
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max(1, $n$ ).	

a	The upper or lower triangle of $A$ is overwritten by the upper or lower triangle of $C$ , as specified by the arguments <i>itype</i> and <i>uplo</i> .
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

Forming the reduced matrix *C* is a stable procedure. However, it involves implicit multiplication by  $B^{-1}$  (if *itype* = 1) or *B* (if *itype* = 2 or 3). When the routine is used as a step in the computation of eigenvalues and eigenvectors of the original problem, there may be a significant loss of accuracy if *B* is ill-conditioned with respect to inversion.

The approximate number of floating-point operations is  $n^3$ .

# ?spgst

Reduces a real symmetric-definite generalized eigenvalue problem to the standard form using packed storage.

```
call sspgst ( itype, uplo, n, ap, bp, info )
call dspgst ( itype, uplo, n, ap, bp, info )
```

#### **Discussion**

This routine reduces real symmetric-definite generalized eigenproblems

 $Az = \lambda Bz$ ,  $ABz = \lambda z$ , or  $BAz = \lambda z$ 

to the standard form  $Cy = \lambda y$ , using packed matrix storage. Here *A* is a real symmetric matrix, and *B* is a real symmetric positive-definite matrix. Before calling this routine, call **?ptrf** to compute the Cholesky factorization:  $B = U^T U$  or  $B = LL^T$  (see page 4-16).

#### **Input Parameters**

itype	<b>INTEGER.</b> Must be 1 or 2 or 3. If <i>itype</i> = 1, the generalized eigenproblem is $Az = \lambda Bz$ ; for <i>uplo</i> = 'U': $C = U^{-T}AU^{-1}$ , $z = U^{-1}y$ ; for <i>uplo</i> = 'L': $C = L^{-1}AL^{-T}$ , $z = L^{-T}y$ . If <i>itype</i> = 2, the generalized eigenproblem is $ABz = \lambda z$ ; for <i>uplo</i> = 'U': $C = UAU^{T}$ , $z = U^{-1}y$ ; for <i>uplo</i> = 'L': $C = L^{T}AL$ , $z = L^{-T}y$ . If <i>itype</i> = 3, the generalized eigenproblem is $BAz = \lambda z$ ; for <i>uplo</i> = 'U': $C = UAU^{T}$ , $z = U^{T}y$ . If <i>itype</i> = 3, the generalized eigenproblem is $BAz = \lambda z$ ; for <i>uplo</i> = 'U': $C = UAU^{T}$ , $z = U^{T}y$ ; for <i>uplo</i> = 'U': $C = UAU^{T}$ , $z = U^{T}y$ ;
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , $ap$ stores the packed upper triangle of $A$ ; you must supply $B$ in the factored form $B = U^T U$ . If $uplo = 'L'$ , $ap$ stores the packed lower triangle of $A$ ; you must supply $B$ in the factored form $B = LL^T$ .
п	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).

n

ap, bp	REAL for sspgst
	DOUBLE PRECISION for dspgst.
	Arrays:
	ap(*) contains the packed upper or lower triangle of A.
	The dimension of <i>ap</i> must be at least max $(1, n*(n+1)/2)$ .
	bp(*) contains the packed Cholesky factor of B (as returned by ?pptrf with the same uplo value). The dimension of bp must be at least max(1,
	n*(n+1)/2).

ap	The upper or lower triangle of $A$ is overwritten by the upper or lower triangle of $C$ , as specified by the arguments <i>itype</i> and <i>uplo</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

# **Application Notes**

Forming the reduced matrix *C* is a stable procedure. However, it involves implicit multiplication by  $B^{-1}$  (if *itype* = 1) or *B* (if *itype* = 2 or 3). When the routine is used as a step in the computation of eigenvalues and eigenvectors of the original problem, there may be a significant loss of accuracy if *B* is ill-conditioned with respect to inversion.

The approximate number of floating-point operations is  $n^3$ .

# ?hpgst

Reduces a complex Hermitian-definite generalized eigenvalue problem to the standard form using packed storage.

```
call chpgst ( itype, uplo, n, ap, bp, info )
call zhpgst ( itype, uplo, n, ap, bp, info )
```

#### **Discussion**

This routine reduces real symmetric-definite generalized eigenproblems

 $Az = \lambda Bz$ ,  $ABz = \lambda z$ , or  $BAz = \lambda z$ 

to the standard form  $Cy = \lambda y$ , using packed matrix storage. Here A is a real symmetric matrix, and B is a real symmetric positive-definite matrix. Before calling this routine, you must call **?ptrf** to compute the Cholesky factorization:  $B = U^H U$  or  $B = LL^H$  (see page 4-16).

itype	<b>INTEGER.</b> Must be 1 or 2 or 3. If <i>itype</i> = 1, the generalized eigenproblem is $Az = \lambda Bz$ ; for <i>uplo</i> = 'U': $C = U^{-H}AU^{-1}$ , $z = U^{-1}y$ ; for <i>uplo</i> = 'L': $C = L^{-1}AL^{-H}$ , $z = L^{-H}y$ . If <i>itype</i> = 2, the generalized eigenproblem is $ABz = \lambda z$ ; for <i>uplo</i> = 'U': $C = UAU^{H}$ , $z = U^{-1}y$ ; for <i>uplo</i> = 'L': $C = L^{H}AL$ , $z = L^{-H}y$ . If <i>itype</i> = 3, the generalized eigenproblem is $BAz = \lambda z$ ; for <i>uplo</i> = 'U': $C = UAU^{H}$ , $z = U^{H}y$ . If <i>itype</i> = 3, the generalized eigenproblem is $BAz = \lambda z$ ; for <i>uplo</i> = 'U': $C = UAU^{H}$ , $z = U^{H}y$ ; for <i>uplo</i> = 'L': $C = L^{H}AL$ , $z = Ly$ .
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , $ap$ stores the packed upper triangle of A; you must supply B in the factored form $B = U^H U$ . If $uplo = 'L'$ , $ap$ stores the packed lower triangle of A; you must supply B in the factored form $B = LL^H$ .
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).

	ap, bp	COMPLEX for chpgst
		DOUBLE COMPLEX for zhpgst.
		Arrays:
		ap(*) contains the packed upper or lower triangle of A.
		The dimension of a must be at least $\max(1, \frac{n(n+1)}{2})$ .
		bp(*) contains the packed Cholesky factor of B
		(as returned by <b>?pptrf</b> with the same <i>uplo</i> value).
		The dimension of <b>b</b> must be at least $\max(1, n^*(n+1)/2)$ .
Output Parameters		
	ар	The upper or lower triangle of $A$ is overwritten by the upper or lower triangle of $C$ , as specified by the arguments <i>itype</i> and <i>uplo</i> .

info

INTEGER. If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value.

#### **Application Notes**

Forming the reduced matrix *C* is a stable procedure. However, it involves implicit multiplication by  $B^{-1}$  (if *itype* = 1) or *B* (if *itype* = 2 or 3). When the routine is used as a step in the computation of eigenvalues and eigenvectors of the original problem, there may be a significant loss of accuracy if *B* is ill-conditioned with respect to inversion.

The approximate number of floating-point operations is  $n^3$ .

# ?sbgst

Reduces a real symmetric-definite generalized eigenproblem for banded matrices to the standard form using the factorization performed by ?pbstf.

```
call ssbgst ( vect, uplo, n, ka, kb, ab, ldab, bb, ldbb, x, ldx,
  work, info )
call dsbgst ( vect, uplo, n, ka, kb, ab, ldab, bb, ldbb, x, ldx,
  work, info )
```

### **Discussion**

To reduce the real symmetric-definite generalized eigenproblem  $Az = \lambda Bz$  to the standard form  $Cy = \lambda y$ , where *A*, *B* and *C* are banded, this routine must be preceded by a call to <u>spbstf/dpbstf</u>, which computes the split Cholesky factorization of the positive-definite matrix *B*:  $B = S^T S$ . The split Cholesky factorization, compared with the ordinary Cholesky factorization, allows the work to be approximately halved.

This routine overwrites A with  $C = X^T A X$ , where  $X = S^{-1}Q$  and Q is an orthogonal matrix chosen (implicitly) to preserve the bandwidth of A. The routine also has an option to allow the accumulation of X, and then, if z is an eigenvector of C, Xz is an eigenvector of the original system.

vect	CHARACTER*1. Must be 'N' or 'V'.
	If <b>vect</b> = 'N', then matrix X is not returned;
	If <b>vect</b> = $V'$ , then matrix X is returned.
uplo	CHARACTER*1. Must be 'U' or 'L'.
	If $uplo = 'U'$ , <i>ab</i> stores the upper triangular part of A.
	If $uplo = 'L'$ , <i>ab</i> stores the lower triangular part of A.
n	<b>INTEGER.</b> The order of the matrices A and B $(n \ge 0)$ .
ka	<b>INTEGER.</b> The number of super- or sub-diagonals in A
	$(ka \ge 0).$

kb	<b>INTEGER.</b> The number of super- or sub-diagonals in $B$ ( $ka \ge kb \ge 0$ ).
ab,bb,work	REAL for ssbgst DOUBLE PRECISION for dsbgst ab (ldab, *) is an array containing either upper or lower triangular part of the symmetric matrix A (as specified by uplo) in band storage format. The second dimension of the array ab must be at least max(1, n). bb (ldbb, *) is an array containing the banded split Cholesky factor of B as specified by uplo, n and kb and returned by spbstf/dpbstf. The second dimension of the array bb must be at least max(1, n). work(*) is a workspace array, DIMENSION at least max(1, 2*n)
ldab	<b>INTEGER.</b> The first dimension of the array <i>ab</i> ; must be at least <i>ka</i> +1.
ldbb	<b>INTEGER.</b> The first dimension of the array <i>bb</i> ; must be at least <i>kb</i> +1.
ldx	The first dimension of the output array x. Constraints: if $vect =  N $ , then $ldx \ge 1$ ; if $vect =  V $ , then $ldx \ge max(1, n)$ .
Output Parame	ters
ab	On exit, this array is overwritten by the upper or lower triangle of $C$ as specified by <u>uplo</u> .
x	REAL for ssbgst DOUBLE PRECISION for dsbgst Array. If $vect = V'$ , then $x (ldx, *)$ contains the <i>n</i> by <i>n</i> matrix $X = S^{-1}Q$ . If $vect = N'$ , then <i>x</i> is not referenced. The second dimension of <i>x</i> must be:

at least max(1, *n*), if *vect* = 'V'; at least 1, if *vect* = 'N'. info

**INTEGER.** If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value.

## **Application Notes**

Forming the reduced matrix *C* involves implicit multiplication by  $B^{-1}$ . When the routine is used as a step in the computation of eigenvalues and eigenvectors of the original problem, there may be a significant loss of accuracy if *B* is ill-conditioned with respect to inversion. The total number of floating-point operations is approximately  $6n^{2*}kb$ , when vect = 'N'. Additional  $(3/2)n^{3*}(kb/ka)$  operations are required when vect = 'V'. All these estimates assume that both *ka* and *kb* are much less than *n*.

# ?hbgst

Reduces a complex Hermitian-definite generalized eigenproblem for banded matrices to the standard form using the factorization performed by <code>?pbstf</code>.

```
call chbgst ( vect, uplo, n, ka, kb, ab, ldab, bb, ldbb, x, ldx,
  work, rwork, info )
call zhbgst ( vect, uplo, n, ka, kb, ab, ldab, bb, ldbb, x, ldx,
  work, rwork, info )
```

#### **Discussion**

To reduce the complex Hermitian-definite generalized eigenproblem  $Az = \lambda Bz$  to the standard form  $Cy = \lambda y$ , where *A*, *B* and *C* are banded, this routine must be preceded by a call to <u>cpbstf/zpbstf</u>, which computes the split Cholesky factorization of the positive-definite matrix  $B: B = S^H S$ . The split Cholesky factorization, compared with the ordinary Cholesky factorization, allows the work to be approximately halved.

This routine overwrites A with  $C = X^H A X$ , where  $X = S^{-1}Q$  and Q is a unitary matrix chosen (implicitly) to preserve the bandwidth of A. The routine also has an option to allow the accumulation of X, and then, if z is an eigenvector of C, Xz is an eigenvector of the original system.

vect	CHARACTER*1. Must be 'N' or 'V'.
	If $vect = 'N'$ , then matrix X is not returned;
	If $vect = V'$ , then matrix X is returned.
uplo	CHARACTER*1. Must be 'U' or 'L'.
	If $uplo = 'U'$ , <i>ab</i> stores the upper triangular part of A.
	If $uplo = 'L'$ , <i>ab</i> stores the lower triangular part of A.
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> $(n \ge 0)$ .
ka	<b>INTEGER.</b> The number of super- or sub-diagonals in A
	$(ka \ge 0).$

kb	<b>INTEGER.</b> The number of super- or sub-diagonals in $B$ ( $ka \ge kb \ge 0$ ).
ab,bb,work	COMPLEX for chbgst DOUBLE COMPLEX for zhbgst ab (ldab, *) is an array containing either upper or lower triangular part of the Hermitian matrix $A$ (as specified by $uplo$ ) in band storage format. The second dimension of the array $ab$ must be at least max $(1, n)$ . bb (ldbb, *) is an array containing the banded split Cholesky factor of $B$ as specified by $uplo$ , $n$ and $kb$ and returned by cpbstf/zpbstf. The second dimension of the array $bb$ must be at least max $(1, n)$ . work(*) is a workspace array, DIMENSION at least max $(1, n)$
ldab	<b>INTEGER.</b> The first dimension of the array $ab$ ; must be at least $ka$ +1.
ldbb	<b>INTEGER</b> . The first dimension of the array $bb$ ; must be at least $kb$ +1.
ldx	The first dimension of the output array x. Constraints: if $vect =  N $ , then $ldx \ge 1$ ; if $vect =  V $ , then $ldx \ge max(1, n)$ .
rwork	REAL for chbgst DOUBLE PRECISION for zhbgst Workspace array, DIMENSION at least max(1, <i>n</i> )

ab	On exit, this array is overwritten by the upper or lower triangle of $C$ as specified by <i>uplo</i> .
x	COMPLEX for chbgst DOUBLE COMPLEX for zhbgst Array.
	If $vect = V'$ , then $x (ldx, *)$ contains the <i>n</i> by <i>n</i> matrix $X = S^{-1}Q$ . If $vect = N'$ , then $x$ is not referenced.

The second dimension of x must be: at least max(1, n), if vect = V'; at least 1, if vect = N'.

INTEGER.

info

If info = 0, the execution is successful.

If info = -i, the *i*th parameter had an illegal value.

### **Application Notes**

Forming the reduced matrix *C* involves implicit multiplication by  $B^{-1}$ . When the routine is used as a step in the computation of eigenvalues and eigenvectors of the original problem, there may be a significant loss of accuracy if *B* is ill-conditioned with respect to inversion. The total number of floating-point operations is approximately  $20n^{2*}kb$ , when vect = 'N'. Additional  $5n^{3*}(kb/ka)$  operations are required when vect = 'V'. All these estimates assume that both *ka* and *kb* are much less

than <u>n</u>.

# ?pbstf

Computes a split Cholesky factorization of a real symmetric or complex Hermitian positive-definite banded matrix used in ?sbgst/?hbgst.

call	spbstf	(	uplo,	n,	kb,	bb,	ldbb,	info	)
call	dpbstf	(	uplo,	n,	kb,	bb,	ldbb,	info	)
call	cpbstf	(	uplo,	n,	kb,	bb,	ldbb,	info	)
call	zpbstf	(	uplo,	n,	kb,	bb,	ldbb,	info	)

#### **Discussion**

This routine computes a split Cholesky factorization of a real symmetric or complex Hermitian positive-definite band matrix *B*. It is to be used in conjunction with <code>?sbgst/?hbgst</code>.

The factorization has the form  $B = S^T S$  (or  $B = S^H S$  for complex flavors), where *S* is a band matrix of the same bandwidth as *B* and the following structure: S is upper triangular in the first (n+kb)/2 rows and lower triangular in the remaining rows.

uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , bb stores the upper triangular part of B. If $uplo = 'L'$ , bb stores the lower triangular part of B.
п	<b>INTEGER.</b> The order of the matrix $B$ ( $n \ge 0$ ).
kb	<b>INTEGER.</b> The number of super- or sub-diagonals in $B$ $(kb \ge 0)$ .
bb	REAL for spbstf DOUBLE PRECISION for dpbstf COMPLEX for cpbstf DOUBLE COMPLEX for zpbstf. bb (1dbb,*) is an array containing either upper or lower triangular part of the matrix <i>B</i> (as specified by

uplo) in b	and storage format.
The second	dimension of the array bb must be at least
max(1, <u>n</u> ).	
INTEGER.	The first dimension of <i>bb</i> ; must be at least
<u>kb</u> +1.	

ldbb

bb	On exit, this array is overwritten by the elements of the split Cholesky factor <i>S</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = i$ , then the factorization could not be completed, because the updated element $b_{ii}$ would be the square root of a negative number; hence the matrix <i>B</i> is not positive-definite. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## **Application Notes**

The computed factor *S* is the exact factor of a perturbed matrix B + E, where

$$|E| \le c(\mathbf{kb} + 1)\varepsilon |S^{H}||S|, \quad |e_{ij}| \le c(\mathbf{kb} + 1)\varepsilon \sqrt{b_{ii}b_{jj}}$$

 $c(\mathbf{n})$  is a modest linear function of  $\mathbf{n}$ , and  $\boldsymbol{\varepsilon}$  is the machine precision.

The total number of floating-point operations for real flavors is approximately  $n(kb+1)^2$ . The number of operations for complex flavors is 4 times greater. All these estimates assume that kb is much less than n.

After calling this routine, you can call  $\underline{?sbgst}/\underline{?hbgst}$  to solve the generalized eigenproblem  $Az = \lambda Bz$ , where *A* and *B* are banded and *B* is positive-definite.

# **Nonsymmetric Eigenvalue Problems**

This section describes LAPACK routines for solving nonsymmetric eigenvalue problems, computing the Schur factorization of general matrices, as well as performing a number of related computational tasks.

A *nonsymmetric eigenvalue problem* is as follows: given a nonsymmetric (or non-Hermitian) matrix A, find the *eigenvalues*  $\lambda$  and the corresponding *eigenvectors z* that satisfy the equation

 $Az = \lambda z$  (right eigenvectors z)

or the equation

 $z^{H}A = \lambda z^{H}$  (left eigenvectors z).

Nonsymmetric eigenvalue problems have the following properties:

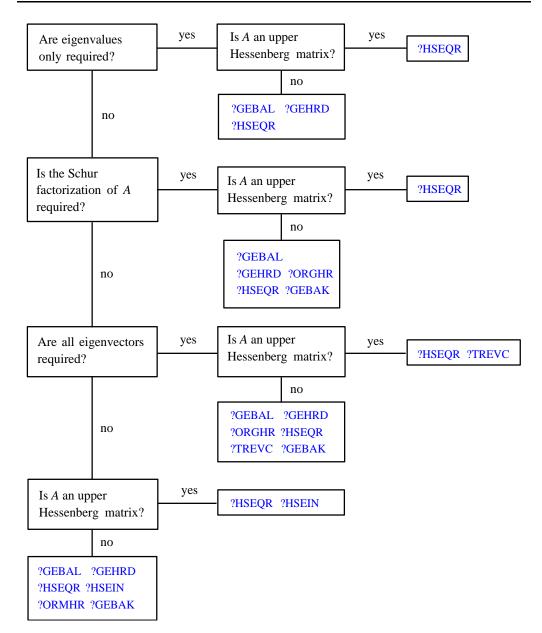
- The number of eigenvectors may be less than the matrix order (but is not less than the number of *distinct eigenvalues* of *A*).
- Eigenvalues may be complex even for a real matrix *A*.
- If a real nonsymmetric matrix has a complex eigenvalue *a+bi* corresponding to an eigenvector *z*, then *a-bi* is also an eigenvalue. The eigenvalue *a-bi* corresponds to the eigenvector whose elements are complex conjugate to the elements of *z*.

To solve a nonsymmetric eigenvalue problem with LAPACK, you usually need to reduce the matrix to the upper Hessenberg form and then solve the eigenvalue problem with the Hessenberg matrix obtained. Table 5-5 lists LAPACK routines for reducing the matrix to the upper Hessenberg form by an orthogonal (or unitary) similarity transformation  $A = QHQ^H$  as well as routines for solving eigenvalue problems with Hessenberg matrices, forming the Schur factorization of such matrices and computing the corresponding condition numbers.

Decision tree in Figure 5-4 helps you choose the right routine or sequence of routines for an eigenvalue problem with a real nonsymmetric matrix. If you need to solve an eigenvalue problem with a complex non-Hermitian matrix, use the decision tree shown in Figure 5-5.

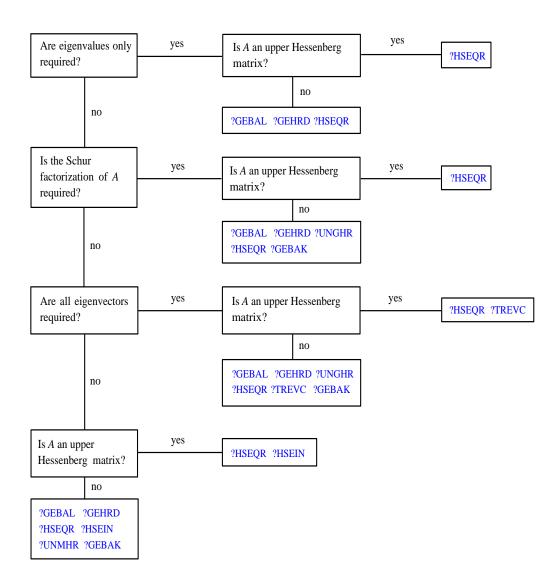
Problems							
Operation performed	Routines for real matrices	Routines for complex matrices					
Reduce to Hessenberg form $A = QHQ^H$	?gehrd,	?gehrd					
Generate the matrix Q	?orghr	?unghr					
Apply the matrix Q	?ormhr	<u>?unmhr</u>					
Balance matrix	?gebal	?gebal					
Transform eigenvectors of balanced matrix to those of the original matrix	?gebak	?gebak					
Find eigenvalues and Schur factorization (QR algorithm)	?hseqr	?hseqr					
Find eigenvectors from Hessenberg form (inverse iteration)	?hsein	?hsein					
Find eigenvectors from Schur factorization	?trevc	?trevc					
Estimate sensitivities of eigenvalues and eigenvectors	<u>?trsna</u>	<u>?trsna</u>					
Reorder Schur factorization	?trexc	?trexc					
Reorder Schur factorization, find the invariant subspace and estimate sensitivities	<u>?trsen</u>	<u>?trsen</u>					
Solves Sylvester's equation.	<u>?trsyl</u>	?trsyl					

# Table 5-5Computational Routines for Solving Nonsymmetric Eigenvalue<br/>Problems



## Figure 5-4 Decision Tree: Real Nonsymmetric Eigenvalue Problems

### Figure 5-5 Decision Tree: Complex Non-Hermitian Eigenvalue Problems



# ?gehrd

Reduces a general matrix to upper Hessenberg form.

call	sgehrd	(	n,	ilo,	ihi,	a,	lda,	tau,	work,	lwork,	info	)
call	dgehrd	(	n,	ilo,	ihi,	a,	lda,	tau,	work,	lwork,	info	)
call	cgehrd	(	n,	ilo,	ihi,	a,	lda,	tau,	work,	lwork,	info	)
call	zgehrd	(	n,	ilo,	ihi,	a,	lda,	tau,	work,	lwork,	info	)

### **Discussion**

The routine reduces a general matrix A to upper Hessenberg form H by an orthogonal or unitary similarity transformation  $A = QHQ^{H}$ . Here H has real subdiagonal elements.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of *elementary reflectors*. Routines are provided to work with Q in this representation.

n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
ilo, ihi	<b>INTEGER.</b> If A has been output by ?gebal, then <i>ilo</i> and <i>ihi</i> must contain the values returned by that routine. Otherwise <i>ilo</i> = 1 and <i>ihi</i> = n. (If $n > 0$ , then 1 $\leq ilo \leq ihi \leq n$ ; if $n = 0$ , <i>ilo</i> = 1 and <i>ihi</i> = 0.)
a, work	REAL for sgehrd DOUBLE PRECISION for dgehrd COMPLEX for cgehrd DOUBLE COMPLEX for zgehrd. Arrays: a ( <i>lda</i> ,*) contains the matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
	work (lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .

lwork	<b>INTEGER.</b> The size of the <i>work</i> array; at least max(1, <i>n</i> ).
	See Application notes for the suggested value of <i>lwork</i> .

a	Overwritten by the upper Hessenberg matrix $H$ and details of the matrix $Q$ . The subdiagonal elements of $H$ are real.
tau	REAL for sgehrd DOUBLE PRECISION for dgehrd COMPLEX for cgehrd DOUBLE COMPLEX for zgehrd. Array, DIMENSION at least max (1, <i>n</i> -1). Contains additional information on the matrix <i>Q</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using lwork = n*blocksize, where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed Hessenberg matrix *H* is exactly similar to a nearby matrix A+E, where  $||E||_2 < c(n)\varepsilon||A||_2$ , c(n) is a modestly increasing function of *n*, and  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations for real flavors is  $(2/3)(ihi - ilo)^2(2ihi + 2ilo + 3n)$ ; for complex flavors it is 4 times greater.

# ?orghr

Generates the real orthogonal matrix Q determined by ?gehrd.

call sorghr ( n, ilo, ihi, a, lda, tau, work, lwork, info )
call dorghr ( n, ilo, ihi, a, lda, tau, work, lwork, info )

### **Discussion**

This routine explicitly generates the orthogonal matrix Q that has been determined by a preceding call to sgehrd/dgehrd. (The routine ?gehrd reduces a real general matrix A to upper Hessenberg form H by an orthogonal similarity transformation,  $A = QHQ^T$ , and represents the matrix Q as a product of *ihi-ilo elementary reflectors*. Here *ilo* and *ihi* are values determined by sgebal/dgebal when balancing the matrix; if the matrix has not been balanced, *ilo* = 1 and *ihi* = n.)

The matrix Q generated by **?orghr** has the structure:

$$Q = \begin{bmatrix} I & 0 & 0 \\ 0 & Q_{22} & 0 \\ 0 & 0 & I \end{bmatrix}$$

where  $Q_{22}$  occupies rows and columns *ilo* to *ihi*.

n	<b>INTEGER.</b> The order of the matrix $Q$ ( $n \ge 0$ ).
ilo, ihi	<b>INTEGER.</b> These must be the same parameters <i>ilo</i> and <i>ihi</i> , respectively, as supplied to ?gehrd. (If $n > 0$ , then $1 \le ilo \le ihi \le n$ ; if $n = 0$ , <i>ilo</i> = 1 and <i>ihi</i> = 0.)
a, tau, work	REAL for sorghr DOUBLE PRECISION for dorghr Arrays:

	<ul> <li>a(lda,*) contains details of the vectors which define the elementary reflectors, as returned by ?gehrd.</li> <li>The second dimension of a must be at least max(1, n).</li> </ul>
	<ul> <li>tau(*) contains further details of the elementary reflectors, as returned by ?gehrd.</li> <li>The dimension of tau must be at least max (1, n-1).</li> </ul>
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, n)$ .
lwork	<pre>INTEGER. The size of the work array; lwork ≥ max(1,ihi-ilo). See Application notes for the suggested value of lwork.</pre>

a	Overwritten by the $n$ by $n$ orthogonal matrix $Q$ .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using lwork = (ihi - ilo)*blocksize, where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

The computed matrix Q differs from the exact result by a matrix E such that  $||E||_2 = O(\varepsilon)$ , where  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations is  $(4/3)(ihi-ilo)^3$ .

The complex counterpart of this routine is <u>?unghr</u>.

# ?ormhr

Multiplies an arbitrary real matrix C by the real orthogonal matrix Q determined by ?gehrd.

### **Discussion**

This routine multiplies a matrix *C* by the orthogonal matrix *Q* that has been determined by a preceding call to sgehrd/dgehrd. (The routine ?gehrd reduces a real general matrix *A* to upper Hessenberg form *H* by an orthogonal similarity transformation,  $A = QHQ^T$ , and represents the matrix *Q* as a product of *ihi-ilo* elementary reflectors. Here *ilo* and *ihi* are values determined by sgebal/dgebal when balancing the matrix; if the matrix has not been balanced, *ilo* = 1 and *ihi* = *n*.)

With ?ormhr, you can form one of the matrix products QC,  $Q^{T}C$ , CQ, or  $CQ^{T}$ , overwriting the result on C (which may be any real rectangular matrix).

A common application of **?ormhr** is to transform a matrix V of eigenvectors of H to the matrix QV of eigenvectors of A.

side	CHARACTER*1. Must be 'L' or 'R'. If <i>side</i> = 'L', then the routine forms $QC$ or $Q^{T}C$ . If <i>side</i> = 'R', then the routine forms $CQ$ or $CQ^{T}$ .
trans	CHARACTER*1. Must be 'N' or 'T'. If $trans =$ 'N', then $Q$ is applied to $C$ . If $trans =$ 'T', then $Q^T$ is applied to $C$ .
m	<b>INTEGER.</b> The number of rows in $C \ (m \ge 0)$ .
n	<b>INTEGER</b> . The number of columns in $C$ ( $n \ge 0$ ).

ilo, ihi	<b>INTEGER.</b> These must be the same parameters <i>ilo</i> and <i>ihi</i> , respectively, as supplied to ?gehrd. If $m > 0$ and <i>side</i> = 'L', then $1 \le ilo \le ihi \le m$ . If $m = 0$ and <i>side</i> = 'L', then <i>ilo</i> = 1 and <i>ihi</i> = 0.
	If $n > 0$ and side = 'R', then $110 = 1$ and $111 = 0$ . If $n > 0$ and side = 'R', then $1 \le 10 \le 1$ ini $\le n$ . If $n = 0$ and side = 'R', then $110 = 1$ and $1$ ini = 0.
a,tau,c,work	REAL for sormhr DOUBLE PRECISION for dormhr Arrays: a(lda,*) contains details of the vectors which define the elementary reflectors, as returned by ?gehrd. The second dimension of a must be at least max(1, m) if side = 'L' and at least max(1, n) if side = 'R'.
	tau(*) contains further details of the <i>elementary</i> reflectors, as returned by ?gehrd. The dimension of tau must be at least max $(1, m-1)$ if side = 'L' and at least max $(1, n-1)$ if side = 'R'.
	c(ldc,*) contains the <i>m</i> by <i>n</i> matrix <i>C</i> . The second dimension of <i>c</i> must be at least max $(1, n)$ .
	work (lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of <i>a</i> ; at least $max(1, m)$ if <i>side</i> = 'L' and at least max $(1, n)$ if <i>side</i> = 'R'.
ldc	<b>INTEGER</b> . The first dimension of $c$ ; at least max(1, $m$ ).
lwork	<pre>INTEGER. The size of the work array. If side = 'L', lwork ≥ max(1,n). If side = 'R', lwork ≥ max(1,m). See Application notes for the suggested value of lwork.</pre>

С	C is overwritten by $QC$ or $Q^TC$ or $CQ^T$ or $CQ$ as specified by <i>side</i> and <i>trans</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.

info

**INTEGER.** If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value.

## **Application Notes**

For better performance, *lwork* should be at least n*blocksize if *side* = 'L' and at least m*blocksize if *side* = 'R', where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed matrix Q differs from the exact result by a matrix E such that  $||E||_2 = O(\varepsilon)||C||_2$ , where  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations is  $2n(ihi-ilo)^2$  if side = 'L';  $2m(ihi-ilo)^2$  if side = 'R'.

The complex counterpart of this routine is <u>?unmhr</u>.

# ?unghr

Generates the complex unitary matrix Q determined by ?gehrd.

call cunghr ( n, ilo, ihi, a, lda, tau, work, lwork, info )
call zunghr ( n, ilo, ihi, a, lda, tau, work, lwork, info )

## **Discussion**

This routine is intended to be used following a call to cgehrd/zgehrd, which reduces a complex matrix A to upper Hessenberg form H by a unitary similarity transformation:  $A = QHQ^H$ . ?gehrd represents the matrix Q as a product of *ihi-ilo* elementary reflectors. Here *ilo* and *ihi* are values determined by cgebal/zgebal when balancing the matrix; if the matrix has not been balanced, *ilo* = 1 and *ihi* = *n*.

Use the routine **?unghr** to generate Q explicitly as a square matrix. The matrix Q has the structure:

$$Q = \begin{bmatrix} I & 0 & 0 \\ 0 & Q_{22} & 0 \\ 0 & 0 & I \end{bmatrix}$$

where  $Q_{22}$  occupies rows and columns *ilo* to *ihi*.

п	<b>INTEGER</b> . The order of the matrix $Q$ ( $n \ge 0$ ).
ilo, ihi	<b>INTEGER.</b> These must be the same parameters <i>ilo</i> and <i>ihi</i> , respectively, as supplied to ?gehrd. (If $n > 0$ , then $1 \le ilo \le ihi \le n$ . If $n = 0$ , then <i>ilo</i> = 1 and <i>ihi</i> = 0.)
a, tau, work	COMPLEX for cunghr DOUBLE COMPLEX for zunghr. Arrays:

	a(lda,*) contains details of the vectors which define the <i>elementary reflectors</i> , as returned by ?gehrd. The second dimension of a must be at least max(1, n).
	tau(*) contains further details of the <i>elementary</i> <i>reflectors</i> , as returned by ?gehrd. The dimension of $tau$ must be at least max $(1, n-1)$ .
	work (lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
lwork	<b>INTEGER</b> . The size of the <i>work</i> array; $lwork \ge max(1, ihi-ilo)$ . See <i>Application notes</i> for the suggested value of <i>lwork</i> .

a	Overwritten by the $n$ by $n$ unitary matrix $Q$ .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For better performance, try using lwork = (ihi - ilo) * blocksize, where blocksize is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed matrix Q differs from the exact result by a matrix E such that  $||E||_2 = O(\varepsilon)$ , where  $\varepsilon$  is the machine precision.

The approximate number of real floating-point operations is  $(16/3)(ihi-ilo)^3$ .

The real counterpart of this routine is <u>?orghr</u>.

## ?unmhr

Multiplies an arbitrary complex matrix C by the complex unitary matrix Q determined by ?gehrd.

#### **Discussion**

This routine multiplies a matrix *C* by the unitary matrix *Q* that has been determined by a preceding call to cgehrd/zgehrd. (The routine ?gehrd reduces a real general matrix *A* to upper Hessenberg form *H* by an orthogonal similarity transformation,  $A = QHQ^H$ , and represents the matrix *Q* as a product of *ihi-ilo* elementary reflectors. Here *ilo* and *ihi* are values determined by cgebal/zgebal when balancing the matrix; if the matrix has not been balanced, *ilo* = 1 and *ihi* = n.)

With ?unmhr, you can form one of the matrix products QC,  $Q^{H}C$ , CQ, or  $CQ^{H}$ , overwriting the result on C (which may be any complex rectangular matrix). A common application of this routine is to transform a matrix V of eigenvectors of H to the matrix QV of eigenvectors of A.

side	CHARACTER*1. Must be 'L' or 'R'.
	If <b>side</b> = 'L', then the routine forms $QC$ or $Q^{H}C$ .
	If <b>side</b> = 'R', then the routine forms $CQ$ or $CQ^{H}$ .
trans	CHARACTER*1. Must be 'N' or 'C'.
	If $trans = 'N'$ , then Q is applied to C.
	If $trans = 'T'$ , then $Q^H$ is applied to C.
m	<b>INTEGER</b> . The number of rows in $C \ (m \ge 0)$ .
n	<b>INTEGER</b> . The number of columns in $C (n \ge 0)$ .

ilo, ihi	<b>INTEGER.</b> These must be the same parameters <i>ilo</i> and <i>ihi</i> , respectively, as supplied to ?gehrd. If $m > 0$ and $side = 'L'$ , then $1 \le ilo \le ihi \le m$ . If $m = 0$ and $side = 'L'$ , then <i>ilo</i> = 1 and <i>ihi</i> = 0. If $n > 0$ and $side = 'R'$ , then $1 \le ilo \le ihi \le n$ . If $n = 0$ and $side = 'R'$ , then <i>ilo</i> = 1 and <i>ihi</i> = 0.
a,tau,c,work	COMPLEX for cummhr DOUBLE COMPLEX for zummhr. Arrays: a (1da,*) contains details of the vectors which define the elementary reflectors, as returned by ?gehrd. The second dimension of a must be at least max(1, m) if side = 'L' and at least max(1, n) if side = 'R'.
	tau(*) contains further details of the elementary reflectors, as returned by ?gehrd. The dimension of $tau$ must be at least max $(1, m-1)$ if <i>side</i> = 'L' and at least max $(1, n-1)$ if <i>side</i> = 'R'.
	c ( <i>ldc</i> , *) contains the <i>m</i> by <i>n</i> matrix <i>C</i> . The second dimension of <i>c</i> must be at least max(1, <i>n</i> ).
	work (lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max(1, $m$ ) if <u>side</u> = 'L' and at least max (1, $n$ ) if <u>side</u> = 'R'.
ldc	<b>INTEGER.</b> The first dimension of $c$ ; at least max(1, m).
lwork	<b>INTEGER.</b> The size of the <i>work</i> array. If <i>side</i> = 'L', <i>lwork</i> $\ge \max(1,n)$ . If <i>side</i> = 'R', <i>lwork</i> $\ge \max(1,m)$ . See Application notes for the suggested value of <i>lwork</i> .

С	C is overwritten by $QC$ or $Q^H C$ or $CQ^H$ or $CQ$ as specified by <i>side</i> and <i>trans</i> .
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.

infoINTEGER.If info = 0, the execution is successful.If info = -i, the *i*th parameter had an illegal value.

## **Application Notes**

For better performance, *lwork* should be at least n*blocksize if *side* = 'L' and at least m*blocksize if *side* = 'R', where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The computed matrix Q differs from the exact result by a matrix E such that  $||E||_2 = O(\varepsilon) ||C||_2$ , where  $\varepsilon$  is the machine precision.

The approximate number of floating-point operations is  $8n(ihi-ilo)^2$  if side = 'L';

 $8m(ihi-ilo)^2$  if side = 'R'.

The real counterpart of this routine is <u>?ormhr</u>.

# ?gebal

Balances a general matrix to improve the accuracy of computed eigenvalues and eigenvectors.

call sgebal ( job, n, a, lda, ilo, ihi, scale, info )
call dgebal ( job, n, a, lda, ilo, ihi, scale, info )
call cgebal ( job, n, a, lda, ilo, ihi, scale, info )
call zgebal ( job, n, a, lda, ilo, ihi, scale, info )

#### **Discussion**

This routine *balances* a matrix *A* by performing either or both of the following two similarity transformations:

(1) The routine first attempts to permute A to block upper triangular form:

$$PAP^{T} = A' = \begin{bmatrix} A'_{11} & A'_{12} & A'_{13} \\ 0 & A'_{22} & A'_{23} \\ 0 & 0 & A'_{33} \end{bmatrix}$$

where *P* is a permutation matrix, and  $A'_{11}$  and  $A'_{33}$  are upper triangular. The diagonal elements of  $A'_{11}$  and  $A'_{33}$  are eigenvalues of *A*. The rest of the eigenvalues of *A* are the eigenvalues of the central diagonal block  $A'_{22}$ , in rows and columns *ilo* to *ihi*. Subsequent operations to compute the eigenvalues of *A* (or its Schur factorization) need only be applied to these rows and columns; this can save a significant amount of work if *ilo* > 1 and *ihi* < *n*. If no suitable permutation exists (as is often the case), the routine sets *ilo* = 1 and *ihi* = *n*, and  $A'_{22}$  is the whole of *A*.

(2) The routine applies a diagonal similarity transformation to A', to make the rows and columns of  $A'_{22}$  as close in norm as possible:

$$A'' = DA' D^{-1} = \begin{bmatrix} I & 0 & 0 \\ 0 & D_{22} & 0 \\ 0 & 0 & I \end{bmatrix} \times \begin{bmatrix} A'_{11} & A'_{12} & A'_{13} \\ 0 & A'_{22} & A'_{23} \\ 0 & 0 & A'_{33} \end{bmatrix} \times \begin{bmatrix} I & 0 & 0 \\ 0 & D_{22}^{-1} & 0 \\ 0 & 0 & I \end{bmatrix}$$

This scaling can reduce the norm of the matrix (that is,  $||A'_{22}|| < ||A'_{22}||$ ), and hence reduce the effect of rounding errors on the accuracy of computed eigenvalues and eigenvectors.

## **Input Parameters**

job	CHARACTER*1. Must be 'N' or 'P' or 'S' or 'B'. If $job = 'N'$ , then A is neither permuted nor scaled (but <i>ilo, ihi, and scale</i> get their values). If $job = 'P'$ , then A is permuted but not scaled. If $job = 'S'$ , then A is scaled but not permuted. If $job = 'B'$ , then A is both scaled and permuted.
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
a	REAL for sgebal DOUBLE PRECISION for dgebal COMPLEX for cgebal DOUBLE COMPLEX for zgebal. Arrays: a (1da, *) contains the matrix A. The second dimension of a must be at least max(1, n). a is not referenced if $job = 'N'$ .
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .

#### **Output Parameters**

a	Overwritten by the balanced matrix ( <i>a</i> is not referenced if $job = 'N'$ ).
ilo, ihi	<b>INTEGER.</b> The values <i>ilo</i> and <i>ihi</i> such that on exit $a(i, j)$ is zero if $i > j$ and $1 \le j < ilo$ or <i>ihi</i> $< i \le n$ . If $job = 'N'$ or 'S', then <i>ilo</i> = 1 and <i>ihi</i> = <i>n</i> .
scale	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors Array, <b>DIMENSION</b> at least max(1, <i>n</i> ).
	Contains details of the permutations and scaling factors.

More precisely, if  $p_j$  is the index of the row and column<br/>interchanged with row and column j, and  $d_j$  is the<br/>scaling factor used to balance row and column j, then<br/> $scale(j) = p_j$  for j = 1, 2, ..., ilo-1, ihi+1, ..., n;<br/> $scale(j) = d_j$  for j = ilo, ilo + 1, ..., ihi.<br/>The order in which the interchanges are made is<br/>n to ihi+1, then 1 to ilo-1.infoINTEGER.<br/>If info = 0, the execution is successful.<br/>If info = -i, the ith parameter had an illegal value.

### **Application Notes**

The errors are negligible, compared with those in subsequent computations.

If the matrix A is balanced by this routine, then any eigenvectors computed subsequently are eigenvectors of the matrix A'' and hence you must call **?gebak** (see page 5-193) to transform them back to eigenvectors of A.

If the Schur vectors of A are required, do not call this routine with job = 'S' or 'B', because then the balancing transformation is not orthogonal (not unitary for complex flavors). If you call this routine with job = 'P', then any Schur vectors computed subsequently are Schur vectors of the matrix A'', and you'll need to call ?gebak (with *side* = 'R') to transform them back to Schur vectors of A.

The total number of floating-point operations is proportional to  $n^2$ .

# ?gebak

Transforms eigenvectors of a balanced matrix to those of the original nonsymmetric matrix.

call sgebak ( job,side,n,ilo,ihi,scale,m,v,ldv,info )
call dgebak ( job,side,n,ilo,ihi,scale,m,v,ldv,info )
call cgebak ( job,side,n,ilo,ihi,scale,m,v,ldv,info )
call zgebak ( job,side,n,ilo,ihi,scale,m,v,ldv,info )

## **Discussion**

This routine is intended to be used after a matrix A has been balanced by a call to ?gebal, and eigenvectors of the balanced matrix  $A'_{22}$  have subsequently been computed.

For a description of balancing, see **?gebal** (page 5-190). The balanced matrix A'' is obtained as  $A'' = DPAP^TD^{-1}$ , where *P* is a permutation matrix and *D* is a diagonal scaling matrix. This routine transforms the eigenvectors as follows:

if x is a right eigenvector of A'', then  $P^T D^{-1}x$  is a right eigenvector of A; if x is a left eigenvector of A'', then  $P^T Dy$  is a left eigenvector of A.

job	CHARACTER*1. Must be 'N' or 'P' or 'S' or 'B'. The same parameter <i>job</i> as supplied to ?gebal.
side	CHARACTER*1. Must be 'L' or 'R'. If <i>side</i> = 'L', then left eigenvectors are transformed. If <i>side</i> = 'R', then right eigenvectors are transformed.
n	<b>INTEGER.</b> The number of rows of the matrix of eigenvectors $(n \ge 0)$ .
ilo, ihi	<b>INTEGER.</b> The values <i>ilo</i> and <i>ihi</i> , as returned by <b>?gebal.</b> (If $n > 0$ , then $1 \le ilo \le ihi \le n$ ; if $n = 0$ , then <i>ilo</i> = 1 and <i>ihi</i> = 0.)

scale	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors Array, <b>DIMENSION</b> at least max(1, <i>n</i> ).
	Contains details of the permutations and/or the scaling factors used to balance the original general matrix, as returned by ?gebal.
m	<b>INTEGER</b> . The number of columns of the matrix of eigenvectors $(m \ge 0)$ .
V	REAL for sgebak DOUBLE PRECISION for dgebak COMPLEX for cgebak DOUBLE COMPLEX for zgebak. Arrays: v (1dv,*) contains the matrix of left or right eigenvectors to be transformed. The second dimension of v must be at least max(1, m).
ldv	<b>INTEGER</b> . The first dimension of $v$ ; at least max $(1, n)$ .

v	Overwritten by the transformed eigenvectors.
info	INTEGER.
	If $info = 0$ , the execution is successful.
	If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## **Application Notes**

The errors in this routine are negligible.

The approximate number of floating-point operations is approximately proportional to m*n.

## ?hseqr

Computes all eigenvalues and (optionally) the Schur factorization of a matrix reduced to Hessenberg form.

```
call shseqr (job,compz,n,ilo,ihi,h,ldh,wr,wi,z,ldz,work,lwork,info)
call dhseqr (job,compz,n,ilo,ihi,h,ldh,wr,wi,z,ldz,work,lwork,info)
call chseqr (job,compz,n,ilo,ihi,h,ldh,w,z,ldz,work,lwork,info)
call zhseqr (job,compz,n,ilo,ihi,h,ldh,w,z,ldz,work,lwork,info)
```

### **Discussion**

This routine computes all the eigenvalues, and optionally the Schur factorization, of an upper Hessenberg matrix  $H: H = ZTZ^H$ , where T is an upper triangular (or, for real flavors, quasi-triangular) matrix (the Schur form of H), and Z is the unitary or orthogonal matrix whose columns are the Schur vectors  $z_i$ .

You can also use this routine to compute the Schur factorization of a general matrix *A* which has been reduced to upper Hessenberg form *H*:  $A = QHQ^{H}$ , where *Q* is unitary (orthogonal for real flavors);  $A = (QZ)T(QZ)^{H}$ .

In this case, after reducing A to Hessenberg form by ?gehrd (page 5-178), call ?orghr to form Q explicitly (page 5-180) and then pass Q to ?hseqr with compz = 'V'.

You can also call (page 5-190) to balance the original matrix before reducing it to Hessenberg form by (page 7, so) that the Hessenberg matrix H will have the structure:

$$\begin{bmatrix} H_{11} & H_{12} & H_{13} \\ 0 & H_{22} & H_{23} \\ 0 & 0 & H_{33} \end{bmatrix}$$

where  $H_{11}$  and  $H_{33}$  are upper triangular.

If so, only the central diagonal block  $H_{22}$  (in rows and columns *ilo* to *ihi*) needs to be further reduced to Schur form (the blocks  $H_{12}$  and  $H_{23}$  are also affected). Therefore the values of *ilo* and *ihi* can be supplied to ?hseqr directly. Also, after calling this routine you must call ?gebak (page 5-193) to permute the Schur vectors of the balanced matrix to those of the original matrix.

If ?gebal has not been called, however, then *ilo* must be set to 1 and *ihi* to *n*. Note that if the Schur factorization of *A* is required, ?gebal must not be called with job = 'S' or 'B', because the balancing transformation is not unitary (for real flavors, it is not orthogonal).

**?hseqr** uses a multishift form of the upper Hessenberg *QR* algorithm. The Schur vectors are normalized so that  $||z_i||_2 = 1$ , but are determined only to within a complex factor of absolute value 1 (for the real flavors, to within a factor  $\pm 1$ ).

job	CHARACTER*1. Must be 'E' or 'S'. If $job = 'E'$ , then eigenvalues only are required. If $job = 'S'$ , then the Schur form <i>T</i> is required.
Compz	CHARACTER*1. Must be 'N' or 'I' or 'V'. If $compz =$ 'N', then no Schur vectors are computed (and the array z is not referenced). If $compz =$ 'I', then the Schur vectors of H are computed (and the array z is initialized by the routine). If $compz =$ 'V', then the Schur vectors of A are computed (and the array z must contain the matrix Q on entry).
п	<b>INTEGER.</b> The order of the matrix $H (n \ge 0)$ .
ilo, ihi	<b>INTEGER.</b> If <i>A</i> has been balanced by ?gebal, then <i>ilo</i> and <i>ihi</i> must contain the values returned by ?gebal. Otherwise, <i>ilo</i> must be set to 1 and <i>ihi</i> to <i>n</i> .
h, z, work	REAL for shseqr DOUBLE PRECISION for dhseqr COMPLEX for chseqr DOUBLE COMPLEX for zhseqr.

	Arrays: h(1dh, *) The <i>n</i> by <i>n</i> upper Hessenberg matrix <i>H</i> . The second dimension of <i>h</i> must be at least max(1, <i>n</i> ).
	z (ldz, *) If $compz = 'V'$ , then z must contain the matrix Q from the reduction to Hessenberg form. If $compz = 'I'$ , then z need not be set. If $compz = 'N'$ , then z is not referenced. The second dimension of z must be at least max(1, n) if $compz = 'V'$ or 'I'; at least 1 if $compz = 'N'$ .
	<i>work(lwork)</i> is a workspace array. The dimension of <i>work</i> must be at least max (1, <i>n</i> ).
ldh	<b>INTEGER.</b> The first dimension of $h$ ; at least max $(1, n)$ .
ldz	<b>INTEGER.</b> The first dimension of $z$ ; If $compz = 'N'$ , then $ldz \ge 1$ . If $compz = 'V'$ or 'I', then $ldz \ge max(1,n)$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> . <i>lwork</i> $\geq \max(1,n)$ . If <i>lwork</i> = -1, then a workspace query is assumed; the routine only calculates the optimal size of the <i>work</i> array, returns this value as the first entry of the <i>work</i> array, and no error message related to <i>lwork</i> is issued by xerbla.

W	COMPLEX for chseqr
	DOUBLE COMPLEX for zhseqr.
	Array, DIMENSION at least max $(1, n)$ .
	Contains the computed eigenvalues, unless <i>info</i> >0. The
	eigenvalues are stored in the same order as on the
	diagonal of the Schur form <i>T</i> (if computed).
wr, wi	REAL for shseqr
	DOUBLE PRECISION for dhseqr
	Arrays, DIMENSION at least max (1, <i>n</i> ) each.
	Contain the real and imaginary parts, respectively, of the

	computed eigenvalues, unless <i>info</i> > 0. Complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having positive imaginary part first. The eigenvalues are stored in the same order as on the diagonal of the Schur form $T$ (if computed).
Ζ	If <i>compz</i> = 'V' or 'I', then <i>z</i> contains the unitary (orthogonal) matrix of the required Schur vectors, unless <i>info</i> > 0. If <i>compz</i> = 'N', then <i>z</i> is not referenced.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the optimal <i>lwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info > 0$ , the algorithm has failed to find all the eigenvalues after a total $30(ihi-ilo+1)$ iterations. If info = i, elements 1,2,, <i>ilo</i> -1 and <i>i</i> +1, <i>i</i> +2,, <i>n</i> of <i>wr</i> and <i>wi</i> contain the real and imaginary parts of the eigenvalues which have been found.

## **Application Notes**

The computed Schur factorization is the exact factorization of a nearby matrix H + E, where  $||E||_2 < O(\varepsilon) ||H||_2/s_i$ , and  $\varepsilon$  is the machine precision. If  $\lambda_i$  is an exact eigenvalue, and  $\mu_i$  is the corresponding computed value, then  $|\lambda_i - \mu_i| \leq c(n)\varepsilon ||H||_2/s_i$  where c(n) is a modestly increasing function of n, and  $s_i$  is the reciprocal condition number of  $\lambda_i$ . You can compute the condition numbers  $s_i$  by calling ?trsna (see page 5-210).

The total number of floating-point operations depends on how rapidly the algorithm converges; typical numbers are as follows.

If only eigenvalues are computed:	$7n^3$ for real flavors
	$25n^3$ for complex flavors.
If the Schur form is computed:	$10n^3$ for real flavors
	$35n^3$ for complex flavors.
If the full Schur factorization is computed	
	$70n^3$ for complex flavors.

## ?hsein

Computes selected eigenvectors of an upper Hessenberg matrix that correspond to specified eigenvalues.

```
call shsein ( job, eigsrc, initv, select, n, h, ldh, wr, wi, vl,
    ldvl, vr, ldvr, mm, m, work, ifaill, ifailr, info )
call dhsein ( job, eigsrc, initv, select, n, h, ldh, wr, wi, vl,
    ldvl, vr, ldvr, mm, m, work, ifaill, ifailr, info )
call chsein ( job, eigsrc, initv, select, n, h, ldh, w, vl,
    ldvl, vr, ldvr, mm, m, work, rwork, ifaill, ifailr, info )
call zhsein ( job, eigsrc, initv, select, n, h, ldh, w, vl,
    ldvl, vr, ldvr, mm, m, work, rwork, ifaill, ifailr, info )
```

#### **Discussion**

This routine computes left and/or right eigenvectors of an upper Hessenberg matrix H, corresponding to selected eigenvalues.

The right eigenvector *x* and the left eigenvector *y*, corresponding to an eigenvalue  $\lambda$ , are defined by:  $Hx = \lambda x$  and  $y^H H = \lambda y^H$  (or  $H^H y = \lambda^* y$ ). Here  $\lambda^*$  denotes the conjugate of  $\lambda$ .

The eigenvectors are computed by inverse iteration. They are scaled so that, for a real eigenvector *x*, max $|x_i| = 1$ , and for a complex eigenvector, max $(|\text{Re}x_i| + |\text{Im}x_i|) = 1$ .

If *H* has been formed by reduction of a general matrix A to upper Hessenberg form, then eigenvectors of *H* may be transformed to eigenvectors of *A* by ?ormhr (page 5-182) or ?unmhr (page 5-187).

### **Input Parameters**

job

CHARACTER*1. Must be 'R' or 'L' or 'B'.

If job = 'R', then only right eigenvectors are computed.

If job = 'L', then only left eigenvectors are computed.

If job = 'B', then all eigenvectors are computed.

eigsrc	CHARACTER*1. Must be 'Q' or 'N'. If $eigsrc = 'Q'$ , then the eigenvalues of $H$ were found using ?hseqr (see page 5-195); thus if $H$ has any zero sub-diagonal elements (and so is block triangular), then the <i>j</i> th eigenvalue can be assumed to be an eigenvalue of the block containing the <i>j</i> th row/column. This property allows the routine to perform inverse iteration on just one diagonal block. If $eigsrc = 'N'$ , then no such assumption is made and the routine performs inverse iteration using the whole matrix.
initv	CHARACTER*1. Must be 'N' or 'U'. If <i>initv</i> = 'N', then no initial estimates for the selected eigenvectors are supplied. If <i>initv</i> = 'U', then initial estimates for the selected eigenvectors are supplied in v1 and/or vr.
select	LOGICAL. Array, DIMENSION at least max $(1, n)$ . Specifies which eigenvectors are to be computed. For real flavors: To obtain the real eigenvector corresponding to the real eigenvalue $wr(j)$ , set $select(j)$ to .TRUE. To select the complex eigenvector corresponding to the complex eigenvalue $(wr(j), wi(j))$ with complex conjugate $(wr(j+1), wi(j+1))$ , set $select(j)$ and/or select(j+1) to .TRUE.; the eigenvector corresponding to the first eigenvalue in the pair is computed. For complex flavors: To select the eigenvector corresponding to the eigenvalue $w(j)$ , set $select(j)$ to .TRUE.
n	<b>INTEGER</b> . The order of the matrix $H(n \ge 0)$ .
h,vl,vr,work	REAL for shsein DOUBLE PRECISION for dhsein COMPLEX for chsein DOUBLE COMPLEX for zhsein.

Arrays:

h(ldh, *) The n by n upper Hessenberg matrix H. The second dimension of *h* must be at least  $\max(1, n)$ .

#### vl(ldvl,*)

If initv = V' and job = L' or 'B', then v1 must contain starting vectors for inverse iteration for the left eigenvectors. Each starting vector must be stored in the same column or columns as will be used to store the corresponding eigenvector. If initv = 'N', then v1 need not be set.

The second dimension of  $v_1$  must be at least max(1, mm)if job = 'L' or 'B' and at least 1 if job = 'R'. The array v1 is not referenced if job = 'R'.

#### vr(ldvr,*)

If initv = V' and job = R' or B', then vr must contain starting vectors for inverse iteration for the right eigenvectors. Each starting vector must be stored in the same column or columns as will be used to store the corresponding eigenvector.

If initv = 'N', then vr need not be set. The second dimension of vr must be at least max(1, mm)if job = 'R' or 'B' and at least 1 if job = 'L'. The array *vr* is not referenced if job = 'L'.

work(*) is a workspace array. DIMENSION at least max  $(1, n^*(n+2))$  for real flavors and at least max  $(1, n^*n)$  for complex flavors.

**INTEGER.** The first dimension of h; at least max(1, n).

ldh

W

COMPLEX for chsein

DOUBLE COMPLEX for zhsein. Array, **DIMENSION** at least max (1, *n*). Contains the eigenvalues of the matrix H. If *eigsrc* = 'Q', the array must be exactly as returned by ?hseqr.

wr, wi	<b>REAL</b> for shsein <b>DOUBLE PRECISION</b> for dhsein Arrays, <b>DIMENSION</b> at least max $(1, n)$ each. Contain the real and imaginary parts, respectively, of the eigenvalues of the matrix <i>H</i> . Complex conjugate pairs of values must be stored in consecutive elements of the arrays. If <i>eigsrc</i> = 'Q', the arrays must be exactly as returned by ?hseqr.
ldvl	<b>INTEGER.</b> The first dimension of $vl$ . If $job = 'L'$ or $'B'$ , $ldvl \ge max(1,n)$ . If $job = 'R'$ , $ldvl \ge 1$ .
ldvr	<b>INTEGER.</b> The first dimension of <i>vr</i> . If $job =  \mathbf{R} $ or $ \mathbf{B} $ , $ldvr \ge max(1,n)$ . If $job =  \mathbf{L} $ , $ldvr \ge 1$ .
mm	<b>INTEGER.</b> The number of columns in <i>vl</i> and/or <i>vr</i> . Must be at least <i>m</i> , the actual number of columns required (see <i>Output Parameters</i> below). For real flavors, <i>m</i> is obtained by counting 1 for each selected real eigenvector and 2 for each selected complex eigenvector (see <i>select</i> ). For complex flavors, <i>m</i> is the number of selected eigenvectors (see <i>select</i> ). Constraint: $0 \le mm \le n$ .
rwork	REAL for chsein DOUBLE PRECISION for zhsein. Array, DIMENSION at least max $(1, n)$ .

select	Overwritten for real flavors only. If a complex eigenvector was selected as specified above, then $select(j)$ is set to .TRUE. and $select(j+1)$ to .FALSE.
W	The real parts of some elements of $w$ may be modified, as close eigenvalues are perturbed slightly in searching for independent eigenvectors.

WĽ	Some elements of <i>wr</i> may be modified, as close eigenvalues are perturbed slightly in searching for independent eigenvectors.
vl, vr	If <i>job</i> = 'L' or 'B', <i>vl</i> contains the computed left eigenvectors (as specified by <i>select</i> ). If <i>job</i> = 'R' or 'B', <i>vr</i> contains the computed right eigenvectors (as specified by <i>select</i> ).
	The eigenvectors are stored consecutively in the columns of the array, in the same order as their eigenvalues. For real flavors: a real eigenvector corresponding to a selected real eigenvalue occupies one column; a complex eigenvector corresponding to a selected complex eigenvalue occupies two columns: the first column holds the real part and the second column holds the imaginary part.
m	INTEGER. For real flavors: the number of columns of v1 and/or vr required to store the selected eigenvectors. For complex flavors: the number of selected eigenvectors.
ifaill,ifailr	<pre>INTEGER. Arrays, DIMENSION at least max(1, mm) each. ifaill(i) = 0 if the ith column of vl converged; ifaill(i) = j &gt; 0 if the eigenvector stored in the ith column of vl (corresponding to the jth eigenvalue) failed to converge. ifailr(i) = 0 if the ith column of vr converged; ifailr(i) = j &gt; 0 if the eigenvector stored in the ith column of vr (corresponding to the jth eigenvalue) failed to converge. For real flavors: if the ith and (i+1)th columns of vl contain a selected complex eigenvector, then ifaill(i) and ifaill(i+1) are set to the same value. A similar rule holds for vr and ifailr. The array ifaill is not referenced if job = 'R'.</pre>
	The array <i>ifailr</i> is not referenced if $job = 'L'$ .

info

INTEGER.

If *info* = 0, the execution is successful. If *info* = -*i*, the *i*th parameter had an illegal value. If *info* > 0, then *i* eigenvectors (as indicated by the parameters *ifaill* and/or *ifailr* above) failed to converge. The corresponding columns of *vl* and/or *vr* contain no useful information.

## **Application Notes**

Each computed right eigenvector  $x_i$  is the exact eigenvector of a nearby matrix  $A + E_i$ , such that  $||E_i|| < O(\varepsilon)||A||$ . Hence the residual is small:  $||Ax_i - \lambda_i x_i|| = O(\varepsilon)||A||$ .

However, eigenvectors corresponding to close or coincident eigenvalues may not accurately span the relevant subspaces.

Similar remarks apply to computed left eigenvectors.

# ?trevc

Computes selected eigenvectors of an upper (quasi-) triangular matrix computed by ?hseqr.

```
call strevc ( side, howmny, select, n, t, ldt, vl, ldvl, vr, ldvr,
    mm, m, work, info )
call dtrevc ( side, howmny, select, n, t, ldt, vl, ldvl, vr, ldvr,
    mm, m, work, info )
call ctrevc ( side, howmny, select, n, t, ldt, vl, ldvl, vr, ldvr,
    mm, m, work, rwork, info )
call ztrevc ( side, howmny, select, n, t, ldt, vl, ldvl, vr, ldvr,
    mm, m, work, rwork, info )
```

### **Discussion**

This routine computes some or all of the right and/or left eigenvectors of an upper triangular matrix *T* (or, for real flavors, an upper quasi-triangular matrix *T*). Matrices of this type are produced by the Schur factorization of a general matrix:  $A = QTQ^{H}$ , as computed by ?hseqr (see page 5-195).

The right eigenvector x and the left eigenvector y of T corresponding to an eigenvalue w, are defined by:

 $T x = w x , \qquad y^H T = w y^H$ 

where  $y^H$  denotes the conjugate transpose of y.

The eigenvalues are not input to this routine, but are read directly from the diagonal blocks of T.

This routine returns the matrices X and/or Y of right and left eigenvectors of T, or the products QX and/or QY, where Q is an input matrix.

If Q is the orthogonal/unitary factor that reduces a matrix A to Schur form T, then QX and QY are the matrices of right and left eigenvectors of A.

side	CHARACTER*1. Must be 'R' or 'L' or 'B'. If <i>side</i> = 'R', then only right eigenvectors are computed. If <i>side</i> = 'L', then only left eigenvectors are computed. If <i>side</i> = 'B', then all eigenvectors are computed.
howmny	CHARACTER*1. Must be 'A' or 'B' or 'S'. If howmny = 'A', then all eigenvectors (as specified by side) are computed. If howmny = 'B', then all eigenvectors (as specified by side) are computed and backtransformed by the matrices supplied in v1 and vr. If howmny = 'S', then selected eigenvectors (as specified by side and select) are computed.
select	LOGICAL. Array, DIMENSION at least max $(1, n)$ . If howmny='S', select specifies which eigenvectors are to be computed. If howmny= 'A' or 'B', select is not referenced. For real flavors: If $\varphi$ is a real eigenvalue, the corresponding real eigenvector is computed if select(j) is .TRUE If $\varphi$ and $\varphi_{+1}$ are the real and imaginary parts of a complex eigenvalue, the corresponding complex eigenvector is computed if either select(j) or select(j+1) is .TRUE., and on exit select(j) is set to .TRUE. and select(j+1) is set to .FALSE For complex flavors: The eigenvector corresponding to the j-th eigenvalue is computed if select(j) is .TRUE
n	<b>INTEGER</b> . The order of the matrix $T (n \ge 0)$ .
t,vl,vr,work	REAL for strevc DOUBLE PRECISION for dtrevc COMPLEX for ctrevc DOUBLE COMPLEX for ztrevc. Arrays:

	t(ldt, *) contains the <i>n</i> by <i>n</i> matrix <i>T</i> in Schur canonical form. The second dimension of <i>t</i> must be at least max(1, <i>n</i> ).
	<pre>vl(ldvl,*) If howmny ='B' and side ='L' or 'B', then vl must contain an n by n matrix Q (usually the matrix of Schur vectors returned by ?hseqr). If howmny ='A' or 'S', then vl need not be set. The second dimension of vl must be at least max(1, mm) if side ='L' or 'B' and at least 1 if side ='R'. The array vl is not referenced if side ='R'.</pre>
	<pre>vr (ldvr,*) If howmny = 'B' and side = 'R' or 'B', then vr must contain an n by n matrix Q (usually the matrix of Schur vectors returned by ?hseqr) If howmny = 'A' or 'S', then vr need not be set. The second dimension of vr must be at least max(1, mm) if side = 'R' or 'B' and at least 1 if side = 'L'. The array vr is not referenced if side = 'L'.</pre>
	work(*) is a workspace array. DIMENSION at least max $(1, 3*n)$ for real flavors and at least max $(1, 2*n)$ for complex flavors.
ldt	<b>INTEGER.</b> The first dimension of $t$ ; at least max $(1, n)$ .
ldvl	<b>INTEGER.</b> The first dimension of $vl$ . If $side = 'L'$ or $'B'$ , $ldvl \ge max(1,n)$ . If $side = 'R'$ , $ldvl \ge 1$ .
ldvr	<b>INTEGER.</b> The first dimension of <b>vr</b> . If $side = 'R'$ or $'B'$ , $ldvr \ge max(1,n)$ . If $side = 'L'$ , $ldvr \ge 1$ .
mm	INTEGER. The number of columns in the arrays $vl$ and/or $vr$ . Must be at least $m$ (the precise number of columns required). If howmny = 'A' or 'B', $m = n$ . If howmny = 'S': for real flavors, $m$ is obtained by counting 1 for each selected real eigenvector and 2 for each selected complex eigenvector;

rwork	for complex flavors, m is the number of selected eigenvectors (see select). Constraint: $0 \le m \le n$ . REAL for ctrevc DOUBLE PRECISION for ztrevc. Workspace array, DIMENSION at least max $(1, n)$ .
Output Parame	eters
select	If a complex eigenvector of a real matrix was selected as specified above, then $select(j)$ is set to .TRUE. and $select(j+1)$ to .FALSE.
vl,vr	If <i>side</i> = 'L' or 'B', <i>vl</i> contains the computed left eigenvectors (as specified by <i>howmny</i> and <i>select</i> ). If <i>side</i> = 'R' or 'B', <i>vr</i> contains the computed right eigenvectors (as specified by <i>howmny</i> and <i>select</i> ).
	The eigenvectors are stored consecutively in the columns of the array, in the same order as their eigenvalues. <i>For real flavors</i> : corresponding to each real eigenvalue is a real eigenvector, occupying one column; corresponding to each complex conjugate pair of eigenvalues is a complex eigenvector, occupying two columns; the first column holds the real part and the second column holds the imaginary part.
m	INTEGER. For complex flavors: the number of selected eigenvectors. If howmny = 'A' or 'B', m is set to n. For real flavors: the number of columns of vl and/or vr actually used to store the selected eigenvectors. If howmny = 'A' or 'B', m is set to n.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## **Application Notes**

If  $x_i$  is an exact right eigenvector and  $y_i$  is the corresponding computed eigenvector, then the angle  $\theta(y_i, x_i)$  between them is bounded as follows:  $\theta(y_i, x_i) \leq (c(n)\varepsilon ||T||_2)/\text{sep}_i$  where  $\text{sep}_i$  is the reciprocal condition number of  $x_i$ . The condition number  $\text{sep}_i$  may be computed by calling ?trsna.

## ?trsna

Estimates condition numbers for specified eigenvalues and right eigenvectors of an upper (quasi-) triangular matrix.

```
call strsna ( job, howmny, select, n, t, ldt, vl, ldvl, vr, ldvr,
    s, sep, mm, m, work, ldwork, iwork, info )
call dtrsna ( job, howmny, select, n, t, ldt, vl, ldvl, vr, ldvr,
    s, sep, mm, m, work, ldwork, iwork, info )
call ctrsna ( job, howmny, select, n, t, ldt, vl, ldvl, vr, ldvr,
    s, sep, mm, m, work, ldwork, rwork, info )
call ztrsna ( job, howmny, select, n, t, ldt, vl, ldvl, vr, ldvr,
    s, sep, mm, m, work, ldwork, rwork, info )
```

## Discussion

This routine estimates condition numbers for specified eigenvalues and/or right eigenvectors of an upper triangular matrix T (or, for real flavors, upper quasi-triangular matrix T in canonical Schur form). These are the same as the condition numbers of the eigenvalues and right eigenvectors of an original matrix  $A = ZTZ^H$  (with unitary or, for real flavors, orthogonal Z), from which T may have been derived.

The routine computes the reciprocal of the condition number of an eigenvalue  $\lambda_i$  as  $s_i = |v^H u| / (||u||_E ||v||_E)$ , where *u* and *v* are the right and left eigenvectors of *T*, respectively, corresponding to  $\lambda_i$ . This reciprocal condition number always lies between zero (ill-conditioned) and one (well-conditioned).

An approximate error estimate for a computed eigenvalue  $\lambda_i$  is then given by  $\varepsilon ||T||/s_i$ , where  $\varepsilon$  is the *machine precision*.

To estimate the reciprocal of the condition number of the right eigenvector corresponding to  $\lambda_i$ , the routine first calls ?trexc (see <u>page 5-215</u>) to reorder the eigenvalues so that  $\lambda_i$  is in the leading position:

$$T = Q \begin{bmatrix} \lambda_i & C^H \\ 0 & T_{22} \end{bmatrix} Q^H$$

The reciprocal condition number of the eigenvector is then estimated as  $sep_i$ , the smallest singular value of the matrix  $T_{22} - \lambda_i I$ . This number ranges from zero (ill-conditioned) to very large (well-conditioned).

An approximate error estimate for a computed right eigenvector u corresponding to  $\lambda_i$  is then given by  $\varepsilon \mid \mid T \mid |se_i$ .

job	CHARACTER*1. Must be 'E' or 'V' or 'B'. If job = 'E', then condition numbers for eigenvalues only are computed. If job = 'V', then condition numbers for eigenvectors only are computed. If job = 'B', then condition numbers for both eigenvalues and eigenvectors are computed.
howmny	CHARACTER*1. Must be 'A' or 'S'. If howmny = 'A', then the condition numbers for all eigenpairs are computed. If howmny = 'S', then condition numbers for selected eigenpairs (as specified by select) are computed.
select	LOGICAL. Array, DIMENSION at least max $(1, n)$ if howmny = 'S' and at least 1 otherwise. Specifies the eigenpairs for which condition numbers are to be computed if howmny= 'S'. For real flavors: To select condition numbers for the eigenpair corresponding to the real eigenvalue $\lambda_j$ , select(j) must be set .TRUE.; to select condition numbers for the

	eigenpair corresponding to a complex conjugate pair of eigenvalues $\lambda_j$ and $\lambda_{j+1}$ , $\texttt{select}(j)$ and/or $\texttt{select}(j+1)$ must be set .TRUE. For complex flavors: To select condition numbers for the eigenpair corresponding to the eigenvalue $\lambda_j$ , $\texttt{select}(j)$ must be set .TRUE. select is not referenced if $howmny = 'A'$ .
n	<b>INTEGER.</b> The order of the matrix $T (n \ge 0)$ .
t,vl,vr,work	<pre>REAL for strsna DOUBLE PRECISION for dtrsna COMPLEX for ctrsna DOUBLE COMPLEX for ztrsna. Arrays: t(ldt,*) contains the n by n matrix T. The second dimension of t must be at least max(1, n).</pre>
	<pre>vl(ldvl,*) If job = 'E' or 'B', then vl must contain the left eigenvectors of T (or of any matrix QTQ^H with Q unitary or orthogonal) corresponding to the eigenpairs specified by howmny and select. The eigenvectors must be stored in consecutive columns of vl, as returned by ?trevc or ?hsein. The second dimension of vl must be at least max(1, mm) if job = 'E' or 'B' and at least 1 if job = 'V'. The array vl is not referenced if job = 'V'.</pre>
	vr(ldvr, *) If $job = 'E'$ or 'B', then $vr$ must contain the right eigenvectors of $T$ (or of any matrix $QTQ^H$ with $Q$ unitary or orthogonal) corresponding to the eigenpairs specified by howmny and select. The eigenvectors must be stored in consecutive columns of $vr$ , as returned by ?trevc or ?hsein. The second dimension of $vr$ must be at least max(1, mm) if $job = 'E'$ or 'B' and at least 1 if $job = 'V'$ . The array $vr$ is not referenced if $job = 'V'$ .

	work(ldwork, *) is a workspace array. The second dimension of work must be at least max(1, $n+1$ ) for complex flavors and at least max(1, $n+6$ ) for real flavors if $job = 'V'$ or 'B'; at least 1 if $job = 'E'$ . The array work is not referenced if $job = 'E'$ .
ldt	<b>INTEGER.</b> The first dimension of $t$ ; at least max(1, $n$ ).
ldvl	<b>INTEGER.</b> The first dimension of $vl$ . If $job = 'E'$ or $'B'$ , $ldvl \ge max(1,n)$ . If $job = 'V'$ , $ldvl \ge 1$ .
ldvr	<pre>INTEGER. The first dimension of vr. If job = 'E' or 'B', ldvr≥max(1,n). If job = 'R', ldvr≥1.</pre>
mm	<b>INTEGER.</b> The number of elements in the arrays <i>s</i> and <i>sep</i> , and the number of columns in <i>vl</i> and <i>vr</i> (if used). Must be at least <i>m</i> (the precise number required). If <i>howmny</i> = 'A', <i>m</i> = <i>n</i> ; if <i>howmny</i> = 'S', <i>for real flavors m</i> is obtained by counting 1 for each selected real eigenvalue and 2 for each selected complex conjugate pair of eigenvalues. <i>for complex flavors m</i> is the number of selected eigenpairs (see <i>select</i> ). Constraint: $0 \le m \le n$ .
ldwork	<b>INTEGER.</b> The first dimension of work. If $job = 'V'$ or 'B', $ldwork \ge max(1,n)$ . If $job = 'E'$ , $ldwork \ge 1$ .
rwork	REAL for ctrsna, ztrsna. Array, DIMENSION at least max $(1, n)$ .
iwork	INTEGER for strsna, dtrsna. Array, DIMENSION at least max $(1, n)$ .

sREAL for single-precision flavorsDOUBLE PRECISION for double-precision flavors.Array, DIMENSION at least max(1, mm) if job = 'E' or'B' and at least 1 if job = 'V'.

sep

т

info

Contains the reciprocal condition numbers of the selected eigenvalues if $job = 'E'$ or $'B'$ , stored in consecutive elements of the array. Thus $s(j)$ , $sep(j)$ and the <i>j</i> th columns of $vl$ and $vr$ all correspond to the same eigenpair (but not in general the <i>j</i> th eigenpair unless all eigenpairs have been selected). For real flavors: For a complex conjugate pair of eigenvalues, two consecutive elements of S are set to the same value. The array <i>s</i> is not referenced if $job = 'V'$ .
<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. Array, <b>DIMENSION</b> at least $max(1, mm)$ if $job = 'V'$ or 'B' and at least 1 if $job = 'E'$ . Contains the estimated reciprocal condition numbers of the selected right eigenvectors if $job = 'V'$ or 'B', stored in consecutive elements of the array. <i>For real flavors</i> : for a complex eigenvector, two consecutive elements of <i>sep</i> are set to the same value; if the eigenvalues cannot be reordered to compute <i>sep(j)</i> , then <i>sep(j)</i> is set to zero; this can only occur when the true value would be very small anyway. The array <i>sep</i> is not referenced if $job = 'E'$ .
INTEGER. For complex flavors: the number of selected eigenpairs. If howmny = 'A', m is set to n. For real flavors: the number of elements of s and/or sep actually used to store the estimated condition numbers. If howmny = 'A', m is set to n. INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value.

## **Application Notes**

The computed values  $sep_i$  may overestimate the true value, but seldom by a factor of more than 3.

## ?trexc

*Reorders the Schur factorization of a general matrix.* 

call strexc ( compq, n, t, ldt, q, ldq, ifst, ilst, work, info )
call dtrexc ( compq, n, t, ldt, q, ldq, ifst, ilst, work, info )
call ctrexc ( compq, n, t, ldt, q, ldq, ifst, ilst, info )
call ztrexc ( compq, n, t, ldt, q, ldq, ifst, ilst, info )

### **Discussion**

This routine reorders the Schur factorization of a general matrix  $A = QTQ^H$ , so that the diagonal element or block of *T* with row index *ifst* is moved to row *ilst*.

The reordered Schur form *S* is computed by an unitary (or, for real flavors, orthogonal) similarity transformation:  $S = Z^H T Z$ . Optionally the updated matrix *P* of Schur vectors is computed as P = QZ, giving  $A = PSP^H$ .

COMPq	CHARACTER*1. Must be 'V' or 'N'. If $compq = 'V'$ , then the Schur vectors (Q) are updated. If $compq = 'N'$ , then no Schur vectors are updated.
п	<b>INTEGER.</b> The order of the matrix $T (n \ge 0)$ .
t, q	REAL for strexc DOUBLE PRECISION for dtrexc COMPLEX for ctrexc DOUBLE COMPLEX for ztrexc. Arrays: t(1dt,*) contains the <i>n</i> by <i>n</i> matrix <i>T</i> . The second dimension of <i>t</i> must be at least max(1, <i>n</i> ).
	q(ldq, *) If $compq = 'V'$ , then q must contain Q (Schur vectors). If $compq = 'N'$ , then q is not referenced.

	The second dimension of $q$ must be at least max $(1, n)$ if $compq = 'V'$ and at least 1 if $compq = 'N'$ .	
ldt	<b>INTEGER.</b> The first dimension of $t$ ; at least max $(1, n)$ .	
ldq	<b>INTEGER.</b> The first dimension of $q$ ; If $compq = 'N'$ , then $ldq \ge 1$ . If $compq = 'V'$ , then $ldq \ge max(1,n)$ .	
ifst, ilst	<ul> <li>INTEGER. 1 ≤<i>ifst</i> ≤<i>n</i>; 1 ≤<i>ilst</i> ≤<i>n</i>.</li> <li>Must specify the reordering of the diagonal elements (or blocks, which is possible for real flavors) of the matrix <i>T</i>. The element (or block) with row index <i>ifst</i> is moved to row <i>ilst</i> by a sequence of exchanges between adjacent elements (or blocks).</li> </ul>	
work	REAL for strexc DOUBLE PRECISION for dtrexc. Array, DIMENSION at least max (1, n).	
Output Parameters		
t	Overwritten by the updated matrix S.	
đ	If $compq = V'$ , q contains the updated matrix of Schur vectors.	
ifst, ilst	Overwritten for real flavors only. If <i>ifst</i> pointed to the second row of a 2 by 2 block on entry, it is changed to point to the first row; <i>ilst</i> always points to the first row of the block in its final position (which may differ from its input value by ±1).	

infoINTEGER.If info = 0, the execution is successful.If info = -i, the ith parameter had an illegal value.

#### **Application Notes**

The computed matrix *S* is exactly similar to a matrix T + E, where  $||E||_2 = O(\varepsilon) ||T||_2$ , and  $\varepsilon$  is the machine precision.

Note that if a 2 by 2 diagonal block is involved in the re-ordering, its off-diagonal elements are in general changed; the diagonal elements and the eigenvalues of the block are unchanged unless the block is sufficiently ill-conditioned, in which case they may be noticeably altered. It is possible for a 2 by 2 block to break into two 1 by 1 blocks, that is, for a pair of complex eigenvalues to become purely real.

The values of eigenvalues however are never changed by the re-ordering.

The approximate number of floating-point operations is

for real flavors:	6n(ifst-ilst) 12n(ifst-ilst)	/
for complex flavors:	20n(ifst-ilst) 40n(ifst-ilst)	/

### ?trsen

Reorders the Schur factorization of a matrix and (optionally) computes the reciprocal condition numbers and invariant subspace for the selected cluster of eigenvalues.

```
call strsen (job, compq, select, n, t, ldt, q, ldq, wr, wi, m, s,
    sep, work, lwork, iwork, liwork, info)
call dtrsen (job, compq, select, n, t, ldt, q, ldq, wr, wi, m, s,
    sep, work, lwork, iwork, liwork, info)
call ctrsen (job, compq, select, n, t, ldt, q, ldq, w, m, s,
    sep, work, lwork, info)
call ztrsen (job, compq, select, n, t, ldt, q, ldq, w, m, s,
    sep, work, lwork, info)
```

#### **Discussion**

This routine reorders the Schur factorization of a general matrix  $A = QTQ^H$  so that a selected cluster of eigenvalues appears in the leading diagonal elements (or, for real flavors, diagonal blocks) of the Schur form.

The reordered Schur form *R* is computed by an unitary(orthogonal) similarity transformation:  $R = Z^H T Z$ . Optionally the updated matrix *P* of Schur vectors is computed as P = Q Z, giving  $A = P R P^H$ .

Let

$$R = \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{13} \end{bmatrix}$$

where the selected eigenvalues are precisely the eigenvalues of the leading *m* by *m* submatrix  $T_{11}$ . Let *P* be correspondingly partitioned as  $(Q_1 Q_2)$  where  $Q_1$  consists of the first *m* columns of *Q*. Then  $AQ_1 = Q_1T_{11}$ , and so the *m* columns of  $Q_1$  form an orthonormal basis for the invariant subspace corresponding to the selected cluster of eigenvalues.

Optionally the routine also computes estimates of the reciprocal condition numbers of the average of the cluster of eigenvalues and of the invariant subspace.

job	CHARACTER*1. Must be 'N' or 'E' or 'V' or 'B'. If $job = 'N'$ , then no condition numbers are required. If $job = 'E'$ , then only the condition number for the cluster of eigenvalues is computed. If $job = 'V'$ , then only the condition number for the invariant subspace is computed. If $job = 'B'$ , then condition numbers for both the cluster
	and the invariant subspace are computed.
compq	CHARACTER*1. Must be 'V' or 'N'. If $compq = 'V'$ , then Q of the Schur vectors is updated. If $compq = 'N'$ , then no Schur vectors are updated.
select	LOGICAL. Array, DIMENSION at least max $(1, n)$ . Specifies the eigenvalues in the selected cluster. To select an eigenvalue $\lambda_j$ , <i>select</i> ( <i>j</i> ) must be .TRUE. For real flavors: to select a complex conjugate pair of eigenvalues $\lambda_j$ and $\lambda_{j+1}$ (corresponding 2 by 2 diagonal

	block), <i>select</i> ( <i>j</i> ) and/or <i>select</i> ( <i>j</i> +1) must be . TRUE.; the complex conjugate $\lambda_j$ and $\lambda_{j+1}$ must be either both included in the cluster or both excluded.
n	<b>INTEGER</b> . The order of the matrix $T (n \ge 0)$ .
t, q, work	REAL for strsen DOUBLE PRECISION for dtrsen COMPLEX for ctrsen DOUBLE COMPLEX for ztrsen. Arrays: t (ldt,*) The n by n T. The second dimension of t must be at least max(1, n).
	q(ldq, *) If $compq = 'V'$ , then $q$ must contain $Q$ of Schur vectors. If $compq = 'N'$ , then $q$ is not referenced. The second dimension of $q$ must be at least max $(1, n)$ if compq = 'V' and at least 1 if $compq = 'N'$ .
	work (lwork) is a workspace array. For complex flavors: the array work is not referenced if job = 'N'. The actual amount of workspace required cannot exceed $n^2/4$ if $job = 'E'$ or $n^2/2$ if $job = 'V'$ or 'B'.
ldt	<b>INTEGER</b> . The first dimension of $t$ ; at least max $(1, n)$ .
ldq	<b>INTEGER.</b> The first dimension of $q$ ; If $compq = 'N'$ , then $ldq \ge 1$ . If $compq = 'V'$ , then $ldq \ge max(1,n)$ .
lwork	<b>INTEGER.</b> The dimension of the array work. If $job = 'V'$ or 'B', $lwork \ge max(1,2m(n-m))$ . If $job = 'E'$ , then $lwork \ge max(1,m(n-m))$ If $job = 'N'$ , then $lwork \ge 1$ for complex flavors and $lwork \ge max(1,n)$ for real flavors.
iwork	INTEGER. <i>iwork</i> ( <i>liwork</i> ) is a workspace array. The array <i>iwork</i> is not referenced if $job = "N" or "E"$ . The actual amount of workspace required cannot exceed $n^2/2$ if $job = "V" or "B"$ .

liwork INTEGER. The dimension of the array *iwork*. If job = V' or B',  $liwork \ge max(1, 2m(n-m))$ . If job = 'E' or 'E',  $liwork \ge 1$ . **Output Parameters** Overwritten by the updated matrix *R*. t If compq = V', q contains the updated matrix of Schur q vectors; the first m columns of the Q form an orthogonal basis for the specified invariant subspace. COMPLEX for ctrsen W DOUBLE COMPLEX for ztrsen. Array, **DIMENSION** at least max(1,*n*). The recorded eigenvalues of R. The eigenvalues are stored in the same order as on the diagonal of *R*. wr, wi REAL for strsen DOUBLE PRECISION for dtrsen Arrays, DIMENSION at least max(1,n). Contain the real and imaginary parts, respectively, of the reordered eigenvalues of R. The eigenvalues are stored in the same order as on the diagonal of R. Note that if a complex eigenvalue is sufficiently ill-conditioned, then its value may differ significantly from its value before reordering. INTEGER. т For complex flavors: the number of the specified invariant subspaces, which is the same as the number of selected eigenvalues (see *select*). For real flavors: the dimension of the specified invariant subspace. The value of *m* is obtained by counting 1 for each selected real eigenvalue and 2 for each selected complex conjugate pair of eigenvalues (see *select*). Constraint:  $0 \leq m \leq n$ .

S	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. If $job = 'E'$ or 'B', <i>s</i> is a lower bound on the reciprocal condition number of the average of the selected cluster of eigenvalues. If $m = 0$ or <i>n</i> , then $s = 1$ . <i>For real flavors</i> : if <i>info</i> = 1, then <i>s</i> is set to zero. <i>s</i> is not referenced if <i>job</i> = 'N' or 'V'.
sep	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. If $job = 'V'$ or 'B', <i>sep</i> is the estimated reciprocal condition number of the specified invariant subspace. If $m = 0$ or $n$ , then $sep =   T  $ . For real flavors: if $info = 1$ , then $sep$ is set to zero. sep is not referenced if $job = 'N'$ or 'E'.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th parameter had an illegal value.

#### **Application Notes**

The computed matrix *R* is exactly similar to a matrix T + E, where  $||E||_2 = O(\varepsilon)||T||_2$ , and  $\varepsilon$  is the machine precision. The computed *s* cannot underestimate the true reciprocal condition number by more than a factor of  $(\min(m, n-m))^{1/2}$ ; *sep* may differ from the true value by  $(m^*n-m^2)^{1/2}$ . The angle between the computed invariant subspace and the true subspace is  $O(\varepsilon) ||A||_2/sep$ . Note that if a 2 by 2 diagonal block is involved in the re-ordering, its off-diagonal elements are in general changed; the diagonal elements and the eigenvalues of the block are unchanged unless the block is sufficiently ill-conditioned, in which case they may be noticeably altered. It is possible for a 2 by 2 block to break into two 1 by 1 blocks, that is, for a pair of complex eigenvalues to become purely real. The values of eigenvalues however are never changed by the re-ordering.

## ?trsyl

Solves Sylvester's equation for real quasi-triangular or complex triangular matrices.

```
call strsyl ( trana,tranb,isgn,m,n,a,lda,b,ldb,c,ldc,scale,info )
call dtrsyl ( trana,tranb,isgn,m,n,a,lda,b,ldb,c,ldc,scale,info )
call ctrsyl ( trana,tranb,isgn,m,n,a,lda,b,ldb,c,ldc,scale,info )
call ztrsyl ( trana,tranb,isgn,m,n,a,lda,b,ldb,c,ldc,scale,info )
```

#### **Discussion**

This routine solves the Sylvester matrix equation  $op(A)X \pm Xop(B) = \alpha C$ , where op(A) = A or  $A^H$ , and the matrices A and B are upper triangular (or, for real flavors, upper quasi-triangular in canonical Schur form);  $\alpha \le 1$  is a scale factor determined by the routine to avoid overflow in X; A is m by m, Bis n by n, and C and X are both m by n. The matrix X is obtained by a straightforward process of back substitution.

The equation has a unique solution if and only if  $\alpha_i \pm \beta_i \neq 0$ , where  $\{\alpha_i\}$  and  $\{\beta_i\}$  are the eigenvalues of *A* and *B*, respectively, and the sign (+ or  $\rightarrow$ ) is the same as that used in the equation to be solved.

trana	CHARACTER*1. Must be 'N' or 'T' or 'C'.
	If $trana = 'N'$ , then $op(A) = A$ . If $trana = 'T'$ , then $op(A) = A^T$ (real flavors only).
	If $trana = 'C'$ , then $op(A) = A$ (real navors only). If $trana = 'C'$ then $op(A) = A^H$ .
	• • •
tranb	CHARACTER*1. Must be 'N' or 'T' or 'C'.
	If $tranb = 'N'$ , then $op(B) = B$ .
	If $tranb = 'T'$ , then $op(B) = B^T$ (real flavors only).
	If $tranb = 'C'$ , then $op(B) = B^H$ .
isgn	<b>INTEGER.</b> Indicates the form of the Sylvester equation.
	If $isgn = +1$ , $op(A)X + Xop(B) = \alpha C$ .
	If $isgn = -1$ , $op(A)X - Xop(B) = \alpha C$ .

m	<b>INTEGER.</b> The order of <i>A</i> , and the number of rows in <i>X</i> and <i>C</i> ( $m \ge 0$ ).
n	<b>INTEGER.</b> The order of <i>B</i> , and the number of columns in <i>X</i> and <i>C</i> ( $n \ge 0$ ).
a, b, c	REAL for strsyl DOUBLE PRECISION for dtrsyl COMPLEX for ctrsyl DOUBLE COMPLEX for ztrsyl. Arrays: a(1da, *) contains the matrix A. The second dimension of a must be at least max(1, m). b(1db, *) contains the matrix B. The second dimension of b must be at least max(1, n). c(1dc, *) contains the matrix C. The second dimension of c must be at least max(1, n).
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ ; at least max $(1, n)$ .

С	Overwritten by the solution matrix <i>X</i> .
scale	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. The value of the scale factor $\alpha$ .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.
	If $info = 1$ , $A$ and $B$ have common or close eigenvalues perturbed values were used to solve the equation.

#### **Application Notes**

Let *X* be the exact, *Y* the corresponding computed solution, and *R* the residual matrix:  $R = C - (AY \pm YB)$ . Then the residual is always small:

 $||R||_{F} = O(\varepsilon) (||A||_{F} + ||B||_{F}) ||Y||_{F}.$ 

However, *Y* is not necessarily the exact solution of a slightly perturbed equation; in other words, the solution is not backwards stable.

For the forward error, the following bound holds:

 $||Y - X||_F \leq |R||_F \text{ sep}(A, B)$ 

but this may be a considerable overestimate. See [Golub96] for a definition of sep(A, B).

The approximate number of floating-point operations for real flavors is  $m^*n^*(m+n)$ . For complex flavors it is 4 times greater.

#### **Generalized Nonsymmetric Eigenvalue Problems**

This section describes LAPACK routines for solving generalized nonsymmetric eigenvalue problems, reordering the generalized Schur factorization of a pair of matrices, as well as performing a number of related computational tasks.

A generalized nonsymmetric eigenvalue problem is as follows: given a pair of nonsymmetric (or non-Hermitian) n-by-n matrices A and B, find the generalized eigenvalues  $\lambda$  and the corresponding generalized eigenvectors x and y that satisfy the equations

 $Ax = \lambda Bx$  (right generalized eigenvectors x)

and

 $y^{H}A = \lambda y^{H}B$  (left generalized eigenvectors y).

<u>Table 5-6</u> lists LAPACK routines used to solve the generalized nonsymmetric eigenvalue problems and the generalized Sylvester equation.

# Table 5-6Computational Routines for Solving Generalized Nonsymmetric<br/>Eigenvalue Problems

Routine name	Operation performed
?gghrd	Reduces a pair of matrices to generalized upper Hessenberg form using orthogonal/unitary transformations.
?ggbal	Balances a pair of general real or complex matrices.
?ggbak	Forms the right or left eigenvectors of a generalized eigenvalue problem.
?hgeqz	Implements the QZ method for finding the generalized eigenvalues of the matrix pair (H,T).
?tgevc	Computes some or all of the right and/or left generalized eigenvectors of a pair of upper triangular matrices
?tgexc	Reorders the generalized Schur decomposition of a pair of matrices (A,B) so that one diagonal block of (A,B) moves to another row index.
?tgsen	Reorders the generalized Schur decomposition of a pair of matrices (A,B) so that a selected cluster of eigenvalues appears in the leading diagonal blocks of (A,B).
?tgsyl	Solves the generalized Sylvester equation.
?tgsna	Estimates reciprocal condition numbers for specified eigenvalues and/or eigenvectors of a pair of matrices in generalized real Schur canonical form.

# ?gghrd

Reduces a pair of matrices to generalized upper Hessenberg form using orthogonal/unitary transformations.

#### Discussion

This routine reduces a pair of real/complex matrices (A,B) to generalized upper Hessenberg form using orthogonal/unitary transformations, where A is a general matrix and B is upper triangular. The form of the generalized eigenvalue problem is  $Ax = \lambda Bx$ , and B is typically made upper triangular by computing its *QR* factorization and moving the orthogonal matrix *Q* to the left side of the equation.

This routine simultaneously reduces A to a Hessenberg matrix H:

 $Q^H A \ Z = H$ 

and transforms B to another upper triangular matrix T:

$$Q^H B \ Z = T$$

in order to reduce the problem to its standard form  $Hy = \lambda Ty$  where  $y = Z^H x$ .

The orthogonal/unitary matrices Q and Z are determined as products of Givens rotations. They may either be formed explicitly, or they may be postmultiplied into input matrices  $Q_I$  and  $Z_I$ , so that

$$Q_I A Z_I^H = (Q_I Q) H (Z_I Z)^H$$
$$Q_I B Z_I^H = (Q_I Q) T (Z_I Z)^H$$

If  $Q_I$  is the orthogonal matrix from the *QR* factorization of *B* in the original equation  $Ax = \lambda Bx$ , then **?gghrd** reduces the original problem to generalized Hessenberg form.

compq	CHARACTER*1. Must be 'N', 'I', or 'V'.
	If $compq = 'N'$ , matrix Q is not computed.
	If $compq = 'I'$ , Q is initialized to the unit matrix, and
	the orthogonal/unitary matrix $Q$ is returned;
	If $compq = V'$ , Q must contain an orthogonal/unitary
	matrix $Q_1$ on entry, and the product $Q_1Q$ is returned.
compz	CHARACTER*1. Must be 'N', 'I', or 'V'.
	If $compz = 'N'$ , matrix Z is not computed.
	If $compz = 'I'$ , Z is initialized to the unit matrix, and
	the orthogonal/unitary matrix $Z$ is returned;
	If $compz = V'$ , Z must contain an orthogonal/unitary matrix $Z_1$ on entry, and the product $Z_1Z$ is returned.
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
ilo, ihi	INTEGER. <i>ilo</i> and <i>ihi</i> mark the rows and columns of
	A which are to be reduced. It is assumed that A is already
	upper triangular in rows and columns 1: <u>i10</u> -1 and
	<i>ihi</i> +1: <i>n</i> . Values of <i>ilo</i> and <i>ihi</i> are normally set by a
	previous call to ?ggbal; otherwise they should be set to
	1 and <i>n</i> respectively. Constraint:
	If $n > 0$ , then $1 \le i lo \le i h i \le n$ ;
	if $n = 0$ , then $ilo = 1$ and $ihi = 0$ .
a, b, q, z	REAL for sgghrd
	DOUBLE PRECISION for dgghrd
	COMPLEX for cgghrd
	DOUBLE COMPLEX for zgghrd.
	Arrays:
	a(lda,*) contains the <i>n</i> -by- <i>n</i> general matrix A.
	The second dimension of $a$ must be at least max $(1, n)$ .
	b(ldb, *) contains the <i>n</i> -by- <i>n</i> upper triangular matrix <i>B</i> .
	The second dimension of $b$ must be at least max $(1, n)$ .

	q(ldq, *) If $compq = 'N'$ , then $q$ is not referenced. If $compq = 'I'$ , then, on entry, $q$ need not be set. If $compq = 'V'$ , then $q$ must contain the orthogonal/unitary matrix $Q_1$ , typically from the $QR$ factorization of $B$ . The second dimension of $q$ must be at least max $(1, n)$ .
	z (ldz, *) If $compq = 'N'$ , then z is not referenced. If $compq = 'I'$ , then, on entry, z need not be set. If $compq = 'V'$ , then z must contain the orthogonal/unitary matrix $Z_1$ . The second dimension of z must be at least max $(1, n)$ .
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .
ldq	<b>INTEGER.</b> The first dimension of $q$ ; If $compq = 'N'$ , then $ldq \ge 1$ . If $compq = 'I'$ or 'V', then $ldq \ge max(1,n)$ .
ldz	<b>INTEGER.</b> The first dimension of $z$ ; If $compq = 'N'$ , then $ldz \ge 1$ . If $compq = 'I'$ or 'V', then $ldz \ge max(1,n)$ .

a	On exit, the upper triangle and the first subdiagonal of $A$ are overwritten with the upper Hessenberg matrix $H$ , and the rest is set to zero.
b	On exit, overwritten by the upper triangular matrix $T = Q^H B Z$ . The elements below the diagonal are set to zero.
q	If $compq = 'I'$ , then $q$ contains the orthogonal/unitary matrix $Q$ , where $Q^{H}$ is the product of the Givens transformations which are applied to $A$ and $B$ on the left; If $compq = 'V'$ , then $q$ is overwritten by the product $Q_{1}Q$ .

Ζ	If $compq = 'I'$ , then z contains the orthogonal/unitary matrix Z, which is the product of the Givens transformations which are applied to A and B on the right; If $compq = 'V'$ , then z is overwritten by the product $Z_1Z$ .
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

# ?ggbal

Balances a pair of general real or complex matrices.

#### **Discussion**

This routine balances a pair of general real/complex matrices (A,B). This involves, first, permuting A and B by similarity transformations to isolate eigenvalues in the first 1 to *ilo*-1 and last *ihi*+1 to *n* elements on the diagonal; and second, applying a diagonal similarity transformation to rows and columns *ilo* to *ihi* to make the rows and columns as close in norm as possible. Both steps are optional.

Balancing may reduce the 1-norm of the matrices, and improve the accuracy of the computed eigenvalues and/or eigenvectors in the generalized eigenvalue problem  $Ax = \lambda Bx$ .

job	CHARACTER*1. Specifies the operations to be performed
	on A and B. Must be 'N' or 'P' or 'S' or 'B'.
	If $job = 'N'$ , then no operations are done; simply set
	<i>ilo</i> =1, <i>ihi</i> = <i>n</i> , <i>lscale</i> ( <i>i</i> ) =1.0 and <i>rscale</i> ( <i>i</i> )=1.0 for
	i = 1,, <i>n</i> .
	If $job = 'P'$ , then permute only.
	If $job = 'S'$ , then scale only.
	If $job = 'B'$ , then both permute and scale.
n	<b>INTEGER</b> . The order of the matrices A and $B (n \ge 0)$ .

a, b	REAL for sggbal
	DOUBLE PRECISION for dggbal
	COMPLEX for cggbal
	DOUBLE COMPLEX for zggbal.
	Arrays:
	a(lda, *) contains the matrix A.
	The second dimension of a must be at least $max(1, n)$ .
	b(ldb, *) contains the matrix B.
	The second dimension of $b$ must be at least max $(1, n)$ .
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .
work	<b>REAL</b> for single precision flavors
	DOUBLE PRECISION for double precision flavors.
	Workspace array, DIMENSION at least max(1, 6n).

a, b	Overwritten by the balanced matrices A and B, respectively. If $job = 'N'$ , a and b are not referenced.
ilo, ihi	<b>INTEGER.</b> <i>ilo</i> and <i>ihi</i> are set to integers such that on exit $a(i, j)=0$ and $b(i, j)=0$ if $i>j$ and $j=1,,ilo-1$ or $i=ihi+1,,n$ .
	If $job = 'N'or 'S'$ , then $ilo = 1$ and $ihi = n$ .
lscale,rscale	REAL for single precision flavors DOUBLE PRECISION for double precision flavors. Arrays, DIMENSION at least max(1, n).
	<b>Iscale</b> contains details of the permutations and scaling factors applied to the left side of $A$ and $B$ . If $P_j$ is the index of the row interchanged with row $j$ , and $D_j$ is the scaling factor applied to row $j$ , then
	$lscale(j) = P_j, \text{ for } j = 1,, ilo-1$ = $D_j, \text{ for } j = ilo,, ihi$ = $P_j, \text{ for } j = ihi+1,, n.$ rscale contains details of the permutations and scaling factors applied to the right side of A and B.

If  $P_j$  is the index of the column interchanged with column j, and  $D_j$  is the scaling factor applied to column j, then

$$\begin{aligned} \textbf{rscale}(j) &= P_j \text{, for } j = 1, ..., ilo-1 \\ &= D_j \text{, for } j = ilo, ..., ihi \\ &= P_j \text{, for } j = ihi+1, ..., n \end{aligned}$$

The order in which the interchanges are made is n to ihi+1, then 1 to ilo-1.

info

INTEGER.

If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value.

# ?ggbak

Forms the right or left eigenvectors of a generalized eigenvalue problem.

```
call sggbak(job, side, n, ilo, ihi, lscale, rscale, m, v, ldv, info)
call dggbak(job, side, n, ilo, ihi, lscale, rscale, m, v, ldv, info)
call cggbak(job, side, n, ilo, ihi, lscale, rscale, m, v, ldv, info)
call zggbak(job, side, n, ilo, ihi, lscale, rscale, m, v, ldv, info)
```

#### **Discussion**

This routine forms the right or left eigenvectors of a real/complex generalized eigenvalue problem

 $Ax = \lambda Bx$ 

by backward transformation on the computed eigenvectors of the balanced pair of matrices output by <u>?ggbal</u>.

job	CHARACTER*1. Specifies the type of backward transformation required. Must be 'N', 'P', 'S', or 'B'.
	If $job = 'N'$ , then no operations are done; return.
	If $job = 'P'$ , then do backward transformation for permutation only.
	If $job = S'$ , then do backward transformation for scaling only.
	If $job = 'B'$ , then do backward transformation for both permutation and scaling.
	This argument must be the same as the argument <i>job</i> supplied to ?ggbal.
side	CHARACTER*1. Must be 'L' or 'R'.
	If $side = 'L'$ , then v contains left eigenvectors. If $side = 'R'$ , then v contains right eigenvectors.
n	<b>INTEGER</b> . The number of rows of the matrix $V (n \ge 0)$ .

ilo, ihi	<b>INTEGER.</b> The integers <i>ilo</i> and <i>ihi</i> determined by <b>?gebal.</b> Constraint: If $n > 0$ , then $1 \le ilo \le ihi \le n$ ; if $n = 0$ , then <i>ilo</i> = 1 and <i>ihi</i> = 0.
lscale,rscale	<b>REAL</b> for single precision flavors <b>DOUBLE PRECISION</b> for double precision flavors. Arrays, <b>DIMENSION</b> at least $max(1, n)$ .
	The array <i>lscale</i> contains details of the permutations and/or scaling factors applied to the left side of $A$ and $B$ , as returned by ?ggbal.
	The array <i>rscale</i> contains details of the permutations and/or scaling factors applied to the right side of <i>A</i> and <i>B</i> , as returned by ?ggbal.
m	<b>INTEGER.</b> The number of columns of the matrix $V$ ( $m \ge 0$ ).
V	REAL for sggbak DOUBLE PRECISION for dggbak COMPLEX for cggbak DOUBLE COMPLEX for zggbak. Array $v(ldv, *)$ . Contains the matrix of right or left eigenvectors to be transformed, as returned by ?tgevc. The second dimension of $v$ must be at least max $(1, m)$ .
ldv	<b>INTEGER</b> . The first dimension of $v$ ; at least max $(1, n)$ .
Output Parame	ters
17	Overwritten by the transformed eigenvectors

v	Overwritten by the transformed eigenvectors
info	INTEGER.
	If $info = 0$ , the execution is successful.
	If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## ?hgeqz

Implements the QZ method for finding the generalized eigenvalues of the matrix pair (H,T).

#### **Discussion**

This routine computes the eigenvalues of a real/complex matrix pair (H,T), where *H* is an upper Hessenberg matrix and *T* is upper triangular, using the double-shift version (for real flavors) or single-shift version (for complex flavors) of the *QZ* method.

Matrix pairs of this type are produced by the reduction to generalized upper Hessenberg form of a real/complex matrix pair (A,B):

 $A = Q_I H Z_I^H, \qquad B = Q_I T Z_I^H,$ 

as computed by ?gghrd.

#### For real flavors:

If job = 'S', then the Hessenberg-triangular pair (*H*,*T*) is also reduced to generalized Schur form,

 $H = Q \ S \ Z^T, \qquad T = Q \ P \ Z^T,$ 

where Q and Z are orthogonal matrices, P is an upper triangular matrix, and S is a quasi-triangular matrix with 1-by-1 and 2-by-2 diagonal blocks. The 1-by-1 blocks correspond to real eigenvalues of the matrix pair (H,T) and the 2-by-2 blocks correspond to complex conjugate pairs of eigenvalues.

Additionally, the 2-by-2 upper triangular diagonal blocks of P

corresponding to 2-by-2 blocks of *S* are reduced to positive diagonal form, that is, if S(j+1,j) is non-zero, then P(j+1,j) = P(j,j+1) = 0, P(j,j) > 0, and P(j+1,j+1) > 0.

#### For complex flavors:

If job = 'S', then the Hessenberg-triangular pair (*H*,*T*) is also reduced to generalized Schur form,

 $H = Q \ S \ Z^H, \qquad T = Q \ P \ Z^H,$ 

where Q and Z are unitary matrices, and S and P are upper triangular.

#### For all function flavors:

Optionally, the orthogonal/unitary matrix Q from the generalized Schur factorization may be postmultiplied into an input matrix  $Q_I$ , and the orthogonal/unitary matrix Z may be postmultiplied into an input matrix  $Z_I$ . If  $Q_I$  and  $Z_I$  are the orthogonal/unitary matrices from **?gghrd** that reduced the matrix pair (A,B) to generalized upper Hessenberg form, then the output matrices  $Q_I Q$  and  $Z_I Z$  are the orthogonal/unitary factors from the generalized Schur factorization of (A,B):

 $A = (Q_l Q) S (Z_l Z)^H, \quad B = (Q_l Q) P (Z_l Z)^H.$ 

To avoid overflow, eigenvalues of the matrix pair (H,T) (equivalently, of (A,B)) are computed as a pair of values (*alpha,beta*). For chgeqz/zhgeqz, *alpha* and *beta* are complex, and for shgeqz/dhgeqz, *alpha* is complex and *beta* real. If *beta* is nonzero,  $\lambda = alpha / beta$  is an eigenvalue of the generalized nonsymmetric eigenvalue problem (GNEP)

 $Ax = \lambda Bx$ 

and if *alpha* is nonzero,  $\mu = beta / alpha$  is an eigenvalue of the alternate form of the GNEP

 $\mu A y = B y \, .$ 

Real eigenvalues (for real flavors) or the values of *alpha* and *beta* for the i-th eigenvalue (for complex flavors) can be read directly from the generalized Schur form:

alpha = S(i,i), beta = P(i,i).

job	CHARACTER*1. Specifies the operations to be
	performed. Must be 'E' or 'S'.
	If $job = 'E'$ , then compute eigenvalues only;
	If $job = 'S'$ , then compute eigenvalues and the Schur
	form.
compq	CHARACTER*1. Must be 'N', 'I', or 'V'.
	If $compq = 'N'$ , left Schur vectors (q) are not
	computed;
	If $compq = 'I'$ , q is initialized to the unit matrix and
	the matrix of left Schur vectors of $(H,T)$ is returned;
	If $compq = V'$ , q must contain an orthogonal/unitary
	matrix $Q_1$ on entry and the product $Q_1Q$ is returned.
compz	CHARACTER*1. Must be 'N', 'I', or 'V'.
-	If $compz = 'N'$ , left Schur vectors (q) are not
	computed;
	If $compz = 'I'$ , z is initialized to the unit matrix and
	the matrix of right Schur vectors of $(H,T)$ is returned;
	If $compz = V'$ , z must contain an orthogonal/unitary
	matrix $Z_I$ on entry and the product $Z_I Z$ is returned.
n	<b>INTEGER</b> . The order of the matrices <i>H</i> , <i>T</i> , <i>Q</i> , and <i>Z</i>
11	$(n \ge 0)$ .
ilo, ihi	INTEGER. <i>ilo</i> and <i>ihi</i> mark the rows and columns of
	<i>H</i> which are in Hessenberg form. It is assumed that <i>H</i> is
	already upper triangular in rows and columns 1: <i>i1o</i> -1
	and $ihi+1:n$ . Constraint:
	If $n > 0$ , then $1 \le i lo \le i hi \le n$ ;
	if $n = 0$ , then $ilo = 1$ and $ihi = 0$ .
h,t,q,z,work	REAL for shgeqz
	DOUBLE PRECISION for dhgeqz
	COMPLEX for chgeqz
	DOUBLE COMPLEX for zhgeqz.
	Arrays:
	On entry, $h(ldh, *)$ contains the <i>n</i> -by- <i>n</i> upper
	Hessenberg matrix <i>H</i> .
	The second dimension of $h$ must be at least max $(1, n)$ .

	On entry, $t(ldt, *)$ contains the <i>n</i> -by- <i>n</i> upper triangular matrix <i>T</i> . The second dimension of <i>t</i> must be at least max $(1, n)$ .
	q ( $ldq$ , *): On entry, if $compq = 'V'$ , this array contains the orthogonal/unitary matrix $Q_I$ used in the reduction of ( $A,B$ ) to generalized Hessenberg form. If $compq = 'N'$ , then $q$ is not referenced. The second dimension of $q$ must be at least max(1, $n$ ).
	z (ldz, *): On entry, if $compz = 'V'$ , this array contains the orthogonal/unitary matrix $Z_I$ used in the reduction of (A,B) to generalized Hessenberg form. If $compz = 'N'$ , then z is not referenced. The second dimension of z must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
ldh	<b>INTEGER.</b> The first dimension of $h$ ; at least max $(1, n)$ .
ldt	<b>INTEGER</b> . The first dimension of $t$ ; at least max $(1, n)$ .
ldq	<b>INTEGER.</b> The first dimension of $q$ ; If $compq = 'N'$ , then $ldq \ge 1$ . If $compq = 'I'$ or 'V', then $ldq \ge max(1,n)$ .
ldz	<b>INTEGER.</b> The first dimension of $z$ ; If $compq = 'N'$ , then $ldz \ge 1$ . If $compq = 'I'$ or 'V', then $ldz \ge max(1,n)$ .
lwork	<b>INTEGER.</b> The dimension of the array work. <i>lwork</i> $\geq \max(1,n)$ .
rwork	REAL for chgeqz DOUBLE PRECISION for zhgeqz. Workspace array, DIMENSION at least max(1, <i>n</i> ). Used in complex flavors only.

h	For real flavors: If $job = 'S'$ , then, on exit, <i>h</i> contains the upper quasi-triangular matrix <i>S</i> from the generalized Schur factorization; 2-by-2 diagonal blocks (corresponding to complex conjugate pairs of eigenvalues) are returned in standard form, with $h(i,i) = h(i+1, i+1)$ and h(i+1, i) * h(i, i+1) < 0. If $job = 'E'$ , then on exit the diagonal blocks of <i>h</i> match those of <i>S</i> , but the rest of <i>h</i> is unspecified.
	For complex flavors: If $job = 'S'$ , then, on exit, <i>h</i> contains the upper triangular matrix <i>S</i> from the generalized Schur factorization. If $job = 'E'$ , then on exit the diagonal of <i>h</i> matches that of <i>S</i> , but the rest of <i>h</i> is unspecified.
t	If $job = "S"$ , then, on exit, $t$ contains the upper triangular matrix $P$ from the generalized Schur factorization. <i>For real flavors</i> : 2-by-2 diagonal blocks of $P$ corresponding to 2-by-2 blocks of $S$ are reduced to positive diagonal form, that is, if $h(j+1,j)$ is non-zero, then $t(j+1,j)=t(j,j+1)=0$ and t(j,j) and $t(j+1,j+1)$ will be positive.
	If $job = 'E'$ , then on exit the diagonal blocks of $t$ match those of $P$ , but the rest of $t$ is unspecified.
	For complex flavors: If $job = 'E'$ , then on exit the diagonal of $t$ matches that of $P$ , but the rest of $t$ is unspecified.
alphar,alphai	REAL for shgeqz; DOUBLE PRECISION for dhgeqz. Arrays, DIMENSION at least max(1,n). The real and imaginary parts, respectively, of each scalar <i>alpha</i> defining an eigenvalue of GNEP.

	If <i>alphai</i> (j) is zero, then the j-th eigenvalue is real; if positive, then the j-th and (j+1)-th eigenvalues are a complex conjugate pair, with <i>alphai</i> (j+1) = $-alphai$ (j).
alpha	COMPLEX for chgeqz; DOUBLE COMPLEX for zhgeqz. Array, DIMENSION at least max $(1,n)$ . The complex scalars <i>alpha</i> that define the eigenvalues of GNEP. <i>alphai</i> (i) = $S(i,i)$ in the generalized Schur factorization.
beta	REAL for shgeqz DOUBLE PRECISION for dhgeqz COMPLEX for chgeqz DOUBLE COMPLEX for zhgeqz. Array, DIMENSION at least max(1,n). For real flavors: The scalars beta that define the eigenvalues of GNEP. Together, the quantities $alpha = (alphar(j), alphai(j))$ and $beta = beta(j)$ represent the j-th eigenvalue of the matrix pair (A,B), in one of the forms $\lambda = alpha/beta$ or $\mu = beta/alpha$ . Since either $\lambda$ or $\mu$ may overflow, they should not, in general, be computed.
	For complex flavors: The real non-negative scalars <i>beta</i> that define the eigenvalues of GNEP. <i>beta</i> (i) = $P(i,i)$ in the generalized Schur factorization. Together, the quantities <i>alpha</i> = <i>alpha</i> (j) and <i>beta</i> = <i>beta</i> (j) represent the j-th eigenvalue of the matrix pair ( <i>A</i> , <i>B</i> ), in one of the forms $\lambda = alpha/beta$ or $\mu = beta/alpha$ . Since either $\lambda$ or $\mu$ may overflow, they should not, in general, be computed.
q	On exit, if $compq = 'I', q$ is overwritten by the orthogonal/unitary matrix of left Schur vectors of the pair ( <i>H</i> , <i>T</i> ), and if $compq = 'V', q$ is overwritten by the orthogonal/unitary matrix of left Schur vectors of ( <i>A</i> , <i>B</i> ).

Ζ	On exit, if $compz = 'I'$ , z is overwritten by the orthogonal/unitary matrix of right Schur vectors of the pair ( <i>H</i> , <i>T</i> ), and if $compz = 'V'$ , z is overwritten by the orthogonal/unitary matrix of right Schur vectors of ( <i>A</i> , <i>B</i> ).
work(1)	If $info \ge 0$ , on exit, $work(1)$ contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = 1,,n$ , the QZ iteration did not converge. (H,T) is not in Schur form, but $alphar(i)$ , $alphai(i)$ (for real flavors), $alpha(i)$ (for complex flavors), and beta(i), $i=info+1,,n$ should be correct.
	If $info = n+1,,2n$ , the shift calculation failed. ( <i>H</i> , <i>T</i> ) is not in Schur form, but $alphar(i)$ , $alphai(i)$ (for real flavors), $alpha(i)$ (for complex flavors), and beta(i), $i = info - n+1,,n$ should be correct.

### ?tgevc

Computes some or all of the right and/or left generalized eigenvectors of a pair of upper triangular matrices.

#### Discussion

This routine computes some or all of the right and/or left eigenvectors of a pair of real/complex matrices (S, P), where S is quasi-triangular (for real flavors) or upper triangular (for complex flavors) and P is upper triangular.

Matrix pairs of this type are produced by the generalized Schur factorization of a real/complex matrix pair (A, B):

 $A = Q S Z^H , \qquad B = Q P Z^H$ 

as computed by ?gghrd plus ?hgeqz.

The right eigenvector x and the left eigenvector y of (S, P) corresponding to an eigenvalue w are defined by:

Sx = wPx,  $y^H S = wy^H P$ 

The eigenvalues are not input to this routine, but are computed directly from the diagonal blocks or diagonal elements of *S* and *P*.

This routine returns the matrices *X* and/or *Y* of right and left eigenvectors of (S,P), or the products *ZX* and/or *QY*, where *Z* and *Q* are input matrices. If *Q* and *Z* are the orthogonal/unitary factors from the generalized Schur factorization of a matrix pair (A,B), then *ZX* and *QY* are the matrices of right and left eigenvectors of (A,B).

input Paramete	515
side	CHARACTER*1. Must be 'R', 'L', or 'B'. If <i>side</i> = 'R', compute right eigenvectors only. If <i>side</i> = 'L', compute left eigenvectors only. If <i>side</i> = 'B', compute both right and left eigenvectors.
howmny	CHARACTER*1. Must be 'A', 'B', or 'S'. If howmny = 'A', compute all right and/or left eigenvectors. If howmny = 'B', compute all right and/or left eigenvectors, backtransformed by the matrices in vr and/or v1. If howmny = 'S', compute selected right and/or left eigenvectors, specified by the logical array select.
select	LOGICAL. Array, DIMENSION at least max $(1, n)$ . If howmny ='S', select specifies the eigenvectors to be computed. If howmny= 'A'Or 'B', select is not referenced. For real flavors: If $\omega$ is a real eigenvalue, the corresponding real eigenvector is computed if select(j) is .TRUE If $\omega$ and $\omega_{+1}$ are the real and imaginary parts of a complex eigenvalue, the corresponding complex eigenvector is computed if either select(j) or select(j+1) is .TRUE., and on exit select(j) is set to .TRUE. and select(j+1) is set to .FALSE For complex flavors: The eigenvector corresponding to the j-th eigenvalue is computed if select(j) is .TRUE
п	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
s,p,vl,vr,wor.	k REAL for stgevc DOUBLE PRECISION for dtgevc COMPLEX for ctgevc DOUBLE COMPLEX for ztgevc. Arrays:

s(lds, *) contains the matrix *S* from a generalized Schur factorization as computed by ?hgeqz. This matrix is upper quasi-triangular for real flavors, and upper triangular for complex flavors. The second dimension of *s* must be at least max(1, *n*).

p(ldp, *) contains the upper triangular matrix P from a generalized Schur factorization as computed by ?hgeqz.

For real flavors, 2-by-2 diagonal blocks of *P* corresponding to 2-by-2 blocks of *S* must be in positive diagonal form.

For complex flavors, *P* must have real diagonal elements.

The second dimension of p must be at least max(1, n).

If side = 'L' or 'B' and howmny = 'B',

vl(ldvl,*) must contain an *n*-by-*n* matrix *Q* (usually the orthogonal/unitary matrix *Q* of left Schur vectors returned by ?hgeqz). The second dimension of vl must be at least max(1, *mm*). If *side* = 'R', *vl* is not referenced.

If *side* = 'R' or 'B' and *howmny* = 'B',

vr(ldvr,*) must contain an n-by-n matrix Z (usually the orthogonal/unitary matrix Z of right Schur vectors returned by ?hgeqz). The second dimension of vr must be at least max(1, mm). If side = 'L', vr is not referenced.

work(*) is a workspace array.

**DIMENSION** at least max (1, 6*n) for real flavors and at least max (1, 2*n) for complex flavors.

lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max(1, $n$ ).
ldb	<b>INTEGER</b> . The first dimension of $b$ ; at least max $(1, n)$ .
ldvl	<b>INTEGER</b> . The first dimension of $v1$ ;
	If $side = 'L' or 'B'$ , then $ldvl \ge max(1,n)$ .
	If $side =  \mathbf{R} $ , then $ dv  \ge 1$ .

ldvr	<b>INTEGER.</b> The first dimension of $vr$ ; If $side = 'R' or 'B'$ , then $ldvr \ge max(1,n)$ . If $side = 'L'$ , then $ldvr \ge 1$ .
mm	<b>INTEGER.</b> The number of columns in the arrays $vl$ and/or $vr$ ( $mm \ge m$ ).
rwork	REAL for ctgevc DOUBLE PRECISION for ztgevc. Workspace array, DIMENSION at least max (1, 2*n). Used in complex flavors only.

v1	On exit, if <i>side</i> = 'L'or 'B', <i>vl</i> contains: if <i>howmny</i> = 'A', the matrix <i>Y</i> of left eigenvectors of ( <i>S</i> , <i>P</i> ); if <i>howmny</i> = 'B', the matrix <i>QY</i> ; if <i>howmny</i> = 'S', the left eigenvectors of ( <i>S</i> , <i>P</i> ) specified by <i>select</i> , stored consecutively in the columns of <i>vl</i> , in the same order as their eigenvalues. <i>For real flavors</i> : A complex eigenvector corresponding to a complex eigenvalue is stored in two consecutive columns, the first holding the real part, and the second the imaginary part.
vr	On exit, if <i>side</i> = 'R'or 'B', <i>vr</i> contains: if <i>howmny</i> = 'A', the matrix <i>X</i> of right eigenvectors of ( <i>S</i> , <i>P</i> ); if <i>howmny</i> = 'B', the matrix <i>ZX</i> ; if <i>howmny</i> = 'S', the right eigenvectors of ( <i>S</i> , <i>P</i> ) specified by <i>select</i> , stored consecutively in the columns of <i>vr</i> , in the same order as their eigenvalues. <i>For real flavors</i> : A complex eigenvector corresponding to a complex eigenvalue is stored in two consecutive columns, the first holding the real part, and the second the imaginary part.

m	INTEGER. The number of columns in the arrays $vl$
	and/or vr actually used to store the eigenvectors.
	If howmny = 'A' or 'B', m is set to n.
	For real flavors:
	Each selected real eigenvector occupies one column and
	each selected complex eigenvector occupies two
	columns.
	For complex flavors:
	Each selected eigenvector occupies one column.
info	INTEGER.
	If $info = 0$ , the execution is successful.
	If $info = -i$ , the <i>i</i> th parameter had an illegal value.
	For real flavors:
	If $info = i > 0$ , the 2-by-2 block $(i:i+1)$ does not have a
	complex eigenvalue.

т

## ?tgexc

Reorders the generalized Schur decomposition of a pair of matrices (A,B)so that one diagonal block of (A,B) moves to another row index.

#### **Discussion**

This routine reorders the generalized real-Schur/Schur decomposition of a real/complex matrix pair (A, B) using an orthogonal/unitary equivalence transformation

$$(A, B) = Q (A, B) Z^H,$$

so that the diagonal block of (A, B) with row index *ifst* is moved to row *ilst*.

Matrix pair (A, B) must be in generalized real-Schur/Schur canonical form (as returned by <u>?gges</u>), i.e. A is block upper triangular with 1-by-1 and 2-by-2 diagonal blocks and B is upper triangular.

Optionally, the matrices Q and Z of generalized Schur vectors are updated.

$$Q(in) * A(in) * Z(in)' = Q(out) * A(out) * Z(out)'$$
  
 $Q(in) * B(in) * Z(in)' = Q(out) * B(out) * Z(out)'.$ 

#### **Input Parameters**

wantq, wantz LOGICAL.
If wantq = . TRUE . , update the left transformation
matrix Q;

	If wantq = .FALSE., do not update Q; If wantz = .TRUE., update the right transformation matrix Z;
	If $wantz = .FALSE.$ , do not update Z.
n	<b>INTEGER.</b> The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
a, b, q, z	REAL for stgexc DOUBLE PRECISION for dtgexc COMPLEX for ctgexc DOUBLE COMPLEX for ztgexc. Arrays: a(lda,*) contains the matrix A. The second dimension of a must be at least max(1, n).
	b(1db, *) contains the matrix <i>B</i> . The second dimension of <i>b</i> must be at least max $(1, n)$ .
	q(ldq, *) If wantq = .FALSE., then q is not referenced. If wantq = .TRUE., then q must contain the orthogonal/unitary matrix Q. The second dimension of q must be at least max(1, n).
	z (ldz, *) If wantz = .FALSE., then z is not referenced. If wantz = .TRUE., then z must contain the orthogonal/unitary matrix Z. The second dimension of z must be at least max(1, n).
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max(1, $n$ ).
ldq	<b>INTEGER.</b> The first dimension of $q$ ; If want $q = .$ FALSE., then $ldq \ge 1$ . If want $q = .$ TRUE., then $ldq \ge max(1,n)$ .
ldz	<b>INTEGER.</b> The first dimension of $z$ ; If want $z = .$ FALSE., then $ldz \ge 1$ . If want $z = .$ TRUE., then $ldz \ge max(1,n)$ .

ifst, ilst	<b>INTEGER.</b> Specify the reordering of the diagonal blocks of $(A, B)$ . The block with row index <i>ifst</i> is moved to row <i>ilst</i> , by a sequence of swapping between adjacent blocks. Constraint: $1 \leq ifst$ , <i>ilst</i> $\leq n$ .
work	REAL for stgexc; DOUBLE PRECISION for dtgexc. Workspace array, DIMENSION ( <i>lwork</i> ). Used in real flavors only.
lwork	<b>INTEGER</b> . The dimension of <i>work</i> ; must be at least $4n + 16$ .

a, b	Overwritten by the updated matrices A and B.
ifst, ilst	Overwritten for real flavors only. If <i>ifst</i> pointed to the second row of a 2 by 2 block on entry, it is changed to point to the first row; <i>ilst</i> always points to the first row of the block in its final position (which may differ from its input value by ±1).
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = 1$ , the transformed matrix pair ( <i>A</i> , <i>B</i> ) would be too far from generalized Schur form; the problem is ill-conditioned. ( <i>A</i> , <i>B</i> ) may have been partially reordered, and <i>ilst</i> points to the first row of the current position of the block being moved.

### ?tgsen

Reorders the generalized Schur decomposition of a pair of matrices (A,B)so that a selected cluster of eigenvalues appears in the leading diagonal blocks of (A,B).

lwork, iwork, liwork, info )

#### **Discussion**

This routine reorders the generalized real-Schur/Schur decomposition of a real/complex matrix pair (*A*, *B*) (in terms of an orthogonal/unitary equivalence transformation Q' * (A, B) * Z), so that a selected cluster of eigenvalues appears in the leading diagonal blocks of the pair (*A*, *B*). The leading columns of *Q* and *Z* form orthonormal/unitary bases of the corresponding left and right eigenspaces (deflating subspaces). (*A*, *B*) must be in generalized real-Schur/Schur canonical form (as returned by <u>?gges</u>), that is, *A* and *B* are both upper triangular. **?tgsen** also computes the generalized eigenvalues

$\omega = (alphar(j) + alphai(j)*i)/beta(j)$	(for real flavors)
$\dot{\omega} = alpha(j)/beta(j)$	(for complex flavors)
of the reordered matrix pair (A, B).	

Optionally, the routine computes the estimates of reciprocal condition numbers for eigenvalues and eigenspaces. These are  $Difu[(A_{11}, B_{11}), (A_{22}, B_{22})]$  and  $Difl[(A_{11}, B_{11}), (A_{22}, B_{22})]$ , that is, the separation(s) between the matrix pairs  $(A_{11}, B_{11})$  and  $(A_{22}, B_{22})$  that

correspond to the selected cluster and the eigenvalues outside the cluster, respectively, and norms of "projections" onto left and right eigenspaces with respect to the selected cluster in the (1,1)-block.

```
ijob
                   INTEGER. Specifies whether condition numbers are
                   required for the cluster of eigenvalues (pl and pr) or the
                   deflating subspaces Difu and Difl.
                   If i job =0, only reorder with respect to select;
                   If ijob =1, reciprocal of norms of "projections" onto
                   left and right eigenspaces with respect to the selected
                   cluster (pl and pr);
                   If ijob =2, compute upper bounds on Difu and Difl,
                   using F-norm-based estimate (dif (1:2));
                   If i job =3, compute estimate of Difu and Difl, using
                   1-norm-based estimate (dif (1:2)). This option is
                   about 5 times as expensive as i job = 2;
                   If i job =4, compute p1, pr and dif (i.e., options 0, 1
                   and 2 above). This is an economic version to get it all;
                   If ijob =5, compute pl, pr and dif (i.e., options 0, 1
                   and 3 above).
                   LOGICAL.
wantq, wantz
                   If wantq = . TRUE . , update the left transformation
                   matrix O:
                   If wantq = . FALSE., do not update Q;
                   If wantz = .TRUE., update the right transformation
                   matrix Z;
                   If wantz = . FALSE . , do not update Z.
select
                   LOGICAL.
                   Array, DIMENSION at least max (1, n).
                   Specifies the eigenvalues in the selected cluster.
                   To select an eigenvalue \omega_j, select (j) must be .TRUE.
                   For real flavors: to select a complex conjugate pair of
                   eigenvalues \omega and \omega_{\pm 1} (corresponding 2 by 2 diagonal
```

	block), <i>select</i> ( <i>j</i> ) and/or <i>select</i> ( <i>j</i> +1) must be set to . TRUE.; the complex conjugate $\omega_j$ and $\omega_{j+1}$ must be either both included in the cluster or both excluded.
п	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
a,b,q,z,work	REAL for stgsen DOUBLE PRECISION for dtgsen COMPLEX for ctgsen DOUBLE COMPLEX for ztgsen. Arrays: a (1da, *) contains the matrix A. For real flavors: A is upper quasi-triangular, with (A, B) in generalized real Schur canonical form. For complex flavors: A is upper triangular, in generalized Schur canonical form. The second dimension of a must be at least max(1, n).
	<ul> <li>b(1db,*) contains the matrix B.</li> <li>For real flavors: B is upper triangular, with (A, B) in generalized real Schur canonical form.</li> <li>For complex flavors: B is upper triangular, in generalized Schur canonical form.</li> <li>The second dimension of b must be at least max(1, n).</li> </ul>
	q(ldq, *) If wantq = .TRUE., then q is an n-by-n matrix; If wantq = .FALSE., then q is not referenced. The second dimension of q must be at least max(1, n).
	z (ldz, *) If wantz = .TRUE., then z is an n-by-n matrix; If wantz = .FALSE., then z is not referenced. The second dimension of z must be at least max(1, n).
	<pre>work(lwork) is a workspace array. If ijob=0, work is not referenced.</pre>
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .

ldq	<b>INTEGER.</b> The first dimension of $q$ ; $ldq \ge 1$ . If want $q = .$ TRUE., then $ldq \ge max(1,n)$ .
ldz	<b>INTEGER.</b> The first dimension of $z$ ; $ldz \ge 1$ . If want $z = .$ TRUE., then $ldz \ge max(1,n)$ .
lwork	INTEGER. The dimension of the array work. For real flavors: If $ijob = 1, 2, \text{ or } 4, lwork \ge max(4n+16, 2m(n-m)).$ If $ijob = 3 \text{ or } 5, lwork \ge max(4n+16, 4m(n-m)).$ For complex flavors: If $ijob = 1, 2, \text{ or } 4, lwork \ge max(1, 2m(n-m)).$ If $ijob = 3 \text{ or } 5, lwork \ge max(1, 4m(n-m)).$
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> ( <i>liwork</i> ). If <i>ijob</i> =0, <i>iwork</i> is not referenced.
liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . For real flavors: If $ijob = 1, 2, \text{ or } 4, liwork \ge n+6$ . If $ijob = 3 \text{ or } 5, liwork \ge max(n+6, 2m(n-m))$ . For complex flavors: If $ijob = 1, 2, \text{ or } 4, liwork \ge n+2$ . If $ijob = 3 \text{ or } 5, liwork \ge max(n+2, 2m(n-m))$ .

a, b	Overwritten by the reordered matrices <i>A</i> and <i>B</i> , respectively.
alphar,alphai	REAL for stgsen; DOUBLE PRECISION for dtgsen. Arrays, DIMENSION at least max(1,n). Contain values that form generalized eigenvalues in real flavors. See <i>beta</i> .
alpha	COMPLEX for ctgsen; DOUBLE COMPLEX for ztgsen. Array, DIMENSION at least max(1,n). Contain values that form generalized eigenvalues in complex flavors. See <i>beta</i> .

beta

q

 $\boldsymbol{Z}$ 

т

pl, pr

REAL for stgsen
DOUBLE PRECISION for dtgsen
COMPLEX for ctgsen
DOUBLE COMPLEX for ztgsen.
Array, <b>DIMENSION</b> at least max(1, <i>n</i> ).
For real flavors:
On exit, $(alphar(j) + alphai(j)*i)/beta(j), j=1,,n,$
will be the generalized eigenvalues.
alphar(j) + alphai(j)*i and $beta(j), j=1,,n$ are the
diagonals of the complex Schur form $(S,T)$ that would
result if the 2-by-2 diagonal blocks of the real
generalized Schur form of $(A, B)$ were further reduced to
triangular form using complex unitary transformations.
If <i>alphai</i> (j) is zero, then the j-th eigenvalue is real; if
positive, then the j-th and (j+1)-st eigenvalues are a
complex conjugate pair, with <i>alphai</i> (j+1) negative.
For complex flavors:
The diagonal elements of <i>A</i> and <i>B</i> , respectively, when
the pair $(A,B)$ has been reduced to generalized Schur
form. $alpha(i)/beta(i)$ , $i=1,,n$ are the generalized
eigenvalues.
If wantq = . TRUE., then, on exit, $Q$ has been
postmultiplied by the left orthogonal transformation
matrix which reorder $(A, B)$ . The leading <i>m</i> columns of
Q form orthonormal bases for the specified pair of left
eigenspaces (deflating subspaces).
If $wantz = .TRUE.$ , then, on exit, Z has been
postmultiplied by the left orthogonal transformation
matrix which reorder $(A, B)$ . The leading <i>m</i> columns of Z
form orthonormal bases for the specified pair of left
eigenspaces (deflating subspaces).
<b>INTEGER.</b> The dimension of the specified pair of left
and right eigen-spaces (deflating subspaces); $0 \le m \le n$ .
REAL for single precision flavors;
DOUBLE PRECISION for double precision flavors.
If $i j o b = 1, 4, \text{ or } 5, p1$ and pr are lower bounds on the

	reciprocal of the norm of "projections" onto left and right eigenspaces with respect to the selected cluster. $0 < p1, pr \leq 1$ . If $m = 0$ or $m = n$ , $p1 = pr = 1$ . If $ijob = 0, 2$ or $3, p1$ and $pr$ are not referenced
dif	<b>REAL</b> for single precision flavors; <b>DOUBLE PRECISION</b> for double precision flavors. Array, <b>DIMENSION</b> (2). If $ijob \ge 2$ , $dif(1:2)$ store the estimates of Difu and Difl. If $ijob = 2$ or 4, $dif(1:2)$ are F-norm-based upper bounds on Difu and Difl. If $ijob = 3$ or 5, $dif(1:2)$ are 1-norm-based estimates of Difu and Difl. If $m = 0$ or $n$ , dif(1:2) = F-norm([A, B]). If $ijob = 0$ or 1, $dif$ is not referenced.
work(1)	If <i>ijob</i> is not 0 and <i>info</i> = 0, on exit, <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
iwork(1)	If <i>ijob</i> is not 0 and <i>info</i> = 0, on exit, <i>iwork</i> (1) contains the minimum value of <i>liwork</i> required for optimum performance. Use this <i>liwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = 1$ , Reordering of $(A, B)$ failed because the transformed matrix pair $(A, B)$ would be too far from generalized Schur form; the problem is very ill-conditioned. $(A, B)$ may have been partially reordered. If requested, 0 is returned in <i>dif</i> (*), <i>p1</i> and <i>pr</i> .

# ?tgsyl

Solves the generalized Sylvester equation.

### **Discussion**

This routine solves the generalized Sylvester equation:

A R - L B = scale * CD R - L E = scale * F

where R and L are unknown *m*-by-*n* matrices, (A, D), (B, E) and (C, F) are given matrix pairs of size *m*-by-*m*, *n*-by-*n* and *m*-by-*n*, respectively, with real/complex entries. (A, D) and (B, E) must be in generalized real-Schur/Schur canonical form, that is, A, B are upper quasi-triangular/triangular and D, E are upper triangular.

The solution (*R*, *L*) overwrites (*C*, *F*). The factor *scale*,  $0 \le scale \le 1$ , is an output scaling factor chosen to avoid overflow.

In matrix notation the above equation is equivalent to the following: solve Zx = scale * b, where Z is defined as

$$Z = \begin{pmatrix} kron(I_n, A) - kron(B', I_m) \\ kron(I_n, D) - kron(E', I_m) \end{pmatrix}$$

Here  $I_k$  is the identity matrix of size k and X' is the transpose/conjugate-transpose of X. kron(X, Y) is the Kronecker product between the matrices X and Y.

If trans = 'T' (for real flavors), or trans = 'C' (for complex flavors), the routine ?tgsyl solves the transposed/conjugate-transposed system Z'y = scale * b, which is equivalent to solve for R and L in

A'R + D'L = scale * CRB' + LE' = scale * (-F)

This case (trans = 'T' for stgsyl/dtgsyl or trans = 'C' for ctgsyl/ztgsyl) is used to compute an one-norm-based estimate of Dif[(A,D), (B,E)], the separation between the matrix pairs (A,D) and (B,E), using slacon/clacon.

If  $ijob \ge 1$ , ?tgsyl computes a Frobenius norm-based estimate of Dif[(A,D), (B,E)]. That is, the reciprocal of a lower bound on the reciprocal of the smallest singular value of Z. This is a level 3 BLAS algorithm.

trans	CHARACTER*1. Must be 'N', 'T', or 'C'. If <i>trans</i> = 'N', solve the generalized Sylvester equation. If <i>trans</i> = 'T', solve the 'transposed' system (for real flavors only). If <i>trans</i> = 'C', solve the 'conjugate transposed' system (for complex flavors only).
ijob	<pre>INTEGER. Specifies what kind of functionality to be performed: If ijob =0, solve the generalized Sylvester equation only; If ijob =1, perform the functionality of ijob =0 and ijob =3; If ijob =2, perform the functionality of ijob =0 and ijob =4; If ijob =3, only an estimate of Dif[(A,D), (B,E)] is computed (look ahead strategy is used);</pre>

	If $ijob = 4$ , only an estimate of Dif[( <i>A</i> , <i>D</i> ), ( <i>B</i> , <i>E</i> )] is computed (?gecon on sub-systems is used). If $trans = 'T'or 'C'$ , $ijob$ is not referenced.
m	<b>INTEGER.</b> The order of the matrices <i>A</i> and <i>D</i> , and the row dimension of the matrices <i>C</i> , <i>F</i> , <i>R</i> and <i>L</i> .
n	<b>INTEGER.</b> The order of the matrices <i>B</i> and <i>E</i> , and the column dimension of the matrices <i>C</i> , <i>F</i> , <i>R</i> and <i>L</i> .
a,b,c,d,e,f,wo	Drk REAL for stgsyl DOUBLE PRECISION for dtgsyl COMPLEX for ctgsyl DOUBLE COMPLEX for ztgsyl.
	Arrays: <b>a</b> (1da,*) contains the upper quasi-triangular (for real flavors) or upper triangular (for complex flavors) matrix A. The second dimension of <b>a</b> must be at least max(1, m).
	b(1db, *) contains the upper quasi-triangular (for real flavors) or upper triangular (for complex flavors) matrix <i>B</i> . The second dimension of <i>b</i> must be at least max $(1, n)$ .
	c (ldc, *) contains the right-hand-side of the first matrix equation in the generalized Sylvester equation (as defined by <i>trans</i> ) The second dimension of $c$ must be at least max $(1, n)$ .
	d (1dd, *) contains the upper triangular matrix <i>D</i> . The second dimension of <i>d</i> must be at least max(1, <i>m</i> ).
	e(1de, *) contains the upper triangular matrix E. The second dimension of $e$ must be at least max $(1, n)$ .
	f(ldf,*) contains the right-hand-side of the second matrix equation in the generalized Sylvester equation (as defined by <i>trans</i> ) The second dimension of $f$ must be at least max $(1, n)$ .

work(lwork) is a workspace array. If ijob=0, work is
not referenced.

lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
ldb	<b>INTEGER</b> . The first dimension of $b$ ; at least max $(1, n)$ .
ldc	<b>INTEGER.</b> The first dimension of $c$ ; at least max(1, $m$ ).
ldd	<b>INTEGER.</b> The first dimension of $d$ ; at least max(1, $m$ ).
lde	<b>INTEGER.</b> The first dimension of $e$ ; at least max $(1, n)$ .
ldf	<b>INTEGER.</b> The first dimension of $f$ ; at least max $(1, m)$ .
lwork	<b>INTEGER.</b> The dimension of the array work . lwork $\ge 1$ . If $ijob = 1$ or 2 and $trans = 'N'$ , lwork $\ge 2mn$ .
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least $(m+n+6)$ for real flavors, and at least $(m+n+2)$ for complex flavors. If <i>ijob</i> =0, <i>iwork</i> is not referenced.

С	If $ijob=0$ , 1, or 2, overwritten by the solution <i>R</i> . If $ijob=3$ or 4 and $trans = 'N', c$ holds <i>R</i> , the solution achieved during the computation of the Dif-estimate.
f	If $ijob=0$ , 1, or 2, overwritten by the solution <i>L</i> . If $ijob=3$ or 4 and $trans = 'N'$ , <i>f</i> holds <i>L</i> , the solution achieved during the computation of the Dif-estimate.
dif	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. On exit, <i>dif</i> is the reciprocal of a lower bound of the reciprocal of the Dif-function, i.e. <i>dif</i> is an upper bound of $\text{Dif}[(A,D), (B,E)] = \text{sigma}_{\min}(Z)$ , where Z as in (2). If <i>ijob</i> = 0, or <i>trans</i> = 'T'(for real flavors), or <i>trans</i> = 'C'(for complex flavors), <i>dif</i> is not touched.

scale	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. On exit, <i>scale</i> is the scaling factor in the generalized Sylvester equation. If $0 < scale < 1$ , <i>c</i> and <i>f</i> hold the solutions <i>R</i> and <i>L</i> , respectively, to a slightly perturbed system but the input matrices <i>A</i> , <i>B</i> , <i>D</i> and <i>E</i> have not been changed. If <i>scale</i> = 0, <i>c</i> and <i>f</i> hold the solutions <i>R</i> and <i>L</i> , respectively, to the homogeneous system with C = F = 0. Normally, <i>scale</i> = 1.
work(1)	If <i>ijob</i> is not 0 and <i>info</i> = 0, on exit, <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info > 0$ , ( <i>A</i> , <i>D</i> ) and ( <i>B</i> , <i>E</i> ) have common or close eigenvalues.

# ?tgsna

Estimates reciprocal condition numbers for specified eigenvalues and/or eigenvectors of a pair of matrices in generalized real Schur canonical form.

call stgsna ( job, howmny, select, n, a, lda, b, ldvr, s, dif, mm, m, work, lwork,	
call dtgsna ( job, howmny, select, n, a, lda, b, ldvr, s, dif, mm, m, work, lwork,	
call ctgsna ( job, howmny, select, n, a, lda, b, ldvr, s, dif, mm, m, work, lwork,	
<pre>call ztgsna ( job, howmny, select, n, a, lda, b,</pre>	

### **Discussion**

The real flavors stgsna/dtgsna of this routine estimate reciprocal condition numbers for specified eigenvalues and/or eigenvectors of a matrix pair (A, B) in generalized real Schur canonical form (or of any matrix pair ( $Q A Z^T, Q B Z^T$ ) with orthogonal matrices Q and Z. (A, B) must be in generalized real Schur form (as returned by sgges/dgges), that is, A is block upper triangular with 1-by-1 and 2-by-2 diagonal blocks. B is upper triangular.

The complex flavors ctgsna/ztgsna estimate reciprocal condition numbers for specified eigenvalues and/or eigenvectors of a matrix pair (A, B). (A, B) must be in generalized Schur canonical form, that is, A and B are both upper triangular.

```
jobCHARACTER*1. Specifies whether condition numbers<br/>are required for eigenvalues or eigenvectors .<br/>Must be 'E' or 'V' or 'B'.<br/>If job = 'E', for eigenvalues only (compute s ).
```

	If $job = 'V'$ , for eigenvectors only (compute <i>dif</i> ). If $job = 'B'$ , for both eigenvalues and eigenvectors (compute both <i>s</i> and <i>dif</i> ).
howmny	CHARACTER*1. Must be 'A' or 'S'. If <i>howmny</i> = 'A', compute condition numbers for all eigenpairs. If <i>howmny</i> = 'S', compute condition numbers for selected eigenpairs specified by the logical array select.
select	LOGICAL. Array, DIMENSION at least max $(1, n)$ . If howmny = 'S', select specifies the eigenpairs for which condition numbers are required. If howmny= 'A', select is not referenced. For real flavors: To select condition numbers for the eigenpair corresponding to a real eigenvalue $\omega_{j}$ , select(j) must be set to .TRUE.; to select condition numbers corresponding to a complex conjugate pair of eigenvalues $\omega_{j+1}$ , either select(j) or select(j+1) must be set to .TRUE. For complex flavors: To select condition numbers for the corresponding j-th eigenvalue and/or eigenvector, select(j) must be set to .TRUE
п	<b>INTEGER.</b> The order of the square matrix pair $(A, B)$ $(n \ge 0)$ .
a,b,vl,vr,wo	The second dimension of a must be at least max $(1, n)$ .

	<b>b</b> ( <i>ldb</i> , *) contains the upper triangular matrix $B$ in the pair ( $A$ , $B$ ).
	The second dimension of <i>b</i> must be at least $\max(1, n)$ .
	If $job = 'E'$ or 'B',
	vl(ldvl,*) must contain left eigenvectors of $(A, B)$ , corresponding to the eigenpairs specified by howmny and select. The eigenvectors must be stored in consecutive columns of $vl$ , as returned by ?tgevc. If $job = 'V', vl$ is not referenced. The second dimension of $vl$ must be at least max $(1, m)$ .
	If $job = 'E'$ or 'B',
	<pre>vr(ldvr,*) must contain right eigenvectors of (A, B), corresponding to the eigenpairs specified by howmny and select. The eigenvectors must be stored in</pre>
	consecutive columns of $vr$ , as returned by ?tgevc. If $job = 'V'$ , $vr$ is not referenced.
	The second dimension of $vr$ must be at least max $(1, m)$ .
	<pre>work(lwork) is a workspace array. If job = 'E', work is not referenced.</pre>
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER</b> . The first dimension of $b$ ; at least max $(1, n)$ .
ldvl	<b>INTEGER.</b> The first dimension of $vl$ ; $ldvl \ge 1$ . If $job = 'E'$ or 'B', then $ldvl \ge max(1,n)$ .
ldvr	<b>INTEGER.</b> The first dimension of $vr$ ; $ldvr \ge 1$ . If $job = 'E'or 'B'$ , then $ldvr \ge max(1,n)$ .
mm	<b>INTEGER.</b> The number of elements in the arrays $s$ and dif $(mm \ge m)$ .
lwork	<b>INTEGER.</b> The dimension of the array work. For real flavors: $lwork \ge n$ . If $job = 'V'$ or 'B', $lwork \ge 2n(n+2)+16$ . For complex flavors: $lwork \ge 1$ .
	If $job = V'$ or $B'$ , $lwork \ge 2n^2$ .

iwork

INTEGER. Workspace array, DIMENSION at least (n+6)for real flavors, and at least (n+2) for complex flavors. If *ijob* = 'E', *iwork* is not referenced.

Output Farameters		
S	REAL for single-precision flavors DOUBLE PRECISION for double-precision flavors. Array, DIMENSION (mm). If $job = 'E'$ or 'B', contains the reciprocal condition numbers of the selected eigenvalues, stored in consecutive elements of the array. If $job = 'V'$ , $s$ is not referenced. For real flavors: For a complex conjugate pair of eigenvalues two consecutive elements of $s$ are set to the same value. Thus, $s(j)$ , $dif(j)$ , and the j-th columns of $vl$ and $vr$ all correspond to the same eigenpair (but not in general the j-th eigenpair, unless all eigenpairs are selected).	
dif	REAL for single-precision flavors DOUBLE PRECISION for double-precision flavors. Array, DIMENSION (mm). If $job = "V"$ or "B", contains the estimated reciprocal condition numbers of the selected eigenvectors, stored in consecutive elements of the array. If the eigenvalues cannot be reordered to compute $dif(j)$ , $dif(j)$ is set to 0; this can only occur when the true value would be very small anyway. If $job = "E"$ , $dif$ is not referenced. For real flavors: For a complex eigenvector, two consecutive elements of dif are set to the same value. For complex flavors: For each eigenvalue/vector specified by <i>select</i> , <i>dif</i> stores a Frobenius norm-based estimate of Difl.	

m	<b>INTEGER.</b> The number of elements in the arrays $s$ and <i>dif</i> used to store the specified condition numbers; for each selected eigenvalue one element is used. If <i>howmny</i> = 'A', <i>m</i> is set to <i>n</i> .
work(1)	<pre>work(1)If job is not 'E' and info = 0, on exit, work(1) contains the minimum value of lwork required for optimum performance. Use this lwork for subsequent runs.</pre>
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

# **Generalized Singular Value Decomposition**

This section describes LAPACK computational routines used for finding the generalized singular value decomposition (GSVD) of two matrices *A* and *B* as

$$\begin{split} U^{H}AQ &= D_{1} \, \ast \, (0 \ R), \\ V^{H}BQ &= D_{2} \, \ast \, (0 \ R), \end{split}$$

where U, V, and Q are orthogonal/unitary matrices, R is a nonsingular upper triangular matrix, and  $D_1$ ,  $D_2$  are "diagonal" matrices of the structure detailed in the routines description section.

# Table 5-7Computational Routines for Generalized Singular Value<br/>Decomposition

Routine name	Operation performed
?ggsvp	Computes the preprocessing decomposition for the generalized SVD
?tgsja	Computes the generalized SVD of two upper triangular or trapezoidal matrices

You can use routines listed in the above table as well as the driver routine ?ggsvd to find the GSVD of a pair of general rectangular matrices.

# ?ggsvp

*Computes the preprocessing decomposition for the generalized SVD.* 

#### **Discussion**

This routine computes orthogonal matrices U, V and Q such that

$$U^{H}A Q = \begin{pmatrix} n-k-l & k & l \\ k & 0 & A_{12} & A_{13} \\ 0 & 0 & A_{23} \\ m-k-l & 0 & 0 \end{pmatrix}, \text{ if } \underline{m-k-l} \ge 0$$

$$= \begin{array}{ccc} n-k-l & k & l \\ k & \begin{pmatrix} 0 & A_{12} & A_{13} \\ 0 & 0 & A_{23} \end{pmatrix}, & \text{if } m-k-l < 0 \\ n-k-l <$$

$$V^{H}BQ = \begin{pmatrix} n-k-l & k & l \\ l & 0 & 0 & B_{13} \\ p-l & 0 & 0 & 0 \end{pmatrix}$$

where the *k*-by-*k* matrix  $A_{12}$  and 1-by-1 matrix  $B_{13}$  are nonsingular upper triangular;  $A_{23}$  is 1-by-1 upper triangular if  $m-k-1 \ge 0$ , otherwise  $A_{23}$  is (m-k)-by-1 upper trapezoidal. The sum k+1 is equal to the effective numerical rank of the (m+p)-by-*n* matrix  $(A^H, B^H)^H$ .

This decomposition is the preprocessing step for computing the Generalized Singular Value Decomposition (GSVD), see subroutine ?ggsvd.

jobu	CHARACTER*1. Must be 'U' or 'N'. If <i>jobu</i> = 'U', orthogonal/unitary matrix U is computed. If <i>jobu</i> = 'N', U is not computed.
jobv	CHARACTER*1. Must be 'V' or 'N'. If <i>jobv</i> = 'V', orthogonal/unitary matrix V is computed. If <i>jobv</i> = 'N', V is not computed.
jobq	CHARACTER*1. Must be 'Q' or 'N'. If $jobq = 'Q'$ , orthogonal/unitary matrix Q is computed. If $jobq = 'N'$ , Q is not computed.
m	<b>INTEGER</b> . The number of rows of the matrix $A \ (m \ge 0)$ .
р	<b>INTEGER</b> . The number of rows of the matrix $B (p \ge 0)$ .
n	<b>INTEGER</b> . The number of columns of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
a,b,tau,work	REAL for sggsvp DOUBLE PRECISION for dggsvp COMPLEX for cggsvp DOUBLE COMPLEX for zggsvp. Arrays: a(lda,*) contains the <i>m</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
	b(1db, *) contains the <i>p</i> -by- <i>n</i> matrix <i>B</i> . The second dimension of <i>b</i> must be at least max $(1, n)$ .
	tau(*) is a workspace array. The dimension of $tau$ must be at least max $(1, n)$ .
	<pre>work(*) is a workspace array. The dimension of work must be at least max(1, 3n, m, p).</pre>

lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max(1, $p$ ).
tola, tolb	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. <b>tola</b> and <b>tolb</b> are the thresholds to determine the effective numerical rank of matrix <i>B</i> and a subblock of <i>A</i> . Generally, they are set to <b>tola</b> = $\max(m, n)^*   A   * MACHEPS,$ <b>tolb</b> = $\max(p, n)^*   B   * MACHEPS.$ The size of <b>tola</b> and <b>tolb</b> may affect the size of backward errors of the decomposition.
ldu	<b>INTEGER.</b> The first dimension of the output array $u$ . $ldu \ge max(1, m)$ if $jobu = 'U'$ ; $ldu \ge 1$ otherwise.
ldv	<b>INTEGER.</b> The first dimension of the output array $v$ . $ldv \ge max(1, p)$ if $jobv = V'$ ; $ldv \ge 1$ otherwise.
ldq	<b>INTEGER.</b> The first dimension of the output array $q$ . $ldq \ge max(1, n)$ if $jobq = 'Q'$ ; $ldq \ge 1$ otherwise.
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least $max(1, n)$ .
rwork	REAL for cggsvp DOUBLE PRECISION for zggsvp. Workspace array, DIMENSION at least max(1, 2n). Used in complex flavors only.

a	Overwritten by the triangular (or trapezoidal) matrix described in the <i>Discussion</i> section.
Ь	Overwritten by the triangular matrix described in the <i>Discussion</i> section.
k, 1	<b>INTEGER.</b> On exit, $k$ and $l$ specify the dimension of subblocks. The sum $k + l$ is equal to effective numerical rank of $(A^H, B^H)^H$ .

u, v, q	REAL for sggsvp
	DOUBLE PRECISION for dggsvp
	COMPLEX for cggsvp
	DOUBLE COMPLEX for zggsvp.
	Arrays:
	If $jobu = U'$ , $u(ldu, *)$ contains the
	orthogonal/unitary matrix U.
	The second dimension of $u$ must be at least max $(1, m)$ .
	If $jobu = 'N'$ , u is not referenced.
	If $jobv = 'V'$ , $v(ldv, *)$ contains the orthogonal/unitary matrix V. The second dimension of v must be at least max $(1, m)$ . If $jobv = 'N'$ , v is not referenced.
	If $jobq = 'Q'$ , $q(ldq, *)$ contains the orthogonal/unitary matrix $Q$ . The second dimension of $q$ must be at least max $(1, n)$ . If $jobq = 'N'$ , $q$ is not referenced.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. 'If $info = -i$ , the <i>i</i> th parameter had an illegal value.

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# ?tgsja

Computes the generalized SVD of two upper triangular or trapezoidal matrices.

call stgsja ( jobu, jobv, jobq, m, p, n, k, l, a, lda, b, ldb, tola, tolb, alpha, beta, u, ldu, v, ldv, q, ldq, work, ncycle, info ) call dtgsja ( jobu, jobv, jobq, m, p, n, k, l, a, lda, b, ldb, tola, tolb, alpha, beta, u, ldu, v, ldv, q, ldq, work, ncycle, info ) call ctgsja ( jobu, jobv, jobq, m, p, n, k, l, a, lda, b, ldb, tola, tolb, alpha, beta, u, ldu, v, ldv, q, ldq, work, ncycle, info ) call ztgsja ( jobu, jobv, jobq, m, p, n, k, l, a, lda, b, ldb, tola, tolb, alpha, beta, u, ldu, v, ldv, q, ldq, work, ncycle, info ) call ztgsja ( jobu, jobv, jobq, m, p, n, k, l, a, lda, b, ldb, tola, tolb, alpha, beta, u, ldu, v, ldv, q, ldq, work, ncycle, info )

#### **Discussion**

This routine computes the generalized singular value decomposition (GSVD) of two real/complex upper triangular (or trapezoidal) matrices A and B. On entry, it is assumed that matrices A and B have the following forms, which may be obtained by the preprocessing subroutine?ggsvp from a general *m*-by-*n* matrix A and *p*-by-*n* matrix B:

$$A = \frac{l}{m-k-l} \begin{pmatrix} n-k-l & k & l \\ k & 0 & A_{12} & A_{13} \\ 0 & 0 & A_{23} \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{if } m-k-l \ge 0$$

$$= \begin{array}{ccc} n-k-l & k & l \\ k & \left( \begin{array}{ccc} 0 & A_{12} & A_{13} \\ 0 & 0 & A_{23} \end{array} \right), & \text{if } m-k-l < 0 \end{array}$$

$$B = \frac{l}{p-l} \begin{pmatrix} 0 & 0 & B_{13} \\ 0 & 0 & 0 \end{pmatrix}$$

where the *k*-by-*k* matrix  $A_{12}$  and 1-by-1 matrix  $B_{13}$  are nonsingular upper triangular;  $A_{23}$  is 1-by-1 upper triangular if  $m-k-1 \ge 0$ , otherwise  $A_{23}$  is (m-k)-by-1 upper trapezoidal.

On exit,

$$U^H A Q = D_1^*(0 R)$$
,  $V^H B Q = D_2^*(0 R)$ ,  
where *U*, *V* and *Q* are orthogonal/unitary matrices, *R* is a nonsingular upper  
triangular matrix, and  $D_1$  and  $D_2$  are "diagonal" matrices, which are of the  
following structures:

If  $m-k-1 \geq 0$ ,

$$D_{1} = \binom{k}{l} \binom{l}{I} \begin{pmatrix} 0 & 0 \\ 0 & C \\ 0 & 0 \end{pmatrix}$$
$$D_{2} = \binom{l}{p-l} \binom{k}{0} \begin{pmatrix} 0 & S \\ 0 & 0 \end{pmatrix}$$
$$\frac{n-k-l}{k} \begin{pmatrix} 0 & R_{11} & R_{12} \\ 0 & 0 & R_{22} \end{pmatrix}$$

where

$$C = \text{diag} (alpha(k+1),...,alpha(k+1))$$
  

$$S = \text{diag} (beta(k+1),...,beta(k+1))$$
  

$$C^{2} + S^{2} = I$$
  
*R* is stored in a(1:k+1, n-k-1+1:n) on exit.

If m-k-1 < 0,  $k \quad m-k \quad k+l-m$  $D_1 = \begin{cases} k \begin{pmatrix} I & 0 & 0 \\ 0 & C & 0 \end{pmatrix} \\ k & m-k & k+l-m \\ m-k & \begin{pmatrix} 0 & S & 0 \\ 0 & 0 & I \\ p-l & \begin{pmatrix} 0 & 0 & I \\ 0 & 0 & 0 \end{pmatrix} \\ n-k-l \quad k & m-k \quad k+l-m \\ \begin{pmatrix} 0 & R_{11} & R_{12} & R_{13} \\ 0 & 0 & R_{22} & R_{23} \\ 0 & 0 & 0 & R_{33} \end{pmatrix}$ 

where

C = diag ( alpha(k+1),...,alpha(m)), S = diag ( beta(k+1),...,beta(m)), $C^2 + S^2 = I$ 

On exit,  $\begin{pmatrix} R_{11}R_{12}R_{13} \\ 0 & R_{22}R_{23} \end{pmatrix}$  is stored in a(1:m, n-k-l+1:n) and  $R_{33}$  is stored

in *b*(*m*-*k*+1:1, *n*+*m*-*k*-1+1:*n*).

The computation of the orthogonal/unitary transformation matrices U, V or Q is optional. These matrices may either be formed explicitly, or they may be postmultiplied into input matrices  $U_1$ ,  $V_1$ , or  $Q_1$ .

jobu	CHARACTER*1. Must be 'U', 'I', or 'N'. If $jobu = 'U'$ , u must contain an orthogonal/unitary matrix $U_1$ on entry. If $jobu = 'I'$ , u is initialized to the unit matrix. If $jobu = 'N'$ , u is not computed.	
jobv	CHARACTER*1. Must be 'V', 'I', or 'N'. If $jobv = 'V'$ , $v$ must contain an orthogonal/unitary matrix $V_I$ on entry. If $jobv = 'I'$ , $v$ is initialized to the unit matrix. If $jobv = 'N'$ , $v$ is not computed.	
jobq	CHARACTER*1. Must be 'Q', 'I', or 'N'. If $jobq = 'Q'$ , $q$ must contain an orthogonal/unitary matrix $Q_1$ on entry. If $jobq = 'I'$ , $q$ is initialized to the unit matrix. If $jobq = 'N'$ , $q$ is not computed.	
m	<b>INTEGER.</b> The number of rows of the matrix $A \ (m \ge 0)$ .	
р	<b>INTEGER.</b> The number of rows of the matrix $B (p \ge 0)$ .	
п	<b>INTEGER.</b> The number of columns of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).	
k, l	<b>INTEGER.</b> Specify the subblocks in the input matrices <i>A</i> and <i>B</i> , whose GSVD is going to be computed by ?tgsja.	
a,b,u,v,q,work	CREAL for stgsja DOUBLE PRECISION for dtgsja COMPLEX for ctgsja DOUBLE COMPLEX for ztgsja. Arrays: a(1da, *) contains the <i>m</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ). b(1db, *) contains the <i>p</i> -by- <i>n</i> matrix <i>B</i> . The second dimension of <i>b</i> must be at least max(1, <i>n</i> ).	

	If $jobu = 'U'$ , $u(ldu, *)$ must contain a matrix $U_I$ (usually the orthogonal/unitary matrix returned by ?ggsvp). The second dimension of $u$ must be at least max $(1, m)$ .
	If $jobv = V'$ , $v(ldv, *)$ must contain a matrix $V_l$ (usually the orthogonal/unitary matrix returned by ?ggsvp). The second dimension of $v$ must be at least max $(1, p)$ .
	If $jobq = Q'$ , $q(ldq, *)$ must contain a matrix $Q_I$ (usually the orthogonal/unitary matrix returned by ?ggsvp). The second dimension of $q$ must be at least max $(1, n)$ .
	work(*) is a workspace array. The dimension of work must be at least $max(1, 2n)$ .
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, m)$ .
ldb	<b>INTEGER</b> . The first dimension of $b$ ; at least max $(1, p)$ .
ldu	<b>INTEGER.</b> The first dimension of the array $u$ . $ldu \ge max(1, m)$ if $jobu = 'U'$ ; $ldu \ge 1$ otherwise.
ldv	<b>INTEGER.</b> The first dimension of the array $v$ . $ldv \ge max(1, p)$ if $jobv = V'$ ; $ldv \ge 1$ otherwise.
ldq	<b>INTEGER.</b> The first dimension of the array $q$ . $ldq \ge max(1, n)$ if $jobq = Q'$ ; $ldq \ge 1$ otherwise.
tola, tolb	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. <i>tola</i> and <i>tolb</i> are the convergence criteria for the Jacobi-Kogbetliantz iteration procedure. Generally, they are the same as used in ?ggsvp : <i>tola</i> = max( $m$ , $n$ )*   $A$    *MACHEPS, <i>tolb</i> = max( $p$ , $n$ )*   $B$    *MACHEPS.

а	On exit, $a(n-k+1:n, 1:min(k+1, m))$ contains the
	triangular matrix R or part of R.

Ь	On exit, if necessary, $b(m-k+1: 1, n+m-k-1+1: n))$ contains a part of <i>R</i> .
alpha, beta	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. Arrays, <b>DIMENSION</b> at least $max(1,n)$ . Contain the generalized singular value pairs of A and B.
	alpha(1:k) = 1, beta(1:k) = 0,
	and if $m-k-1 \ge 0$ , alpha(k+1:k+1) = diag(C), beta(k+1:k+1) = diag(S),
	or if $m-k-1 < 0$ , alpha(k+1:m) = C, $alpha(m+1:k+1) = 0beta(k+1:m) = S$ , $beta(m+1:k+1) = 1$ .
	Furthermore, if $k+1 < n$ , alpha(k+1+1:n) = 0 and beta(k+1+1:n) = 0.
u	If $jobu = 'I'$ , <i>u</i> contains the orthogonal/unitary matrix <i>U</i> . If $jobu = 'U'$ , <i>u</i> contains the product $U_IU$ . If $jobu = 'N'$ , <i>u</i> is not referenced.
v	If $jobv = 'I', v$ contains the orthogonal/unitary matrix U. If $jobv = 'V', v$ contains the product $V_I V$ . If $jobv = 'N', v$ is not referenced.
đ	If $jobq = 'I'$ , $q$ contains the orthogonal/unitary matrix $U$ . If $jobq = 'Q'$ , $q$ contains the product $Q_IQ$ . If $jobq = 'N'$ , $q$ is not referenced.
ncycle	<b>INTEGER</b> . The number of cycles required for convergence.

INTEGER. If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value. If info = 1, the procedure does not converge after MAXIT cycles.

info

# **Driver Routines**

Each of the LAPACK driver routines solves a complete problem. To arrive at the solution, driver routines typically call a sequence of appropriate <u>computational routines</u>. Driver routines are described in the following sections:

Linear Least Squares (LLS) Problems Generalized LLS Problems Symmetric Eigenproblems Nonsymmetric Eigenproblems Singular Value Decomposition Generalized Symmetric Definite Eigenproblems Generalized Nonsymmetric Eigenproblems

### Linear Least Squares (LLS) Problems

This section describes LAPACK driver routines used for solving linear least-squares problems. <u>Table 5-8</u> lists routines described in more detail below.

Table 5-6	Driver Routines for Solving LLS Problems
Routine Name	Operation performed
?gels	Uses QR or LQ factorization to solve a overdetermined or underdetermined linear system with full rank matrix.
?gelsy	Computes the minimum-norm solution to a linear least squares problem using a complete orthogonal factorization of A.
?gelss	Computes the minimum-norm solution to a linear least squares problem using the singular value decomposition of A.
?gelsd	Computes the minimum-norm solution to a linear least squares problem using the singular value decomposition of A and a divide and conquer method.

#### Table 5-8 Driver Routines for Solving LLS Problems

# ?gels

Uses QR or LQ factorization to solve a overdetermined or underdetermined linear system with full rank matrix.

call sgels ( trans, m, n, nrhs, a, lda, b, ldb, work, lwork, info ) call dgels ( trans, m, n, nrhs, a, lda, b, ldb, work, lwork, info ) call cgels ( trans, m, n, nrhs, a, lda, b, ldb, work, lwork, info ) call zgels ( trans, m, n, nrhs, a, lda, b, ldb, work, lwork, info )

#### **Discussion**

This routine solves overdetermined or underdetermined real/complex linear systems involving an m-by-n matrix A, or its transpose/conjugate-transpose, using a QR or LQ factorization of A. It is assumed that A has full rank.

The following options are provided:

1. If trans = 'N' and  $m \ge n$ : find the least squares solution of an overdetermined system, that is, solve the least squares problem minimize  $|| b - A x ||_2$ 

2. If trans = 'N' and m < n: find the minimum norm solution of an underdetermined system A X = B.

3. If *trans* = 'T' or 'C' and  $m \ge n$ : find the minimum norm solution of an undetermined system  $A^H X = B$ .

4. If trans = 'T' or 'C' and m < n: find the least squares solution of an overdetermined system, that is, solve the least squares problem minimize  $|| b - A^H x ||_2$ 

Several right hand side vectors b and solution vectors x can be handled in a single call; they are stored as the columns of the *m*-by-*nrhs* right hand side matrix B and the *n*-by-*nrh* solution matrix X.

trans	CHARACTER*1. Must be 'N', 'T', or 'C'. If $trans =$ 'N', the linear system involves matrix A; If $trans =$ 'T', the linear system involves the transposed matrix $A^T$ (for real flavors only); If $trans =$ 'C', the linear system involves the conjugate-transposed matrix $A^H$ (for complex flavors only).
m	<b>INTEGER</b> . The number of rows of the matrix $A \ (m \ge 0)$ .
n	<b>INTEGER</b> . The number of columns of the matrix $A$ ( $n \ge 0$ ).
nrhs	<b>INTEGER</b> . The number of right-hand sides; the number of columns in <i>B</i> ( <i>nrhs</i> $\ge$ 0).
a, b, work	<pre>REAL for sgels DOUBLE PRECISION for dgels COMPLEX for cgels DOUBLE COMPLEX for zgels. Arrays: a(lda,*) contains the m-by-n matrix A. The second dimension of a must be at least max(1, n). b(ldb,*) contains the matrix B of right hand side vectors, stored columnwise; B is m-by-nrhs if trans = 'N', or n-by-nrhs if trans = 'T'or 'C'. The second dimension of b must be at least max(1, nrhs).</pre>
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
ldb	<b>INTEGER</b> . The first dimension of $b$ ; must be at least max $(1, m, n)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; must be at least min $(m, n) + \max(1, m, n, nrhs)$ . See <i>Application notes</i> for the suggested value of <i>lwork</i> .

а	On exit, overwritten by the factorization data as follows:
	if $m \ge n$ , array a contains the details of the $QR$ factorization of the matrix A as returned by <u>?geqrf</u> ; if $m < n$ , array a contains the details of the $LQ$ factorization of the matrix A as returned by <u>?gelqf</u> .
b	Overwritten by the solution vectors, stored columnwise: If $trans = 'N'$ and $m \ge n$ , rows 1 to n of b contain the least squares solution vectors; the residual sum of squares for the solution in each column is given by the sum of squares of elements $n+1$ to m in that column; If $trans = 'N'$ and $m < n$ , rows 1 to n of b contain the minimum norm solution vectors; if $trans = 'T'$ or 'C' and $m \ge n$ , rows 1 to m of b contain the minimum norm solution vectors; if $trans = 'T'$ or 'C' and $m < n$ , rows 1 to m of b contain the least squares solution vectors; the residual sum of squares for the solution in each column is given by the sum of squares of elements $m+1$ to n in that column.
work(1)	If <i>info</i> = 0, on exit <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.
	in the function parameter had an megal value.

#### **Application Notes**

For better performance, try using

*lwork* =min (*m*, *n*) +max(1, *m*, *n*, *nrhs*)**blocksize*, where *blocksize* is a machine-dependent value (typically, 16 to 64) required for optimum performance of the *blocked algorithm*.

If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work(1)* and use this value for subsequent runs.

# ?gelsy

Computes the minimum-norm solution to a linear least squares problem using a complete orthogonal factorization of A.

### Discussion

This routine computes the minimum-norm solution to a real/complex linear least squares problem:

minimize  $|| b - A x ||_2$ 

using a complete orthogonal factorization of A. A is an m-by-n matrix which may be rank-deficient.

Several right hand side vectors b and solution vectors x can be handled in a single call; they are stored as the columns of the *m*-by-*nrhs* right hand side matrix B and the *n*-by-*nrhs* solution matrix X.

The routine first computes a *QR* factorization with column pivoting:

$$AP = Q \begin{pmatrix} R_{11}R_{12} \\ 0 & R_{22} \end{pmatrix}$$

with  $R_{11}$  defined as the largest leading submatrix whose estimated condition number is less than 1/rcond. The order of  $R_{11}$ , *rank*, is the effective rank of *A*.

Then,  $R_{22}$  is considered to be negligible, and  $R_{12}$  is annihilated by orthogonal/unitary transformations from the right, arriving at the complete orthogonal factorization:

$$AP = Q \begin{pmatrix} T_{11} \\ 0 & 0 \end{pmatrix} Z$$

The minimum-norm solution is then

$$x = PZ^H \begin{pmatrix} T_{11}^{-1} Q_1^H b \\ 0 \end{pmatrix}$$

where  $Q_1$  consists of the first *rank* columns of Q. This routine is basically identical to the original **?gelsx** except three differences:

- The call to the subroutine <u>?geqpf</u> has been substituted by the call to the subroutine <u>?geqp3</u>. This subroutine is a BLAS-3 version of the *QR* factorization with column pivoting.
- Matrix *B* (the right hand side) is updated with BLAS-3.
- The permutation of matrix *B* (the right hand side) is faster and more simple.

m	<b>INTEGER.</b> The number of rows of the matrix $A \ (m \ge 0)$ .
п	<b>INTEGER.</b> The number of columns of the matrix $A$ ( $n \ge 0$ ).
nrhs	<b>INTEGER.</b> The number of right-hand sides; the number of columns in <i>B</i> ( <i>nrhs</i> $\ge$ 0).
a, b, work	REAL for sgelsy DOUBLE PRECISION for dgelsy COMPLEX for cgelsy DOUBLE COMPLEX for zgelsy. Arrays: a(lda,*) contains the <i>m</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).

	<ul> <li>b(1db,*) contains the <i>m</i>-by-<i>nrhs</i> right hand side matrix <i>B</i>.</li> <li>The second dimension of <i>b</i> must be at least max(1, <i>nrhs</i>).</li> </ul>
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max(1, $m$ ).
ldb	<b>INTEGER</b> . The first dimension of $b$ ; must be at least max $(1, m, n)$ .
jpvt	INTEGER. Array, DIMENSION at least $max(1, n)$ .
	On entry, if $jpvt(i) \neq 0$ , the <i>i</i> th column of A is permuted to the front of AP, otherwise the <i>i</i> th column of A is a free column.
rcond	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors.
	<i>rcond</i> is used to determine the effective rank of <i>A</i> , which is defined as the order of the largest leading triangular submatrix $R_{11}$ in the <i>QR</i> factorization with pivoting of <i>A</i> , whose estimated condition number < $1/rcond$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array. See <i>Application notes</i> for the suggested value of <i>lwork</i> .
rwork	REAL for cgelsy DOUBLE PRECISION for zgelsy. Workspace array, DIMENSION at least max(1, 2n). Used in complex flavors only.

a	On exit, overwritten by the details of the complete orthogonal factorization of <i>A</i> .
b	Overwritten by the <i>n</i> -by- <i>nrhs</i> solution matrix $X$ .
jpvt	On exit, if $jpvt(i) = k$ , then the <i>i</i> th column of AP was the <i>k</i> th column of A.

rank	INTEGER.
	The effective rank of A, that is, the order of the
	submatrix $R_{11}$ . This is the same as the order of the
	submatrix $T_{11}$ in the complete orthogonal factorization
	of A.
info	INTEGER.
	If <i>info</i> = 0, the execution is successful.
	If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

For real flavors:

The unblocked strategy requires that:

 $lwork \geq max(mn+3n+1, 2*mn + nrhs),$ 

where  $mn = \min(m, n)$ .

The block algorithm requires that:

 $lwork \ge max(mn+2n+nb*(n+1), 2*mn+nb*nrhs),$ 

where *nb* is an upper bound on the blocksize returned by *ilaenv* for the routines sgeqp3/dgeqp3, stzrzf/dtzrzf, stzrqf/dtzrqf, sormqr/dormqr, and sormrz/dormrz.

For complex flavors:

The unblocked strategy requires that:

 $lwork \ge mn + max(2*mn, n+1, mn + nrhs),$ 

where  $mn = \min(m, n)$ .

The block algorithm requires that:

 $lwork \ge mn + max(2*mn, nb*(n+1), mn+mn*nb, mn+nb*nrhs)$ , where nb is an upper bound on the blocksize returned by ilaenv for the routines cgeqp3/zgeqp3, ctzrzf/ztzrzf, ctzrqf/ztzrqf, cunmqr/zunmqr, and cunmrz/zunmrz.

# ?gelss

Computes the minimum-norm solution to a linear least squares problem using the singular value decomposition of A.

### Discussion

This routine computes the minimum norm solution to a real linear least squares problem:

minimize  $|| b - A x ||_2$ 

using the singular value decomposition (SVD) of A. A is an *m*-by-*n* matrix which may be rank-deficient.

Several right hand side vectors *b* and solution vectors *x* can be handled in a single call; they are stored as the columns of the *m*-by-*nrhs* right hand side matrix *B* and the *n*-by-*nrhs* solution matrix *X*.

The effective rank of *A* is determined by treating as zero those singular values which are less than *rcond* times the largest singular value.

m	<b>INTEGER</b> . The number of rows of the matrix $A \ (m \ge 0)$ .
n	<b>INTEGER</b> . The number of columns of the matrix $A$ $(n \ge 0)$ .
nrhs	<b>INTEGER.</b> The number of right-hand sides; the number of columns in $B$ ( <i>nrhs</i> $\ge$ 0).

a, b, work	REAL for sgelss
	DOUBLE PRECISION for dgelss
	COMPLEX for cgelss
	DOUBLE COMPLEX for zgelss.
	Arrays:
	a(lda, *) contains the <i>m</i> -by- <i>n</i> matrix A.
	The second dimension of a must be at least $max(1, n)$ .
	b(1db, *) contains the <i>m</i> -by- <i>nrhs</i> right hand side matrix <i>B</i> .
	The second dimension of <i>b</i> must be at least
	max(1, <i>nrhs</i> ).
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; must be at least max $(1, m, n)$ .
rcond	<b>REAL</b> for single-precision flavors
	DOUBLE PRECISION for double-precision flavors.
	<b>rcond</b> is used to determine the effective rank of A. Singular values $s(i) \leq rcond * s(1)$ are treated as zero. If <b>rcond</b> < 0, machine precision is used instead.
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; <i>lwork</i> $\ge$ 1. See <i>Application notes</i> for the suggested value of <i>lwork</i> .
rwork	REAL for cgelss
	DOUBLE PRECISION for zgelss.
	Workspace array used in complex flavors only.
	<b>DIMENSION</b> at least $max(1, 5*min(m, n))$ .

a	On exit, the first $\min(m, n)$ rows of <i>A</i> are overwritten with its right singular vectors, stored row-wise.
b	Overwritten by the <i>n</i> -by- <i>nrhs</i> solution matrix $X$ .
	If $m \ge n$ and $rank = n$ , the residual sum-of-squares for the solution in the <i>i</i> -th column is given by the sum of squares of elements $n+1:m$ in that column.

S	<b>REAL</b> for single precision flavors <b>DOUBLE PRECISION</b> for double precision flavors. Array, <b>DIMENSION</b> at least max(1, min( <i>m</i> , <i>n</i> )). The singular values of <i>A</i> in decreasing order. The condition number of <i>A</i> in the 2-norm is $k_2(A) = s(1) / s(min(m, n))$ .
rank	<b>INTEGER.</b> The effective rank of <i>A</i> , that is, the number of singular values which are greater than $rcond * s(1)$ .
work(1)	If <i>info</i> = 0, on exit, <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = i, then the algorithm for computing the SVD failed to converge; i indicates the number of off-diagonal elements of an intermediate bidiagonal form which did not converge to zero.</pre>

## **Application Notes**

For real flavors:

 $lwork \ge 3 * \min(m, n) + \max(2 * \min(m, n), \max(m, n), nrhs)$ 

For complex flavors:

 $lwork \ge 2 * min(m, n) + max(m, n, nrhs)$ 

For good performance, *lwork* should generally be larger. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

# ?gelsd

Computes the minimum-norm solution to a linear least squares problem using the singular value decomposition of A and a divide and conquer method.

## **Discussion**

This routine computes the minimum-norm solution to a real linear least squares problem:

minimize  $|| b - A x ||_2$ 

using the singular value decomposition (SVD) of A. A is an *m*-by-*n* matrix which may be rank-deficient.

Several right hand side vectors *b* and solution vectors *x* can be handled in a single call; they are stored as the columns of the *m*-by-*nrhs* right hand side matrix *B* and the *n*-by-*nrhs* solution matrix *X*.

The problem is solved in three steps:

- 1. Reduce the coefficient matrix A to bidiagonal form with Householder transformations, reducing the original problem into a "bidiagonal least squares problem" (BLS).
- 2. Solve the BLS using a divide and conquer approach.
- 3. Apply back all the Householder transformations to solve the original least squares problem.

The effective rank of *A* is determined by treating as zero those singular values which are less than *rcond* times the largest singular value.

т	<b>INTEGER</b> . The number of rows of the matrix $A \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns of the matrix $A$ ( $n \ge 0$ ).
nrhs	<b>INTEGER</b> . The number of right-hand sides; the number of columns in <i>B</i> ( <i>nrhs</i> $\ge$ 0).
a, b, work	<pre>REAL for sgelsd DOUBLE PRECISION for dgelsd COMPLEX for cgelsd DOUBLE COMPLEX for zgelsd. Arrays: a(lda,*) contains the m-by-n matrix A. The second dimension of a must be at least max(1, n). b(ldb,*) contains the m-by-nrhs right hand side matrix B.</pre>
	The second dimension of $b$ must be at least max $(1, nrhs)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
ldb	<b>INTEGER</b> . The first dimension of $b$ ; must be at least max $(1, m, n)$ .
rcond	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors.
	<b>rcond</b> is used to determine the effective rank of A. Singular values $s(i) \leq rcond * s(1)$ are treated as zero. If <b>rcond</b> < 0, machine precision is used instead.
lwork	<b>INTEGER</b> . The size of the <i>work</i> array; <i>lwork</i> $\ge$ 1. See <i>Application notes</i> for the suggested value of <i>lwork</i> .
iwork	<b>INTEGER</b> . Workspace array. See <i>Application notes</i> for the suggested dimension of <i>iwork</i> .
rwork	REAL for cgelsd DOUBLE PRECISION for zgelsd.
	Workspace array, used in complex flavors only. See

Application notes for the suggested dimension of *rwork*.

#### **Output Parameters**

a	On exit, A has been overwritten.
b	Overwritten by the <i>n</i> -by- <i>nrhs</i> solution matrix <i>X</i> .
	If $m \ge n$ and $rank = n$ , the residual sum-of-squares for the solution in the <i>i</i> -th column is given by the sum of squares of elements $n+1:m$ in that column.
S	<b>REAL</b> for single precision flavors <b>DOUBLE PRECISION</b> for double precision flavors. Array, <b>DIMENSION</b> at least max(1, min( <i>m</i> , <i>n</i> )). The singular values of <i>A</i> in decreasing order. The condition number of <i>A</i> in the 2-norm is $k_2(A) = \mathbf{s}(1) / \mathbf{s}(\min(m, n))$ .
rank	<b>INTEGER.</b> The effective rank of <i>A</i> , that is, the number of singular values which are greater than $rcond * s(1)$ .
work(1)	If <i>info</i> = 0, on exit, <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , then the algorithm for computing the SVD failed to converge; <i>i</i> indicates the number of off-diagonal elements of an intermediate bidiagonal form which did not converge to zero.

## **Application Notes**

The divide and conquer algorithm makes very mild assumptions about floating point arithmetic. It will work on machines with a guard digit in add/subtract. It could conceivably fail on hexadecimal or decimal machines without guard digits, but we know of none. The exact minimum amount of workspace needed depends on m, n and nrhs. The size *lwork* of the workspace array *work* must be as given below.

For real flavors: If  $m \ge n$ ,  $lwork \ge 12n + 2n*smlsiz + 8n*nlvl + n*nrhs + (smlsiz+1)^2$ ; If m < n,  $lwork \ge 12m + 2m*smlsiz + 8m*nlvl + m*nrhs + (smlsiz+1)^2$ ; For complex flavors: If  $m \ge n$ ,  $lwork \ge 2n + n*nrhs$ ; If m < n,  $lwork \ge 2m + m*nrhs$ ; where smlsiz is returned by it second and is equal to the maximum

where *smlsiz* is returned by *ilaenv* and is equal to the maximum size of the subproblems at the bottom of the computation tree (usually about 25), and  $nlvl = INT(\log_2(\min(m, n)/(smlsiz+1))) + 1$ .

For good performance, *lwork* should generally be larger. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The dimension of the workspace array *iwork* must be at least  $3 \min(m, n) * nlvl + 11 \min(m, n)$ .

The dimension *lrwork* of the workspace array *rwork* (for complex flavors) must be at least:

If  $m \ge n$ ,  $lrwork \ge 10n + 2n*smlsiz + 8n*nlvl + 3*smlsiz*nrhs + (smlsiz+1)^2$ ; If m < n,  $lrwork \ge 10m + 2m*smlsiz + 8m*nlvl + 3*smlsiz*nrhs + (smlsiz+1)^2$ .

## **Generalized LLS Problems**

This section describes LAPACK driver routines used for solving generalized linear least-squares problems. <u>Table 5-9</u> lists routines described in more detail below.

Table 5-9	Driver Routines for Solving Generalized LLS Problems
Routine Name	Operation performed
?gglse	Solves the linear equality-constrained least squares problem using a generalized RQ factorization.
?ggglm	Solves a general Gauss-Markov linear model problem using a generalized QR factorization.

# ?gglse

Solves the linear equality-constrained least squares problem using a generalized RQ factorization.

call	sgglse	(	m,	n,	p,	a,	lda,	b,	ldb,	C,	d,	x,	work,	lwork,	info	)
call	dgglse	(	m,	n,	p,	a,	lda,	b,	ldb,	C,	d,	x,	work,	lwork,	info	)
call	cgglse	(	m,	n,	p,	a,	lda,	b,	ldb,	C,	d,	x,	work,	lwork,	info	)
call	zgglse	(	m,	n,	p,	a,	lda,	b,	ldb,	c,	d,	х,	work,	lwork,	info	)

## **Discussion**

This routine solves the linear equality-constrained least squares (LSE) problem:

minimize  $|| c - A x ||_2$  subject to B x = d

where A is an m-by-n matrix, B is a p-by-n matrix, c is a given m-vector, and d is a given p-vector.

It is assumed that  $p \leq n \leq m+p$ , and

$$\operatorname{rank}(B) = p$$
 and  $\operatorname{rank}\begin{pmatrix} A\\ B \end{pmatrix} = n$ .

These conditions ensure that the LSE problem has a unique solution, which is obtained using a generalized RQ factorization of the matrices B and A.

m	<b>INTEGER</b> . The number of rows of the matrix $A \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
p	<b>INTEGER.</b> The number of rows of the matrix $B$ $(0 \leq p \leq n \leq m+p).$
a,b,c,d,work	REAL for sgglse DOUBLE PRECISION for dgglse COMPLEX for cgglse DOUBLE COMPLEX for zgglse.
	Arrays: a(lda,*) contains the <i>m</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
	b(1db, *) contains the <i>p</i> -by- <i>n</i> matrix <i>B</i> . The second dimension of <i>b</i> must be at least max $(1, n)$ .
	c(*), dimension at least max $(1, m)$ , contains the right hand side vector for the least squares part of the LSE problem.
	d(*), dimension at least max(1, p), contains the right hand side vector for the constrained equation. work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, p)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; $lwork \ge max(1, m+n+p)$ . See Application notes for the suggested value of <i>lwork</i> .

x	REAL for sgglse
	DOUBLE PRECISION for dgglse
	COMPLEX for cgglse
	DOUBLE COMPLEX for zgglse.
	Array, DIMENSION at least $max(1, n)$ .
	On exit, contains the solution of the LSE problem.
a,b,d	On exit, these arrays are overwritten.
С	On exit, the residual sum-of-squares for the solution is given by the sum of squares of elements $n-p+1$ to m of vector c.
work(1)	If <i>info</i> = 0, on exit, <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance. Use this <i>lwork</i> for subsequent runs.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## **Application Notes**

For optimum performance use
 lwork ≥ p+min(m, n)+max(m, n)*nb,
where nb is an upper bound for the optimal blocksizes for ?geqrf,
?gerqf, ?ormqr/?unmqr and ?ormrq/?unmrq.

# ?ggglm

Solves a general Gauss-Markov linear model problem using a generalized QR factorization.

call sggglm ( n, m, p, a, lda, b, ldb, d, x, y, work, lwork, info )
call dggglm ( n, m, p, a, lda, b, ldb, d, x, y, work, lwork, info )
call cggglm ( n, m, p, a, lda, b, ldb, d, x, y, work, lwork, info )
call zggglm ( n, m, p, a, lda, b, ldb, d, x, y, work, lwork, info )

### **Discussion**

This routine solves a general Gauss-Markov linear model (GLM) problem: minimize_x  $||y||_2$  subject to d = Ax + Bywhere A is an *n*-by-*m* matrix, B is an *n*-by-*p* matrix, and d is a given *n*-vector.

It is assumed that  $m \leq n \leq m+p$ , and

 $\operatorname{rank}(A) = \mathbf{m}$  and  $\operatorname{rank}(A B) = \mathbf{n}$ .

Under these assumptions, the constrained equation is always consistent, and there is a unique solution x and a minimal 2-norm solution y, which is obtained using a generalized QR factorization of A and B. In particular, if matrix B is square nonsingular, then the problem GLM is equivalent to the following weighted linear least squares problem minimize  $||| B^{-1}(d - Ax)||$ 

minimize_x  $|| B^{-1}(d-Ax) ||_2$ .

п	INTEGER. The number of rows of the matrices A and B $(n \ge 0)$ .
m	<b>INTEGER.</b> The number of columns in $A \ (m \ge 0)$ .
2	<b>INTEGER.</b> The number of columns in $B$ ( $p \ge n - m$ ).
p	INTEGER. The number of columns in $D$ ( $p \ge n - m$ ).
a,b,d,work	REAL for sggglm
	DOUBLE PRECISION for dggglm
	COMPLEX for cggglm
	DOUBLE COMPLEX for zggglm.

	Arrays: a(lda,*) contains the n-by-m matrix A. The second dimension of a must be at least max(1, m).
	b(1db, *) contains the <i>n</i> -by- <i>p</i> matrix <i>B</i> . The second dimension of <i>b</i> must be at least max $(1, p)$ .
	d(*), dimension at least max(1, n), contains the left hand side of the GLM equation. work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .
lwork	<b>INTEGER.</b> The size of the <i>work</i> array; $lwork \ge max(1, n+m+p)$ . See Application notes for the suggested value of $lwork$ .

х, у	REAL for sggglm DOUBLE PRECISION for dggglm COMPLEX for cggglm DOUBLE COMPLEX for zggglm. Arrays x(*), y(*). DIMENSION at least max(1, m) for x
	and at least $\max(1, p)$ for y.
	On exit, $\mathbf{x}$ and $\mathbf{y}$ are the solutions of the GLM problem.
a,b,d	On exit, these arrays are overwritten.
work(1)	If <i>info</i> = 0, on exit, <i>work</i> (1) contains the minimum value of <i>lwork</i> required for optimum performance.
info	<b>INTEGER</b> . If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## **Application Notes**

For optimum performance use

 $lwork \ge m + \min(n, p) + \max(n, p) * nb,$ 

where *nb* is an upper bound for the optimal blocksizes for ?geqrf, ?geqf, ?ormqr/?unmqr and ?ormrq/?unmrq.

## Symmetric Eigenproblems

This section describes LAPACK driver routines used for solving symmetric eigenvalue problems. See also <u>computational routines</u> that can be called to solve these problems.

Table 5-10 lists routines described in more detail below.

## Table 5-10 Driver Routines for Solving Symmetric Eigenproblems

Routine Name	Operation performed
?syev/?heev	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric / Hermitian matrix.
?syevd/?heevd	Computes all eigenvalues and (optionally) all eigenvectors of a real symmetric / Hermitian matrix using divide and conquer algorithm.
?syevx/?heevx	Computes selected eigenvalues and, optionally, eigenvectors of a symmetric / Hermitian matrix.
?syevr/?heevr	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric / Hermitian matrix using the Relatively Robust Representations.
?spev/?hpev	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric / Hermitian matrix in packed storage.
?spevd/?hpevd	Uses divide and conquer algorithm to compute all eigenvalues and (optionally) all eigenvectors of a real symmetric / Hermitian matrix held in packed storage.
?spevx/?hpevx	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric / Hermitian matrix in packed storage.
?sbev/?hbev	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric / Hermitian band matrix.
?sbevd/?hbevd	Computes all eigenvalues and (optionally) all eigenvectors of a real symmetric / Hermitian band matrix using divide and conquer algorithm.
<u>?sbevx/?hbevx</u>	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric / Hermitian band matrix.
<u>?stev</u>	Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix.
?stevd	Computes all eigenvalues and (optionally) all eigenvectors of a real symmetric tridiagonal matrix using divide and conquer algorithm.
<u>?stevx</u>	Computes selected eigenvalues and eigenvectors of a real symmetric tridiagonal matrix.
?stevr	Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix using the Relatively Robust Representations.

## ?syev

Computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix.

call ssyev ( jobz, uplo, n, a, lda, w, work, lwork, info )
call dsyev ( jobz, uplo, n, a, lda, w, work, lwork, info )

## **Discussion**

This routine computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix *A*.

jobz	CHARACTER*1. Must be 'N' or 'V'.
	If $jobz = 'N'$ , then only eigenvalues are computed.
	If $jobz = V'$ , then eigenvalues and eigenvectors are
	computed.
uplo	CHARACTER*1. Must be 'U' or 'L'.
	If $uplo = 'U'$ , a stores the upper triangular part of A.
	If $uplo = 'L'$ , a stores the lower triangular part of A.
п	<b>INTEGER.</b> The order of the matrix $A$ ( $n \ge 0$ ).
a, work	REAL for ssyev
	DOUBLE PRECISION for dsyev
	Arrays:
	a(lda,*) is an array containing either upper or lower
	triangular part of the symmetric matrix A, as specified
	by uplo.
	The second dimension of $a$ must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of the array <i>a</i> .
	Must be at least $max(1, n)$ .

lwork	<b>INTEGER</b> . The dimension of the array <i>work</i> . Constraint: $lwork \ge max(1, 3n-1)$ . See <i>Application notes</i> for the suggested value of <i>lwork</i> .
Output Para	meters
a	On exit, if <i>jobz</i> = 'V', then if <i>info</i> = 0, array <i>a</i> contains the orthonormal eigenvectors of the matrix <i>A</i> . If <i>jobz</i> = 'N', then on exit the lower triangle (if <i>uplo</i> = 'L') or the upper triangle (if <i>uplo</i> = 'U') of <i>A</i> , including the diagonal, is overwritten.
W	<b>REAL for ssyev</b> <b>DOUBLE PRECISION for dsyev</b> Array, <b>DIMENSION</b> at least $max(1, n)$ . If <i>info</i> = 0, contains the eigenvalues of the matrix A in ascending order.
work(1)	On exit, if <i>lwork</i> > 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = i, then the algorithm failed to converge; i indicates the number of elements of an intermediate tridiagonal form which did not converge to zero.</pre>

## **Application Notes**

For optimum performance use

 $lwork \ge (nb+2)*n$ ,

where *nb* is the blocksize for ?sytrd returned by ilaenv. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

## ?heev

Computes all eigenvalues and, optionally, eigenvectors of a Hermitian matrix.

call cheev ( jobz, uplo, n, a, lda, w, work, lwork, rwork, info )
call zheev ( jobz, uplo, n, a, lda, w, work, lwork, rwork, info )

## **Discussion**

This routine computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix *A*.

jobz	CHARACTER*1. Must be 'N' or 'V'. If $jobz = 'N'$ , then only eigenvalues are computed. If $jobz = 'V'$ , then eigenvalues and eigenvectors are computed.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , a stores the upper triangular part of A. If $uplo = 'L'$ , a stores the lower triangular part of A.
п	<b>INTEGER.</b> The order of the matrix $A$ ( $n \ge 0$ ).
a, work	COMPLEX for cheev DOUBLE COMPLEX for zheev Arrays: a(lda,*) is an array containing either upper or lower triangular part of the Hermitian matrix A, as specified by uplo. The second dimension of a must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, n)$ .

lwork	<b>INTEGER</b> . The dimension of the array work. Constraint: $lwork \ge max(1, 2n-1)$ . See Application notes for the suggested value of $lwork$ .
rwork	REAL for cheev DOUBLE PRECISION for zheev. Workspace array, DIMENSION at least max(1, 3n-2).
Output Para	meters
a	On exit, if <i>jobz</i> = 'V', then if <i>info</i> = 0, array <i>a</i> contains the orthonormal eigenvectors of the matrix <i>A</i> . If <i>jobz</i> = 'N', then on exit the lower triangle (if <i>uplo</i> = 'L') or the upper triangle (if <i>uplo</i> = 'U') of <i>A</i> , including the diagonal, is overwritten.
W	REAL for cheev DOUBLE PRECISION for zheev Array, DIMENSION at least $max(1, n)$ . If <i>info</i> = 0, contains the eigenvalues of the matrix A in ascending order.
work(1)	On exit, if <i>lwork</i> > 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = i, then the algorithm failed to converge; i indicates the number of elements of an intermediate tridiagonal form which did not converge to zero.</pre>

## **Application Notes**

For optimum performance use

 $lwork \ge (nb+1)*n,$ 

where *nb* is the blocksize for ?hetrd returned by ilaenv. If you are in doubt how much workspace to supply, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

# ?syevd

Computes all eigenvalues and (optionally) all eigenvectors of a real symmetric matrix using divide and conquer algorithm.

call ssyevd (job,uplo,n,a,lda,w,work,lwork,iwork,liwork,info)
call dsyevd (job,uplo,n,a,lda,w,work,lwork,iwork,liwork,info)

### **Discussion**

This routine computes all the eigenvalues, and optionally all the eigenvectors, of a real symmetric matrix *A*. In other words, it can compute the spectral factorization of *A* as:  $A = Z\Lambda Z^{T}$ .

Here  $\Lambda$  is a diagonal matrix whose diagonal elements are the eigenvalues  $\lambda_i$ , and Z is the orthogonal matrix whose columns are the eigenvectors  $z_i$ . Thus,

 $Az_i = \lambda_i z_i$  for i = 1, 2, ..., n.

If the eigenvectors are requested, then this routine uses a divide and conquer algorithm to compute eigenvalues and eigenvectors. However, if only eigenvalues are required, then it uses the Pal-Walker-Kahan variant of the QL or QR algorithm.

job	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , a stores the upper triangular part of A. If $uplo = 'L'$ , a stores the lower triangular part of A.
n	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .
a	REAL for ssyevd DOUBLE PRECISION for dsyevd Array, DIMENSION ( <i>1da</i> , *).

	<ul> <li>a (lda,*) is an array containing either upper or lower triangular part of the symmetric matrix A, as specified by uplo.</li> <li>The second dimension of a must be at least max(1, n).</li> </ul>
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, n)$ .
work	REAL for ssyevd DOUBLE PRECISION for dsyevd. Workspace array, DIMENSION at least <i>lwork</i> .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> . Constraints: if $n \le 1$ , then $1 \text{work} \ge 1$ ; if $job = 'N'$ and $n > 1$ , then $1 \text{work} \ge 2n+1$ ; if $job = 'V'$ and $n > 1$ , then $1 \text{work} \ge 3n^2 + (5+2k) * n+1$ , where k is the smallest integer which satisfies $2^k \ge n$ .
iwork	INTEGER. Workspace array, DIMENSION at least <i>liwork</i> .
liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . Constraints: if $n \le 1$ , then <i>liwork</i> $\ge 1$ ; if <i>job</i> = 'N' and $n > 1$ , then <i>liwork</i> $\ge 1$ ; if <i>job</i> = 'V' and $n > 1$ , then <i>liwork</i> $\ge 5n+2$ .

W	REAL for ssyevd
	DOUBLE PRECISION for dsyevd
	Array, DIMENSION at least $max(1, n)$ .
	If $info = 0$ , contains the eigenvalues of the matrix A in
	ascending order.
	See also info.
a	If $job = 'V'$ , then on exit this array is overwritten by the orthogonal matrix Z which contains the eigenvectors of A.

work(1)	On exit, if <i>lwork</i> > 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
iwork(1)	On exit, if <i>liwork</i> > 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = i$ , then the algorithm failed to converge; <i>i</i> indicates the number of elements of an intermediate tridiagonal form which did not converge to zero. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## **Application Notes**

The computed eigenvalues and eigenvectors are exact for a matrix T + E such that  $||E||_2 = O(\varepsilon) ||T||_2$ , where  $\varepsilon$  is the machine precision.

The complex analogue of this routine is <u>?heevd</u>.

## ?heevd

Computes all eigenvalues and (optionally) all eigenvectors of a complex Hermitian matrix using divide and conquer algorithm.

```
call cheevd (job, uplo, n, a, lda, w, work, lwork, rwork, lrwork,
iwork, liwork, info)
call zheevd (job, uplo, n, a, lda, w, work, lwork, rwork, lrwork,
iwork, liwork, info)
```

### **Discussion**

This routine computes all the eigenvalues, and optionally all the eigenvectors, of a complex Hermitian matrix *A*. In other words, it can compute the spectral factorization of *A* as:  $A = Z\Lambda Z^H$ . Here  $\Lambda$  is a real diagonal matrix whose diagonal elements are the eigenvalues  $\lambda_i$ , and *Z* is the (complex) unitary matrix whose columns are the eigenvectors  $z_i$ . Thus,

 $Az_i = \lambda_i z_i$  for i = 1, 2, ..., n.

If the eigenvectors are requested, then this routine uses a divide and conquer algorithm to compute eigenvalues and eigenvectors. However, if only eigenvalues are required, then it uses the Pal-Walker-Kahan variant of the QL or QR algorithm.

job	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , a stores the upper triangular part of A. If $uplo = 'L'$ , a stores the lower triangular part of A.
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .

a	COMPLEX for cheevd DOUBLE COMPLEX for zheevd Array, DIMENSION ( <i>lda</i> , *). <i>a</i> ( <i>lda</i> , *) is an array containing either upper or lower triangular part of the Hermitian matrix <i>A</i> , as specified by <i>uplo</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, n)$ .
work	COMPLEX for cheevd DOUBLE COMPLEX for zheevd. Workspace array, DIMENSION at least <i>lwork</i> .
lwork	<b>INTEGER.</b> The dimension of the array work. Constraints: if $n \le 1$ , then $lwork \ge 1$ ; if $job = 'N'$ and $n > 1$ , then $lwork \ge n+1$ ; if $job = 'V'$ and $n > 1$ , then $lwork \ge n^2+2n$
rwork	REAL for cheevd DOUBLE PRECISION for zheevd Workspace array, DIMENSION at least <i>lrwork</i> .
lrwork	<b>INTEGER.</b> The dimension of the array <i>rwork</i> . Constraints: if $n \le 1$ , then <i>lrwork</i> $\ge 1$ ; if <i>job</i> = 'N' and $n > 1$ , then <i>lrwork</i> $\ge n$ ; if <i>job</i> = 'V' and $n > 1$ , then <i>lrwork</i> $\ge 3n^2 + (4+2k) * n+1$ , where k is the smallest integer which satisfies $2^k \ge n$ .
iwork	INTEGER. Workspace array, DIMENSION at least <i>liwork</i> .
liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . Constraints: if $n \le 1$ , then $liwork \ge 1$ ; if $job =  N $ and $n > 1$ , then $liwork \ge 1$ ; if $job =  V $ and $n > 1$ , then $liwork \ge 5n+2$ .

W	REAL for cheevd DOUBLE PRECISION for zheevd Array, DIMENSION at least $max(1, n)$ . If <i>info</i> = 0, contains the eigenvalues of the matrix A in ascending order. See also <i>info</i> .
a	If $job = V'$ , then on exit this array is overwritten by the unitary matrix Z which contains the eigenvectors of A.
work(1)	On exit, if <i>lwork</i> > 0, then the real part of <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
rwork(1)	On exit, if <i>lrwork</i> > 0, then <i>rwork(1)</i> returns the required minimal size of <i>lrwork</i> .
iwork(1)	On exit, if <i>liwork</i> > 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = i$ , then the algorithm failed to converge; <i>i</i> indicates the number of elements of an intermediate tridiagonal form which did not converge to zero. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## **Application Notes**

The computed eigenvalues and eigenvectors are exact for a matrix A + E such that  $||E||_2 = O(\varepsilon) ||A||_2$ , where  $\varepsilon$  is the machine precision.

The real analogue of this routine is ?syevd.

See also <u>?hpevd</u> for matrices held in packed storage, and <u>?hbevd</u> for banded matrices.

# ?syevx

Computes selected eigenvalues and, optionally, eigenvectors of a symmetric matrix.

## **Discussion**

This routine computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix *A*. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

jobz	CHARACTER*1. Must be 'N' or 'V'. If $jobz = 'N'$ , then only eigenvalues are computed. If $jobz = 'V'$ , then eigenvalues and eigenvectors are computed.
range	CHARACTER*1. Must be 'A', 'V', or 'I'. If <i>range</i> = 'A', all eigenvalues will be found. If <i>range</i> = 'V', all eigenvalues in the half-open interval ( <i>v1</i> , <i>vu</i> ] will be found.
uplo	If <i>range</i> = 'I', the eigenvalues with indices <i>i</i> 1 through <i>iu</i> will be found. CHARACTER*1. Must be 'U' or 'L'. If <i>uplo</i> = 'U', <i>a</i> stores the upper triangular part of <i>A</i> . If <i>uplo</i> = 'L', <i>a</i> stores the lower triangular part of <i>A</i> .
n	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .

a, work	REAL for ssyevx DOUBLE PRECISION for dsyevx.
	<ul> <li>Arrays:</li> <li>a(lda,*) is an array containing either upper or lower triangular part of the symmetric matrix A, as specified by uplo.</li> <li>The second dimension of a must be at least max(1, n).</li> </ul>
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, n)$ .
vl, vu	REAL for ssyevx DOUBLE PRECISION for dsyevx. If <i>range</i> = 'V', the lower and upper bounds of the interval to be searched for eigenvalues; $v1 \le vu$ . Not referenced if <i>range</i> = 'A' or 'I'.
il, iu	<b>INTEGER.</b> If $range = 'I'$ , the indices of the smallest and largest eigenvalues to be returned. Constraints: $1 \le i1 \le iu \le n$ , if $n > 0$ ; i1 = 1 and $iu = 0$ , if $n = 0$ . Not referenced if $range = 'A'$ or 'V'.
abstol	<b>REAL for ssyevx</b> <b>DOUBLE PRECISION for dsyevx.</b> The absolute error tolerance for the eigenvalues . See <i>Application notes</i> for more information.
ldz	<b>INTEGER.</b> The first dimension of the output array $z$ ; $ldz \ge 1$ . If $jobz = V'$ , then $ldz \ge max(1,n)$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> . Constraint: $lwork \ge max(1, 8n)$ . See Application notes for the suggested value of $lwork$ .
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least $max(1, 5n)$ .

a	On exit, the lower triangle (if $uplo = 'L'$ ) or the upper triangle (if $uplo = 'U'$ ) of <i>A</i> , including the diagonal, is overwritten.
m	<b>INTEGER.</b> The total number of eigenvalues found; $0 \le n \le n$ . If $range = 'A', m = n$ , and if range = 'I', m = iu - il + 1.
W	<b>REAL for ssyevx</b> <b>DOUBLE PRECISION for dsyevx</b> Array, <b>DIMENSION</b> at least $max(1, n)$ . The first <i>m</i> elements contain the selected eigenvalues of the matrix <i>A</i> in ascending order.
Ζ	<b>REAL for ssyevx</b> <b>DOUBLE PRECISION for dsyevx.</b> Array $z(ldz, *)$ contains eigenvectors. The second dimension of $z$ must be at least max $(1, m)$ .
	If $jobz = 'V'$ , then if $info = 0$ , the first <i>m</i> columns of <i>z</i> contain the orthonormal eigenvectors of the matrix <i>A</i> corresponding to the selected eigenvalues, with the i-th column of <i>z</i> holding the eigenvector associated with <i>w</i> (i). If an eigenvector fails to converge, then that column of <i>z</i> contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in <i>ifail</i> . If <i>jobz</i> = 'N', then <i>z</i> is not referenced. Note: you must ensure that at least max(1, <i>m</i> ) columns are supplied in the array <i>z</i> ; if <i>range</i> = 'V', the exact value of <i>m</i> is not known in advance and an upper bound must be used.
work(1)	On exit, if <i>lwork</i> > 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
ifail	<b>INTEGER.</b> Array, <b>DIMENSION</b> at least $max(1, n)$ . If $jobz = 'V'$ , then if $info = 0$ , the first <i>m</i> elements of <i>ifail</i> are zero; if $info > 0$ , then <i>ifail</i> contains the indices of the eigenvectors that failed to converge. If $jobz = 'V'$ , then <i>ifail</i> is not referenced.

info

INTEGER.

If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value. If info = i, then *i* eigenvectors failed to converge; their indices are stored in the array *ifail*.

## **Application Notes**

For optimum performance use  $lwork \ge (nb+3)*n$ , where nb is the maximum of the blocksize for ?sytrd and ?ormtr returned by ilaenv. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to

 $abstol + \varepsilon * max(|a|,|b|)$ , where  $\varepsilon$  is the machine precision. If abstol is less than or equal to zero, then  $\varepsilon * |T|$  will be used in its place, where |T| is the 1-norm of the tridiagonal matrix obtained by reducing A to tridiagonal form.

Eigenvalues will be computed most accurately when *abstol* is set to twice the underflow threshold 2*slamch('S'), not zero. If this routine returns with *info* > 0, indicating that some eigenvectors did not converge, try setting *abstol* to 2*slamch('S').

## ?heevx

Computes selected eigenvalues and, optionally, eigenvectors of a Hermitian matrix.

#### **Discussion**

This routine computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix *A*. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then only eigenvalues are computed. If <i>jobz</i> = 'V', then eigenvalues and eigenvectors are computed.
range	CHARACTER*1. Must be 'A', 'V', or 'I'. If <i>range</i> = 'A', all eigenvalues will be found. If <i>range</i> = 'V', all eigenvalues in the half-open interval (v1, vu] will be found.
uplo	If <i>range</i> = 'I', the eigenvalues with indices <i>i</i> 1 through <i>iu</i> will be found. CHARACTER*1. Must be 'U' or 'L'. If <i>uplo</i> = 'U', <i>a</i> stores the upper triangular part of <i>A</i> . If <i>uplo</i> = 'L', <i>a</i> stores the lower triangular part of <i>A</i> .
n	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .

a, work	COMPLEX for cheevx
	DOUBLE COMPLEX for zheevx.
	Arrays: <b>a</b> ( <i>lda</i> , *) is an array containing either upper or lower triangular part of the Hermitian matrix <i>A</i> , as specified by <i>uplo</i> .
	The second dimension of a must be at least $max(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, n)$ .
vl, vu	REAL for cheevx DOUBLE PRECISION for zheevx. If $range = 'V'$ , the lower and upper bounds of the interval to be searched for eigenvalues; $vl \le vu$ . Not referenced if $range = 'A'$ or 'I'.
il, iu	INTEGER. If $range = 'I'$ , the indices of the smallest and largest eigenvalues to be returned. Constraints: $1 \le i1 \le iu \le n$ , if $n > 0$ ; i1 = 1 and $iu = 0$ , if $n = 0$ . Not referenced if $range = 'A'$ or 'V'.
abstol	REAL for cheevx DOUBLE PRECISION for zheevx. The absolute error tolerance for the eigenvalues . See <i>Application notes</i> for more information.
ldz	<b>INTEGER.</b> The first dimension of the output array $z$ ; $ldz \ge 1$ . If $jobz = V'$ , then $ldz \ge max(1,n)$ .
lwork	<b>INTEGER.</b> The dimension of the array work. Constraint: $lwork \ge max(1, 2n-1)$ . See Application notes for the suggested value of $lwork$ .
rwork	REAL for cheevx DOUBLE PRECISION for zheevx. Workspace array, DIMENSION at least $max(1, 7n)$ .
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least $max(1, 5n)$ .

a	On exit, the lower triangle (if $uplo = 'L'$ ) or the upper triangle (if $uplo = 'U'$ ) of A, including the diagonal, is overwritten.
m	<b>INTEGER.</b> The total number of eigenvalues found; $0 \le m \le n$ . If $range = 'A', m = n$ , and if range = 'I', m = iu - il + 1.
W	<b>REAL for cheevx</b> <b>DOUBLE PRECISION for zheevx</b> Array, <b>DIMENSION</b> at least $max(1, n)$ . The first <i>m</i> elements contain the selected eigenvalues of the matrix <i>A</i> in ascending order.
Ζ	COMPLEX for cheevx DOUBLE COMPLEX for zheevx. Array $z(ldz, *)$ contains eigenvectors. The second dimension of $z$ must be at least max $(1, m)$ .
	If $jobz = 'V'$ , then if $info = 0$ , the first <i>m</i> columns of <i>z</i> contain the orthonormal eigenvectors of the matrix <i>A</i> corresponding to the selected eigenvalues, with the i-th column of <i>z</i> holding the eigenvector associated with <i>w</i> (i). If an eigenvector fails to converge, then that column of <i>z</i> contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in <i>ifail</i> . If $jobz = 'N'$ , then <i>z</i> is not referenced. Note: you must ensure that at least max(1, <i>m</i> ) columns are supplied in the array <i>z</i> ; if <i>range</i> = 'V', the exact value of <i>m</i> is not known in advance and an upper bound must be used.
work(1)	On exit, if <i>lwork</i> > 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
ifail	<pre>INTEGER. Array, DIMENSION at least max(1, n). If jobz = 'V', then if info = 0, the first m elements of ifail are zero; if info &gt; 0, then ifail contains the indices of the eigenvectors that failed to converge. If jobz = 'V', then ifail is not referenced.</pre>

info

INTEGER.

If *info* = 0, the execution is successful. If *info* = -*i*, the *i*th parameter had an illegal value. If *info* = *i*, then *i* eigenvectors failed to converge; their indices are stored in the array *ifail*.

## **Application Notes**

For optimum performance use  $lwork \ge (nb+1)*n$ , where nb is the maximum of the blocksize for ?hetrd and ?unmtr returned by ilaenv. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to

 $abstol + \varepsilon * max(|a|,|b|)$ , where  $\varepsilon$  is the machine precision. If abstol is less than or equal to zero, then  $\varepsilon * |T|$  will be used in its place, where |T| is the 1-norm of the tridiagonal matrix obtained by reducing A to tridiagonal form.

Eigenvalues will be computed most accurately when *abstol* is set to twice the underflow threshold 2*slamch('S'), not zero. If this routine returns with *info* > 0, indicating that some eigenvectors did not converge, try setting *abstol* to 2*slamch('S').

# ?syevr

Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix using the Relatively Robust Representations.

#### **Discussion**

This routine computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix *T*. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

Whenever possible, ?syevr calls <u>sstegr/dstegr</u> to compute the eigenspectrum using Relatively Robust Representations. ?stegr computes eigenvalues by the *dqds* algorithm, while orthogonal eigenvectors are computed from various "good"  $LDL^T$  representations (also known as Relatively Robust Representations). Gram-Schmidt orthogonalization is avoided as far as possible. More specifically, the various steps of the algorithm are as follows. For the i-th unreduced block of *T*,

(a) Compute  $T - \mathbf{q} = L_i D_i L_i^T$ , such that  $L_i D_i L_i^T$  is a relatively robust representation;

(b) Compute the eigenvalues,  $\lambda_j$ , of  $L_i D_i L_i^T$  to high relative accuracy by the *dqds* algorithm;

(c) If there is a cluster of close eigenvalues, "choose"  $\sigma_i$  close to the cluster, and go to step (a);

(d) Given the approximate eigenvalue  $\lambda_j$  of  $L_i D_i L_i^T$ , compute the corresponding eigenvector by forming a rank-revealing twisted factorization.

The desired accuracy of the output can be specified by the input parameter *abstol*.

The routine <code>?syevr</code> calls <code>sstegr/dstegr</code> when the full spectrum is requested on machines which conform to the IEEE-754 floating point standard. <code>?syevr</code> calls <code>sstebz/dstebz</code> and <code>sstein/dstein</code> on non-IEEE machines and when partial spectrum requests are made.

jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then only eigenvalues are computed. If <i>jobz</i> = 'V', then eigenvalues and eigenvectors are computed.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'. If <i>range</i> = 'A', the routine computes all eigenvalues. If <i>range</i> = 'V', the routine computes eigenvalues $\lambda_i$ in the half-open interval: $vl < \lambda_i \le vu$ . If <i>range</i> = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
	For <i>range</i> = 'V'or 'I' and <i>iu-il &lt; n-1</i> , sstebz/dstebz and sstein/dstein are called.
п	<b>INTEGER.</b> The order of the matrix $A$ ( $n \ge 0$ ).
a, work	REAL for ssyevr DOUBLE PRECISION for dsyevr. Arrays: a(lda,*) is an array containing either upper or lower triangular part of the symmetric matrix A, as specified by uplo. The second dimension of a must be at least max(1, n).
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, n)$ .

vl, vu	REAL for ssyevr DOUBLE PRECISION for dsyevr. If range = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: v1< vu.
	If $range = 'A'$ or 'I', vl and vu are not referenced.
il, iu	INTEGER. If $range =  \mathbf{I} $ , the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le i1 \le iu \le n$ , if $n > 0$ ; $i1=1$ and $iu=0$ if $n = 0$ .
	If $range = 'A'$ or 'V', <i>il</i> and <i>iu</i> are not referenced.
abstol	<b>REAL</b> for ssyevr <b>DOUBLE PRECISION</b> for dsyevr. The absolute error tolerance to which each eigenvalue/eigenvector is required. If $jobz = 'V'$ , the eigenvalues and eigenvectors output have residual norms bounded by <i>abstol</i> , and the dot products between different eigenvectors are bounded by $abstol.Ifabstol < n\varepsilon    T  _1$ , then $n\varepsilon    T  _1$ will be used in its place, where $\varepsilon$ is the machine precision. The eigenvalues are computed to an accuracy of $\varepsilon    T  _1$ irrespective of $abstol$ . If high relative accuracy is important, set $abstol$ to ?lamch('S').
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ . Constraints: $ldz \ge 1$ if $jobz = 'N'$ ; $ldz \ge max(1, n)$ if $jobz = 'V'$ .
lwork	<b>INTEGER.</b> The dimension of the array work. Constraint: $lwork \ge max(1, 26n)$ . See Application notes for the suggested value of $lwork$ .
iwork	INTEGER. Workspace array, DIMENSION ( <i>liwork</i> ).
liwork	<b>INTEGER</b> . The dimension of the array <i>iwork</i> , <i>lwork</i> $\ge$ max(1, 10 <i>n</i> ).

a	On exit, the lower triangle (if $uplo = 'L'$ ) or the upper triangle (if $uplo = 'U'$ ) of <i>A</i> , including the diagonal, is overwritten.
m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', m = iu - il + 1.
W, Z	<pre>REAL for ssyevr DOUBLE PRECISION for dsyevr. Arrays: w(*), DIMENSION at least max(1, n), contains the selected eigenvalues in ascending order, stored in w(1) to w(m);</pre>
	z(ldz, *), the second dimension of z must be at least max(1, m). If $jobz = 'V'$ , then if $info = 0$ , the first m columns of z contain the orthonormal eigenvectors of the matrix T corresponding to the selected eigenvalues, with the <i>i</i> -th column of z holding the eigenvector associated with $w(i)$ . If $jobz = 'N'$ , then z is not referenced. Note: you must ensure that at least max(1,m) columns are supplied in the array z; if $range = 'V'$ , the exact value of m is not known in advance and an upper bound must be used.
isuppz	INTEGER. Array, DIMENSION at least $2 * \max(1, m)$ . The support of the sign protocology in $-i$ is the indices
	The support of the eigenvectors in z, i.e., the indices indicating the nonzero elements in z. The <i>i</i> -th eigenvector is nonzero only in elements $isuppz(2i-1)$ through $isuppz(2i)$ . Implemented only for range ='A' or 'I' and iu-il = n-1.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .

iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , an internal error has occurred.

## **Application Notes**

For optimum performance use  $lwork \ge (nb+6)*n$ , where nb is the maximum of the blocksize for ?sytrd and ?ormtr returned by ilaenv. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

Normal execution of **?stegr** may create NaNs and infinities and hence may abort due to a floating point exception in environments which do not handle NaNs and infinities in the IEEE standard default manner.

## ?heevr

Computes selected eigenvalues and, optionally, eigenvectors of a Hermitian matrix using the Relatively Robust Representations.

```
call cheevr ( jobz, range, uplo, n, a, lda, vl, vu, il, iu, abstol,
    m, w, z, ldz, isuppz, work, lwork, rwork, lrwork,
    iwork, liwork, info)
call zheevr ( jobz, range, uplo, n, a, lda, vl, vu, il, iu, abstol,
    m, w, z, ldz, isuppz, work, lwork, rwork, lrwork,
    iwork, liwork, info)
```

### **Discussion**

This routine computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix *T*. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

Whenever possible, ?heevr calls <u>cstegr/zstegr</u> to compute the eigenspectrum using Relatively Robust Representations. ?stegr computes eigenvalues by the *dqds* algorithm, while orthogonal eigenvectors are computed from various "good"  $LDL^T$  representations (also known as Relatively Robust Representations). Gram-Schmidt orthogonalization is avoided as far as possible. More specifically, the various steps of the algorithm are as follows. For the i-th unreduced block of *T*,

(a) Compute  $T - \mathbf{q} = L_i D_i L_i^T$ , such that  $L_i D_i L_i^T$  is a relatively robust representation;

(b) Compute the eigenvalues,  $\lambda_j$ , of  $L_i D_i L_i^T$  to high relative accuracy by the *dqds* algorithm;

(c) If there is a cluster of close eigenvalues, "choose"  $\sigma_1$  close to the cluster, and go to step (a);

(d) Given the approximate eigenvalue  $\lambda_j$  of  $L_i D_i L_i^T$ , compute the corresponding eigenvector by forming a rank-revealing twisted factorization.

The desired accuracy of the output can be specified by the input parameter *abstol*.

The routine ?heevr calls <u>cstegr/zstegr</u> when the full spectrum is requested on machines which conform to the IEEE-754 floating point standard. ?heevr calls <u>sstebz/dstebz</u> and <u>cstein/zstein</u> on non-IEEE machines and when partial spectrum requests are made.

jobz	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'. If <i>range</i> = 'A', the routine computes all eigenvalues. If <i>range</i> = 'V', the routine computes eigenvalues $\lambda_i$ in the half-open interval: $vl < \lambda_i \leq vu$ . If <i>range</i> = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
	For <i>range</i> = 'V'or 'I', sstebz/dstebz and cstein/zstein are called.
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
a, work	COMPLEX for cheevr DOUBLE COMPLEX for zheevr. Arrays: a(lda,*) is an array containing either upper or lower triangular part of the Hermitian matrix A, as specified by uplo. The second dimension of a must be at least max(1, n).
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, n)$ .

vl, vu	REAL for cheevr DOUBLE PRECISION for zheevr. If <i>range</i> = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: v1< vu.
	If $range = 'A'$ or 'I', vl and vu are not referenced.
il, iu	INTEGER. If $range =  I $ , the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le i1 \le iu \le n$ , if $n > 0$ ; $i1=1$ and $iu=0$ if $n = 0$ .
	If <b>range</b> = 'A' or 'V', <b>il</b> and <b>iu</b> are not referenced.
abstol	<b>REAL</b> for cheevr <b>DOUBLE PRECISION</b> for zheevr. The absolute error tolerance to which each eigenvalue/eigenvector is required. If $jobz = 'V'$ , the eigenvalues and eigenvectors output have residual norms bounded by <i>abstol</i> , and the dot products between different eigenvectors are bounded by <i>abstol</i> .If <i>abstol</i> < $n\varepsilon    T   _1$ , then $n\varepsilon    T   _1$ willbeused in its place, where $\varepsilon$ is the machine precision. The eigenvalues are computed to an accuracy of $\varepsilon    T   _1$ irrespective of <i>abstol</i> . If high relative accuracy is important, set <i>abstol</i> to ?lamch('S').
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ . Constraints: $ldz \ge 1$ if $jobz = 'N'$ ; $ldz \ge max(1, n)$ if $jobz = 'V'$ .
lwork	<b>INTEGER.</b> The dimension of the array work. Constraint: $lwork \ge max(1, 2n)$ . See Application notes for the suggested value of $lwork$ .
rwork	REAL for cheevr DOUBLE PRECISION for zheevr. Workspace array, DIMENSION ( <i>lrwork</i> ).

lrwork	<b>INTEGER.</b> The dimension of the array <i>rwork</i> ; <i>lwork</i> $\ge \max(1, 24n)$ .
iwork	INTEGER. Workspace array, DIMENSION (liwork).
liwork	<b>INTEGER</b> . The dimension of the array <i>iwork</i> , $lwork \ge max(1, 10n)$ .

a	On exit, the lower triangle (if $uplo = 'L'$ ) or the upper triangle (if $uplo = 'U'$ ) of <i>A</i> , including the diagonal, is overwritten.
m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If $range = 'A', m = n$ , and if $range = 'I'$ , m = iu - il + 1.
W	REAL for cheevr DOUBLE PRECISION for zheevr. Array, DIMENSION at least max $(1, n)$ , contains the selected eigenvalues in ascending order, stored in $w(1)$ to $w(m)$ .
Ζ	COMPLEX for cheevr DOUBLE COMPLEX for zheevr. Array $z(ldz, *)$ ; the second dimension of $z$ must be at least max $(1, m)$ . If $jobz = 'V'$ , then if $info = 0$ , the first $m$ columns of $z$ contain the orthonormal eigenvectors of the matrix $T$ corresponding to the selected eigenvalues, with the <i>i</i> -th column of $z$ holding the eigenvector associated with w(i). If $jobz = 'N'$ , then $z$ is not referenced. Note: you must ensure that at least max $(1,m)$ columns are supplied in the array $z$ ; if $range = 'V'$ , the exact
	value of $m$ is not known in advance and an upper bound must be used.
isuppz	INTEGER. Array, DIMENSION at least 2*max(1, m).

	The support of the eigenvectors in <i>z</i> , i.e., the indices indicating the nonzero elements in <i>z</i> . The <i>i</i> -th eigenvector is nonzero only in elements <i>isuppz</i> (2 <i>i</i> -1) through <i>isuppz</i> (2 <i>i</i> ).
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
rwork(1)	On exit, if <i>info</i> = 0, then <i>rwork(1)</i> returns the required minimal size of <i>lrwork</i> .
iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , an internal error has occurred.

### **Application Notes**

For optimum performance use  $lwork \ge (nb+1)*n$ , where nb is the maximum of the blocksize for ?hetrd and ?unmtr returned by ilaenv. If you are in doubt how much workspace to supply, use a generous value of lwork for the first run. On exit, examine work(1) and use this value for subsequent runs.

Normal execution of **?stegr** may create NaNs and infinities and hence may abort due to a floating point exception in environments which do not handle NaNs and infinities in the IEEE standard default manner.

# ?spev

Computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix in packed storage.

call sspev (jobz, uplo, n, ap, w, z, ldz, work, info)
call dspev (jobz, uplo, n, ap, w, z, ldz, work, info)

## **Discussion**

This routine computes all the eigenvalues and, optionally, eigenvectors of a real symmetric matrix *A* in packed storage.

jobz	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , $ap$ stores the packed upper triangular part of $A$ . If $uplo = 'L'$ , $ap$ stores the packed lower triangular part of $A$ .
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
ap,work	<b>REAL</b> for sspev <b>DOUBLE PRECISION</b> for dspev Arrays: ap(*) contains the packed upper or lower triangle of symmetric matrix A, as specified by <i>uplo</i> . The dimension of <i>ap</i> must be at least max(1, $n*(n+1)/2$ ). <i>work</i> (*) is a workspace array, <b>DIMENSION</b> at least max(1, 3 <i>n</i> ).

ldz

<b>INTEGER</b> . The leading dimension of the output array <i>z</i> .
Constraints:
if $jobz = 'N'$ , then $ldz \ge 1$ ;
if $jobz = V'$ , then $ldz \ge max(1, n)$ .

## **Output Parameters**

Output Parame	
W,Z	REAL for sspev
	DOUBLE PRECISION for dspev
	Arrays:
	w(*), DIMENSION at least max $(1, n)$ .
	If $info = 0$ , w contains the eigenvalues of the matrix A
	in ascending order.
	z(ldz, *). The second dimension of z must be at least $max(1, n)$ .
	If $jobz = 'V'$ , then if $info = 0$ , $z$ contains the orthonormal eigenvectors of the matrix $A$ , with the <i>i</i> -th column of $z$ holding the eigenvector associated with $w(i)$ .
	If $jobz = 'N'$ , then z is not referenced.
ap	On exit, this array is overwritten by the values generated during the reduction to tridiagonal form. The elements of the diagonal and the off-diagonal of the tridiagonal matrix overwrite the corresponding elements of A.
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = i, then the algorithm failed to converge; i indicates the number of elements of an intermediate</pre>

tridiagonal form which did not converge to zero.

# ?hpev

Computes all eigenvalues and, optionally, eigenvectors of a Hermitian matrix in packed storage.

call chpev (jobz, uplo, n, ap, w, z, ldz, work, rwork, info)
call zhpev (jobz, uplo, n, ap, w, z, ldz, work, rwork, info)

## **Discussion**

This routine computes all the eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix *A* in packed storage.

jobz	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are
uplo	computed. CHARACTER*1. Must be 'U' or 'L'. If <i>uplo</i> = 'U', <i>ap</i> stores the packed upper triangular part of <i>A</i> . If <i>uplo</i> = 'L', <i>ap</i> stores the packed lower triangular part of <i>A</i> .
n	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .
ap,work	COMPLEX for chpev DOUBLE COMPLEX for zhpev. Arrays: ap(*) contains the packed upper or lower triangle of Hermitian matrix A, as specified by $uplo$ . The dimension of $ap$ must be at least max $(1, n*(n+1)/2)$ . work(*) is a workspace array, DIMENSION at least max $(1, 2n-1)$ .

ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ .
	Constraints:
	if $jobz = 'N'$ , then $1dz \ge 1$ ;
	if $jobz = V'$ , then $ldz \ge max(1, n)$ .
rwork	REAL for chpev
	DOUBLE PRECISION for zhpev.
	Workspace array, DIMENSION at least $max(1, 3n-2)$ .

W	REAL for chpev DOUBLE PRECISION for zhpev. Array, DIMENSION at least $max(1, n)$ . If <i>info</i> = 0, <i>w</i> contains the eigenvalues of the matrix <i>A</i> in ascending order.
Ζ	COMPLEX for chpev DOUBLE COMPLEX for zhpev. Array $z(ldz, *)$ . The second dimension of $z$ must be at least max $(1, n)$ . If $jobz = 'V'$ , then if $info = 0$ , $z$ contains the orthonormal eigenvectors of the matrix $A$ , with the <i>i</i> -th column of $z$ holding the eigenvector associated with w(i). If $jobz = 'N'$ , then $z$ is not referenced.
ap	On exit, this array is overwritten by the values generated during the reduction to tridiagonal form. The elements of the diagonal and the off-diagonal of the tridiagonal matrix overwrite the corresponding elements of A.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , then the algorithm failed to converge; <i>i</i> indicates the number of elements of an intermediate

tridiagonal form which did not converge to zero.

# ?spevd

Uses divide and conquer algorithm to compute all eigenvalues and (optionally) all eigenvectors of a real symmetric matrix held in packed storage.

call sspevd (job,uplo,n,ap,w,z,ldz,work,lwork,iwork,liwork,info)
call dspevd (job,uplo,n,ap,w,z,ldz,work,lwork,iwork,liwork,info)

### **Discussion**

This routine computes all the eigenvalues, and optionally all the eigenvectors, of a real symmetric matrix *A* (held in packed storage). In other words, it can compute the spectral factorization of *A* as:  $A = Z\Lambda Z^T$ . Here  $\Lambda$  is a diagonal matrix whose diagonal elements are the eigenvalues  $\lambda_i$ , and *Z* is the orthogonal matrix whose columns are the eigenvectors  $z_i$ . Thus,

 $Az_i = \lambda_i z_i$  for i = 1, 2, ..., n.

If the eigenvectors are requested, then this routine uses a divide and conquer algorithm to compute eigenvalues and eigenvectors. However, if only eigenvalues are required, then it uses the Pal-Walker-Kahan variant of the QL or QR algorithm.

job	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , $ap$ stores the packed upper triangular part of $A$ .
	If $uplo = 'L'$ , ap stores the packed lower triangular part of A.
n	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .

ap,work	REAL for sspevd DOUBLE PRECISION for dspevd Arrays: ap(*) contains the packed upper or lower triangle of symmetric matrix A, as specified by uplo. The
	dimension of ap must be at least $max(1, n*(n+1)/2)$ work(*) is a workspace array, DIMENSION at least <i>lwork</i> .
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ . Constraints: if $job = 'N'$ , then $ldz \ge 1$ ; if $job = 'V'$ , then $ldz \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> . Constraints: if $n \le 1$ , then $lwork \ge 1$ ; if $job = 'N'$ and $n > 1$ , then $lwork \ge 2n$ ; if $job = 'V'$ and $n > 1$ , then $lwork \ge 2n^2 + (5+2k) * n+1$ , where k is the smallest integer which satisfies $2^k \ge n$ . If $lwork = -1$ , then a workspace query is assumed; the routine only calculates the optimal size of the <i>work</i> array, returns this value as the first entry of the <i>work</i> array, and no error message related to <i>lwork</i> is issued by xerbla.
iwork	INTEGER. Workspace array, DIMENSION at least <i>liwork</i> .
liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . Constraints: if $n \le 1$ , then <i>liwork</i> $\ge 1$ ; if <i>job</i> = 'N' and $n > 1$ , then <i>liwork</i> $\ge 1$ ; if <i>job</i> = 'V' and $n > 1$ , then <i>liwork</i> $\ge 5n+3$ . If <i>liwork</i> = -1, then a workspace query is assumed; the routine only calculates the optimal size of the <i>iwork</i> array, returns this value as the first entry of the <i>iwork</i> array, and no error message related to <i>liwork</i> is issued by xerbla.

W,Z	REAL for sspevd
	DOUBLE PRECISION for dspevd
	Arrays:
	w(*), DIMENSION at least max $(1, n)$ .
	If <i>info</i> = 0, contains the eigenvalues of the matrix A in ascending order. See also <i>info</i> .
	z(1dz, *). The second dimension of z must be:
	at least 1 if $job = 'N'$ ;
	at least $\max(1, n)$ if $job = 'V'$ .
	If $job = 'V'$ , then this array is overwritten by the orthogonal matrix Z which contains the eigenvectors of A. If $job = 'N'$ , then z is not referenced.
ap	On exit, this array is overwritten by the values generated during the reduction to tridiagonal form. The elements of the diagonal and the off-diagonal of the tridiagonal matrix overwrite the corresponding elements of A.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the optimal <i>lwork</i> .
iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the optimal <i>liwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = i$ , then the algorithm failed to converge; <i>i</i> indicates the number of elements of an intermediate tridiagonal form which did not converge to zero. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## **Application Notes**

The computed eigenvalues and eigenvectors are exact for a matrix T + E such that  $||E||_2 = O(\varepsilon) ||T||_2$ , where  $\varepsilon$  is the machine precision.

The complex analogue of this routine is ?hpevd.

See also <u>?syevd</u> for matrices held in full storage, and <u>?sbevd</u> for banded matrices.

# ?hpevd

Uses divide and conquer algorithm to compute all eigenvalues and (optionally) all eigenvectors of a complex Hermitian matrix held in packed storage.

### **Discussion**

This routine computes all the eigenvalues, and optionally all the eigenvectors, of a complex Hermitian matrix *A* (held in packed storage). In other words, it can compute the spectral factorization of *A* as:  $A = Z\Lambda Z^H$ . Here  $\Lambda$  is a real diagonal matrix whose diagonal elements are the eigenvalues  $\lambda_i$ , and *Z* is the (complex) unitary matrix whose columns are the eigenvectors  $z_i$ . Thus,

 $Az_i = \lambda_i z_i$  for i = 1, 2, ..., n.

If the eigenvectors are requested, then this routine uses a divide and conquer algorithm to compute eigenvalues and eigenvectors. However, if only eigenvalues are required, then it uses the Pal-Walker-Kahan variant of the QL or QR algorithm.

job	CHARACTER*1. Must be 'N' or 'V'.
	If $job = 'N'$ , then only eigenvalues are computed.
	If $job = V'$ , then eigenvalues and eigenvectors are
	computed.
uplo	CHARACTER*1. Must be 'U' or 'L'.

	If $uplo = 'U'$ , $ap$ stores the packed upper triangular part of $A$ . If $uplo = 'L'$ , $ap$ stores the packed lower triangular part of $A$ .
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
ap,work	COMPLEX for chpevd DOUBLE COMPLEX for zhpevd Arrays:
	ap(*) contains the packed upper or lower triangle of Hermitian matrix A, as specified by $uplo$ . The dimension of $ap$ must be at least max $(1, n*(n+1)/2)$ work(*) is a workspace array, DIMENSION at least <i>lwork</i> .
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ . Constraints: if $job = 'N'$ , then $ldz \ge 1$ ; if $job = 'V'$ , then $ldz \ge max(1, n)$ .
lwork	INTEGER. The dimension of the array work. Constraints: if $n \le 1$ , then $lwork \ge 1$ ; if $job = 'N'$ and $n > 1$ , then $lwork \ge n$ ; if $job = 'V'$ and $n > 1$ , then $lwork \ge 2n$
rwork	REAL for chpevd DOUBLE PRECISION for zhpevd Workspace array, DIMENSION at least <i>lrwork</i> .
lrwork	INTEGER. The dimension of the array <i>rwork</i> . Constraints: if $n \le 1$ , then <i>lrwork</i> $\ge 1$ ; if <i>job</i> = 'N' and $n > 1$ , then <i>lrwork</i> $\ge n$ ; if <i>job</i> = 'V' and $n > 1$ , then <i>lrwork</i> $\ge 3n^2 + (4+2k) * n+1$ , where k is the smallest integer which satisfies $2^k \ge n$ .
iwork	INTEGER. Workspace array, DIMENSION at least <i>liwork</i> .

**INTEGER**. The dimension of the array *iwork*. liwork Constraints: if  $n \leq 1$ , then  $liwork \geq 1$ : if job = 'N' and n > 1, then  $liwork \ge 1$ ; if job = V' and n > 1, then  $liwork \ge 5n+2$ . **Output Parameters** REAL for chpevd W DOUBLE PRECISION for zhpevd Array, DIMENSION at least max(1, n). If *info* = 0, contains the eigenvalues of the matrix A in ascending order. See also *info*. COMPLEX for chpevd  $\mathbf{z}$ DOUBLE COMPLEX for zhpevd Array, **DIMENSION** (*ldz*, *). The second dimension of z must be: at least 1 if iob = 'N': at least max(1, n) if job = V'. If job = V', then this array is overwritten by the unitary matrix Z which contains the eigenvectors of A. If job = 'N', then z is not referenced. On exit, this array is overwritten by the values generated ap during the reduction to tridiagonal form. The elements of the diagonal and the off-diagonal of the tridiagonal matrix overwrite the corresponding elements of A.

- work(1) On exit, if lwork > 0, then the real part of work(1)
  returns the required minimal size of lwork.
  rwork(1) On exit, if lrwork > 0, then rwork(1) returns the
  required minimal size of lrwork.
  iwork(1) On exit, if liwork > 0, then iwork(1) returns the
  - required minimal size of *liwork*. INTEGER. If *info* = 0, the execution is successful.

If info = i, then the algorithm failed to converge; *i* 

info

indicates the number of elements of an intermediate tridiagonal form which did not converge to zero. If info = -i, the *i*th parameter had an illegal value.

## **Application Notes**

The computed eigenvalues and eigenvectors are exact for a matrix T + E such that  $||E||_2 = O(\varepsilon) ||T||_2$ , where  $\varepsilon$  is the machine precision.

The real analogue of this routine is <u>?spevd</u>.

See also <u>?heevd</u> for matrices held in full storage, and <u>?hbevd</u> for banded matrices.

## ?spevx

Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix in packed storage.

## **Discussion**

This routine computes selected eigenvalues and, optionally, eigenvectors of a real symmetric matrix *A* in packed storage. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

jobz	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'. If <i>range</i> = 'A', the routine computes all eigenvalues. If <i>range</i> = 'V', the routine computes eigenvalues $\lambda_i$ in the half-open interval: $v1 < \lambda_i \leq vu$ .
	If <i>range</i> = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , $ap$ stores the packed upper triangular part of A. If $uplo = 'L'$ , $ap$ stores the packed lower triangular part of A.
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .

ap, work	<b>REAL for sspevx</b> <b>DOUBLE PRECISION for dspevx</b> Arrays: ap(*) contains the packed upper or lower triangle of the symmetric matrix A, as specified by $uplo$ . The dimension of $m_{1}$ must be at least $max(1 - t(-t))(2)$
	dimension of <i>ap</i> must be at least $max(1, n*(n+1)/2)$ . <i>work(*)</i> is a workspace array, DIMENSION at least $max(1, 8n)$ .
vl, vu	REAL for sspevx DOUBLE PRECISION for dspevx If range = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: vl< vu. If range = 'A' or 'I', vl and vu are not referenced.
il, iu	<b>INTEGER.</b> If <i>range</i> = 'I', the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le i \le i \le n$ , if $n > 0$ ; $i \le 1 = 1$ and $i \le 0$ if $n = 0$ . If <i>range</i> = 'A' or 'V', <i>i</i> s and <i>i</i> s are not referenced.
abstol	REAL for sspevx DOUBLE PRECISION for dspevx The absolute error tolerance to which each eigenvalue is required. See <i>Application notes</i> for details on error tolerance.
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ . Constraints: if $jobz = 'N'$ , then $ldz \ge 1$ ; if $jobz = 'V'$ , then $ldz \ge max(1, n)$ .
iwork	<b>INTEGER</b> . Workspace array, <b>DIMENSION</b> at least max(1, 5 <i>n</i> ).

## **Output Parameters**

ap	On exit, this array is overwritten by the values generated during the reduction to tridiagonal form. The elements of the diagonal and the off-diagonal of the tridiagonal matrix overwrite the corresponding elements of <i>A</i> .
m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', m = iu - il + 1.
W, Ζ	REAL for sspevx DOUBLE PRECISION for dspevx Arrays: w(*), DIMENSION at least max $(1, n)$ . If $info = 0$ , contains the selected eigenvalues of the matrix A in ascending order. z(ldz,*). The second dimension of z must be at least max $(1, m)$ . If $jobz = 'V'$ , then if $info = 0$ , the first m columns of z contain the orthonormal eigenvectors of the matrix A corresponding to the selected eigenvalues, with the <i>i</i> -th column of z holding the eigenvector associated with w(i). If an eigenvector fails to converge, then that column of z contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in <i>ifail</i> . If $jobz = 'N'$ , then z is not referenced. Note: you must ensure that at least max $(1,m)$ columns are supplied in the array z; if $range = 'V'$ , the exact value of m is not known in advance and an upper bound must be used.
ifail	INTEGER. Array, DIMENSION at least max $(1, n)$ . If <i>jobz</i> = 'V', then if <i>info</i> = 0, the first <i>m</i> elements of <i>ifail</i> are zero; if <i>info</i> > 0, the <i>ifail</i> contains the indices the eigenvectors that failed to converge.

If *jobz* = 'N', then *ifail* is not referenced.

info

INTEGER.

If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value. If info = i, then *i* eigenvectors failed to converge; their indices are stored in the array *ifail*.

### **Application Notes**

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to  $abstol + \varepsilon * max(|a|,|b|)$ , where  $\varepsilon$  is the machine precision. If abstol is less than or equal to zero, then  $\varepsilon * ||T/|_1$  will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when abstol is set to twice the underflow threshold 2*?lamch('S'), not zero. If this routine returns with info > 0, indicating that some eigenvectors did not converge, try setting abstol to 2*?lamch('S').

## ?hpevx

Computes selected eigenvalues and, optionally, eigenvectors of a Hermitian matrix in packed storage.

### **Discussion**

This routine computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix *A* in packed storage. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

jobz	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'. If <i>range</i> = 'A', the routine computes all eigenvalues. If <i>range</i> = 'V', the routine computes eigenvalues $\lambda_i$ in the half-open interval: $v1 < \lambda_i \leq vu$ .
	If <i>range</i> = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , $ap$ stores the packed upper triangular part of A. If $uplo = 'L'$ , $ap$ stores the packed lower triangular part of A.
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .

ap, work	COMPLEX for chpevx DOUBLE COMPLEX for zhpevx Arrays: ap(*) contains the packed upper or lower triangle of the Hermitian matrix A, as specified by $uplo$ . The dimension of $ap$ must be at least max $(1, n*(n+1)/2)$ .
	work(*) is a workspace array, DIMENSION at least $max(1, 2n)$ .
vl, vu	REAL for chpevx DOUBLE PRECISION for zhpevx If range = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: v1< vu. If range = 'A' or 'I', v1 and vu are not referenced.
il, iu	INTEGER. If <i>range</i> = 'I', the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le i1 \le iu \le n$ , if $n > 0$ ; $i1=1$ and $iu=0$ if $n = 0$ . If <i>range</i> = 'A' or 'V', <i>i1</i> and <i>iu</i> are not referenced.
abstol	REAL for chpevx DOUBLE PRECISION for zhpevx The absolute error tolerance to which each eigenvalue is required. See <i>Application notes</i> for details on error tolerance.
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ . Constraints: if $jobz = 'N'$ , then $ldz \ge 1$ ; if $jobz = 'V'$ , then $ldz \ge max(1, n)$ .
rwork	REAL for chpevx DOUBLE PRECISION for zhpevx Workspace array, DIMENSION at least max(1, 7n).
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least $max(1, 5n)$ .

ap	On exit, this array is overwritten by the values generated during the reduction to tridiagonal form. The elements of the diagonal and the off-diagonal of the tridiagonal matrix overwrite the corresponding elements of <i>A</i> .
m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If <i>range</i> = 'A', <i>m</i> = <i>n</i> , and if <i>range</i> = 'I', m = iu - il + 1.
W	REAL for chpevx DOUBLE PRECISION for zhpevx Array, DIMENSION at least $max(1, n)$ . If <i>info</i> = 0, contains the selected eigenvalues of the matrix A in ascending order.
Ζ	COMPLEX for chpevx DOUBLE COMPLEX for zhpevx Array $z(ldz, *)$ . The second dimension of $z$ must be at least max $(1, m)$ . If $jobz = 'V'$ , then if $info = 0$ , the first $m$ columns of $z$ contain the orthonormal eigenvectors of the matrix $A$ corresponding to the selected eigenvalues, with the <i>i</i> -th column of $z$ holding the eigenvector associated with w(i). If an eigenvector fails to converge, then that column of $z$ contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in <i>ifail</i> . If $jobz = 'N'$ , then $z$ is not referenced. Note: you must ensure that at least max $(1,m)$ columns are supplied in the array $z$ ; if $range = 'V'$ , the exact value of $m$ is not known in advance and an upper bound must be used.
ifail	<pre>INTEGER. Array, DIMENSION at least max(1, n). If jobz = 'V', then if info = 0, the first m elements of ifail are zero; if info &gt; 0, the ifail contains the indices the eigenvectors that failed to converge. If jobz = 'N', then ifail is not referenced.</pre>

info

INTEGER.

If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value. If info = i, then *i* eigenvectors failed to converge; their indices are stored in the array *ifail*.

### **Application Notes**

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to  $abstol + \varepsilon * max(|a|,|b|)$ , where  $\varepsilon$  is the machine precision. If abstol is less than or equal to zero, then  $\varepsilon * ||T/|_1$  will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when abstol is set to twice the underflow threshold 2*?lamch('S'), not zero. If this routine returns with info > 0, indicating that some eigenvectors did not converge, try setting abstol to 2*?lamch('S').

## ?sbev

Computes all eigenvalues and, optionally, eigenvectors of a real symmetric band matrix.

```
call ssbev (jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, info)
call dsbev (jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, info)
```

### **Discussion**

This routine computes all eigenvalues and, optionally, eigenvectors of a real symmetric band matrix *A*.

jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then only eigenvalues are computed. If <i>jobz</i> = 'V', then eigenvalues and eigenvectors are computed.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , $ab$ stores the upper triangular part of $A$ . If $uplo = 'L'$ , $ab$ stores the lower triangular part of $A$ .
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
kd	<b>INTEGER.</b> The number of super- or sub-diagonals in $A$ ( $kd \ge 0$ ).
ab, work	<pre>REAL for ssbev DOUBLE PRECISION for dsbev. Arrays: ab (1dab,*) is an array containing either upper or lower triangular part of the symmetric matrix A (as specified by uplo) in band storage format. The second dimension of ab must be at least max(1, n). work (*) is a workspace array. The dimension of work must be at least max(1, 3n-2).</pre>

ldab	<b>INTEGER.</b> The leading dimension of <i>ab</i> ; must be at
	least $kd$ +1.
ldz	<b>INTEGER</b> . The leading dimension of the output array $z$ .
	Constraints:
	if $jobz = 'N'$ , then $ldz \ge 1$ ;
	if $jobz = V'$ , then $ldz \ge max(1, n)$ .

W , Z	<pre>REAL for ssbev DOUBLE PRECISION for dsbev Arrays: w(*), DIMENSION at least max(1, n). If info = 0, contains the eigenvalues of the matrix A in ascending order.</pre>
	z(ldz, *). The second dimension of z must be at least max(1, n). If $jobz = 'V'$ , then if $info = 0$ , z contains the orthonormal eigenvectors of the matrix A, with the <i>i</i> -th column of z holding the eigenvector associated with w(i). If $jobz = 'N'$ , then z is not referenced.
ab	On exit, this array is overwritten by the values generated during the reduction to tridiagonal form. If $uplo = 'U'$ , the first superdiagonal and the diagonal of the tridiagonal matrix <i>T</i> are returned in rows <i>kd</i> and <i>kd</i> +1 of <i>ab</i> , and if $uplo = 'L'$ , the diagonal and first subdiagonal of <i>T</i> are returned in the first two rows of <i>ab</i> .
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = i, then the algorithm failed to converge; i indicates the number of elements of an intermediate tridiagonal form which did not converge to zero.</pre>

## ?hbev

Computes all eigenvalues and, optionally, eigenvectors of a Hermitian band matrix.

call chbev(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, rwork, info)
call zhbev(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, rwork, info)

### **Discussion**

This routine computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix A.

jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then only eigenvalues are computed. If <i>jobz</i> = 'V', then eigenvalues and eigenvectors are computed.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , $ab$ stores the upper triangular part of $A$ . If $uplo = 'L'$ , $ab$ stores the lower triangular part of $A$ .
n	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .
kd	<b>INTEGER.</b> The number of super- or sub-diagonals in $A$ ( $kd \ge 0$ ).
ab, work	COMPLEX for chbev DOUBLE COMPLEX for zhbev. Arrays: ab (1dab,*) is an array containing either upper or lower triangular part of the Hermitian matrix A (as specified by uplo) in band storage format. The second dimension of ab must be at least max(1, n). work (*) is a workspace array. The dimension of work must be at least max(1, n).

ldab	<b>INTEGER.</b> The leading dimension of <i>ab</i> ; must be at least $kd + 1$ .
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ . Constraints: if $jobz = 'N'$ , then $ldz \ge 1$ ; if $jobz = 'V'$ , then $ldz \ge max(1, n)$ .
rwork	REAL for chbev DOUBLE PRECISION for zhbev Workspace array, DIMENSION at least max(1, 3 <i>n</i> -2).

W	REAL for chbev DOUBLE PRECISION for zhbev Array, DIMENSION at least max(1, n). If <i>info</i> = 0, contains the eigenvalues in ascending order.
Ζ	COMPLEX for chbev DOUBLE COMPLEX for zhbev. Array $z(ldz, *)$ . The second dimension of $z$ must be at least max $(1, n)$ . If $jobz = 'V'$ , then if $info = 0, z$ contains the orthonormal eigenvectors of the matrix $A$ , with the <i>i</i> -th column of $z$ holding the eigenvector associated with $w(i)$ . If $jobz = 'N'$ , then $z$ is not referenced.
ab	On exit, this array is overwritten by the values generated during the reduction to tridiagonal form. If $uplo = 'U'$ , the first superdiagonal and the diagonal of the tridiagonal matrix <i>T</i> are returned in rows <i>kd</i> and <i>kd</i> +1 of <i>ab</i> , and if $uplo = 'L'$ , the diagonal and first subdiagonal of <i>T</i> are returned in the first two rows of <i>ab</i> .
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = i, then the algorithm failed to converge; i indicates the number of elements of an intermediate tridiagonal form which did not converge to zero.</pre>

## ?sbevd

Computes all eigenvalues and (optionally) all eigenvectors of a real symmetric band matrix using divide and conquer algorithm.

call ssbevd (job, uplo, n, kd, ab, ldab, w, z, ldz, work, lwork, iwork, liwork, info) call dsbevd (job, uplo, n, kd, ab, ldab, w, z, ldz, work, lwork, iwork, liwork, info)

## **Discussion**

This routine computes all the eigenvalues, and optionally all the eigenvectors, of a real symmetric band matrix A. In other words, it can compute the spectral factorization of A as:

 $A = Z\Lambda Z^T$ 

Here  $\Lambda$  is a diagonal matrix whose diagonal elements are the eigenvalues  $\lambda_i$ , and *Z* is the orthogonal matrix whose columns are the eigenvectors  $z_i$ . Thus,

 $Az_i = \lambda_i z_i$  for i = 1, 2, ..., n.

If the eigenvectors are requested, then this routine uses a divide and conquer algorithm to compute eigenvalues and eigenvectors. However, if only eigenvalues are required, then it uses the Pal-Walker-Kahan variant of the QL or QR algorithm.

job	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
uplo	CHARACTER*1. Must be 'U' or 'L'.
	If $uplo = 'U'$ , <i>ab</i> stores the upper triangular part of A.
	If $uplo = 'L'$ , <i>ab</i> stores the lower triangular part of A.

п	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .
kd	<b>INTEGER</b> . The number of super- or sub-diagonals in $A$ ( $kd \ge 0$ ).
ab, work	<ul> <li>REAL for ssbevd</li> <li>DOUBLE PRECISION for dsbevd.</li> <li>Arrays:</li> <li>ab (1dab,*) is an array containing either upper or lower triangular part of the symmetric matrix A (as specified by uplo) in band storage format.</li> <li>The second dimension of ab must be at least max(1, n).</li> </ul>
	<ul><li>work (*) is a workspace array.</li><li>The dimension of work must be at least lwork.</li></ul>
ldab	<b>INTEGER</b> . The leading dimension of $ab$ ; must be at least $kd$ +1.
ldz	INTEGER. The leading dimension of the output array $z$ . Constraints: if $job = 'N'$ , then $ldz \ge 1$ ; if $job = 'V'$ , then $ldz \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> . Constraints: if $n \le 1$ , then $lwork \ge 1$ ; if $job = 'N'$ and $n > 1$ , then $lwork \ge 2n$ ; if $job = 'V'$ and $n > 1$ , then $lwork \ge 3n^2 + (4+2k) * n+1$ , where k is the smallest integer which satisfies $2^k \ge n$ .
iwork	INTEGER. Workspace array, DIMENSION at least <i>liwork</i> .
liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . Constraints: if $n \le 1$ , then <i>liwork</i> $\ge 1$ ; if <i>job</i> = 'N' and $n > 1$ , then <i>liwork</i> $\ge 1$ ; if <i>job</i> = 'V' and $n > 1$ , then <i>liwork</i> $\ge 5n+2$ .

W,Z	REAL for ssbevd
	DOUBLE PRECISION for dsbevd
	Arrays:
	w(*), DIMENSION at least max $(1, n)$ .
	If $info = 0$ , contains the eigenvalues of the matrix A in
	ascending order. See also <i>info</i> .
	z(ldz, *). The second dimension of z must be:
	at least 1 if $job = 'N';$
	at least $max(1, n)$ if $job = V'$ .
	If $job = 'V'$ , then this array is overwritten by the orthogonal matrix Z which contains the eigenvectors of A. The <i>i</i> th column of Z contains the eigenvector which corresponds to the eigenvalue $w(i)$ . If $job = 'N'$ , then z is not referenced.
ab	On exit, this array is overwritten by the values generated during the reduction to tridiagonal form.
work(1)	On exit, if <i>lwork</i> > 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
iwork(1)	On exit, if <i>liwork</i> > 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = i$ , then the algorithm failed to converge; <i>i</i> indicates the number of elements of an intermediate tridiagonal form which did not converge to zero. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

## **Application Notes**

The computed eigenvalues and eigenvectors are exact for a matrix T + E such that  $||E||_2 = O(\varepsilon) ||T||_2$ , where  $\varepsilon$  is the machine precision.

The complex analogue of this routine is <u>?hbevd</u>.

See also <u>?syevd</u> for matrices held in full storage, and <u>?spevd</u> for matrices held in packed storage.

# ?hbevd

Computes all eigenvalues and (optionally) all eigenvectors of a complex Hermitian band matrix using divide and conquer algorithm.

```
call chbevd (job, uplo, n, kd, ab, ldab, w, z, ldz, work, lwork,
rwork, lrwork, iwork, liwork, info)
call zhbevd (job, uplo, n, kd, ab, ldab, w, z, ldz, work, lwork,
rwork, lrwork, iwork, liwork, info)
```

### **Discussion**

This routine computes all the eigenvalues, and optionally all the eigenvectors, of a complex Hermitian band matrix *A*. In other words, it can compute the spectral factorization of *A* as:  $A = Z\Lambda Z^{H}$ . Here  $\Lambda$  is a real diagonal matrix whose diagonal elements are the eigenvalues  $\lambda_i$ , and *Z* is the (complex) unitary matrix whose columns are the eigenvectors  $z_i$ . Thus,

 $Az_i = \lambda_i z_i$  for i = 1, 2, ..., n.

If the eigenvectors are requested, then this routine uses a divide and conquer algorithm to compute eigenvalues and eigenvectors. However, if only eigenvalues are required, then it uses the Pal-Walker-Kahan variant of the QL or QR algorithm.

job	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are
	computed.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , $ab$ stores the upper triangular part of A. If $uplo = 'L'$ , $ab$ stores the lower triangular part of A.
n	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .

kd	<b>INTEGER</b> . The number of super- or sub-diagonals in $A$ ( <i>kd</i> $\ge$ 0).
ab, work	<ul> <li>COMPLEX for chbevd</li> <li>DOUBLE COMPLEX for zhbevd.</li> <li>Arrays:</li> <li>ab (1dab,*) is an array containing either upper or lower triangular part of the Hermitian matrix A (as specified by uplo) in band storage format.</li> <li>The second dimension of ab must be at least max(1, n).</li> </ul>
	<i>work</i> (*) is a workspace array. The dimension of <i>work</i> must be at least <i>lwork</i> .
ldab	<b>INTEGER.</b> The leading dimension of $ab$ ; must be at least $kd+1$ .
ldz	INTEGER. The leading dimension of the output array z. Constraints: if $job = 'N'$ , then $ldz \ge 1$ ; if $job = 'V'$ , then $ldz \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array work. Constraints: if $n \le 1$ , then $lwork \ge 1$ ; if $job = 'N'$ and $n > 1$ , then $lwork \ge n$ ; if $job = 'V'$ and $n > 1$ , then $lwork \ge 2n^2$
rwork	REAL for chbevd DOUBLE PRECISION for zhbevd Workspace array, DIMENSION at least <i>lrwork</i> .
lrwork	<b>INTEGER.</b> The dimension of the array <i>rwork</i> . Constraints: if $n \le 1$ , then $lrwork \ge 1$ ; if $job = 'N'$ and $n > 1$ , then $lrwork \ge n$ ; if $job = 'V'$ and $n > 1$ , then $lrwork \ge 3n^2 + (4+2k) * n+1$ , where k is the smallest integer which satisfies $2^k \ge n$ .
iwork	INTEGER. Workspace array, DIMENSION at least <i>liwork</i> .

liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . Constraints: if $job = 'N'$ or $n \le 1$ , then $liwork \ge 1$ ; if $job = 'V'$ and $n > 1$ , then $liwork \ge 5n+2$ .
Output Parame	eters
W	REAL for chbevd DOUBLE PRECISION for zhbevd Array, DIMENSION at least $max(1, n)$ . If <i>info</i> = 0, contains the eigenvalues of the matrix A in ascending order. See also <i>info</i> .
Ζ	COMPLEX for chbevd DOUBLE COMPLEX for zhbevd Array, DIMENSION $(ldz, *)$ . The second dimension of z must be: at least 1 if $job = 'N'$ ; at least max $(1, n)$ if $job = 'V'$ . If $job = 'V'$ , then this array is overwritten by the unitary matrix Z which contains the eigenvectors of A. The <i>i</i> th column of Z contains the eigenvector which corresponds to the eigenvalue $w(i)$ . If $job = 'N'$ , then z is not referenced.
ab	On exit, this array is overwritten by the values generated during the reduction to tridiagonal form.
work(1)	On exit, if <i>lwork</i> > 0, then the real part of <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
rwork(1)	On exit, if <i>lrwork</i> > 0, then <i>rwork(1)</i> returns the required minimal size of <i>lrwork</i> .
iwork(1)	On exit, if <i>liwork</i> > 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = <i>i</i> , then the algorithm failed to converge; <i>i</i>

indicates the number of elements of an intermediate tridiagonal form which did not converge to zero. If info = -i, the *i*th parameter had an illegal value.

## **Application Notes**

The computed eigenvalues and eigenvectors are exact for a matrix T + E such that  $||E||_2 = O(\varepsilon) ||T||_2$ , where  $\varepsilon$  is the machine precision.

The real analogue of this routine is <u>?sbevd</u>.

See also <u>?heevd</u> for matrices held in full storage, and <u>?hpevd</u> for matrices held in packed storage.

# ?sbevx

Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric band matrix.

### **Discussion**

This routine computes selected eigenvalues and, optionally, eigenvectors of a real symmetric band matrix *A*. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

jobz	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'. If $range = 'A'$ , the routine computes all eigenvalues. If $range = 'V'$ , the routine computes eigenvalues $\lambda_i$ in the half-open interval: $vl < \lambda_i \leq vu$ .
	If <i>range</i> = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , $ab$ stores the upper triangular part of A. If $uplo = 'L'$ , $ab$ stores the lower triangular part of A.
п	<b>INTEGER</b> . The order of the matrix $A$ $(n \ge 0)$ .
kd	<b>INTEGER.</b> The number of super- or sub-diagonals in $A$ ( $kd \ge 0$ ).

ab, work	REAL for ssbevx DOUBLE PRECISION for dsbevx. Arrays:
	<ul> <li>ab (ldab, *) is an array containing either upper or lower triangular part of the symmetric matrix A (as specified by uplo) in band storage format.</li> <li>The second dimension of ab must be at least max(1, n).</li> </ul>
	<pre>work (*) is a workspace array. The dimension of work must be at least max(1, 7n).</pre>
ldab	<b>INTEGER.</b> The leading dimension of <i>ab</i> ; must be at least $kd + 1$ .
vl, vu	<pre>REAL for ssbevx DOUBLE PRECISION for dsbevx. If range = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: v1&lt; vu. If range = 'A' or 'I', v1 and vu are not referenced.</pre>
il, iu	INTEGER. If <i>range</i> = 'I', the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le i1 \le iu \le n$ , if $n > 0$ ; $i1 = 1$ and $iu = 0$ if $n = 0$ . If <i>range</i> = 'A' or 'V', <i>i1</i> and <i>iu</i> are not referenced.
abstol	REAL for chpevx DOUBLE PRECISION for zhpevx The absolute error tolerance to which each eigenvalue is required. See <i>Application notes</i> for details on error tolerance.
ldq, ldz	<b>INTEGER.</b> The leading dimensions of the output arrays $q$ and $z$ , respectively. Constraints: $ldq \ge 1$ , $ldz \ge 1$ ; If $jobz = 'V'$ , then $ldq \ge max(1, n)$ and $ldz \ge max(1, n)$ .
iwork	<b>INTEGER</b> . Workspace array, <b>DIMENSION</b> at least max(1, 5 <i>n</i> ).

m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', m = iu - il + l.
W , Z	<pre>REAL for ssbevx DOUBLE PRECISION for dsbevx Arrays: w(*), DIMENSION at least max(1, n). The first m elements of w contain the selected eigenvalues of the matrix A in ascending order.</pre>
	z(ldz,*). The second dimension of $z$ must be at least max $(1, m)$ . If $jobz = 'V'$ , then if $info = 0$ , the first $m$ columns of $z$ contain the orthonormal eigenvectors of the matrix $A$ corresponding to the selected eigenvalues, with the <i>i</i> -th column of $z$ holding the eigenvector associated with $w(i)$ . If an eigenvector fails to converge, then that column of $z$ contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in <i>ifail</i> . If $jobz = 'N'$ , then $z$ is not referenced. Note: you must ensure that at least max $(1,m)$ columns
	are supplied in the array $z$ ; if <i>range</i> = 'V', the exact value of <i>m</i> is not known in advance and an upper bound must be used.
ab	On exit, this array is overwritten by the values generated during the reduction to tridiagonal form. If $uplo = 'U'$ , the first superdiagonal and the diagonal of the tridiagonal matrix <i>T</i> are returned in rows <i>kd</i> and <i>kd</i> +1 of <i>ab</i> , and if $uplo = 'L'$ , the diagonal and first subdiagonal of <i>T</i> are returned in the first two rows of <i>ab</i> .
ifail	INTEGER. Array, DIMENSION at least max $(1, n)$ . If $jobz = 'V'$ , then if $info = 0$ , the first <i>m</i> elements of

*ifail* are zero; if *info* > 0, the *ifail* contains the indices the eigenvectors that failed to converge. If jobz = 'N', then *ifail* is not referenced.

info

INTEGER.

If *info* = 0, the execution is successful. If *info* = -*i*, the *i*th parameter had an illegal value. If *info* = *i*, then *i* eigenvectors failed to converge; their indices are stored in the array *ifail*.

### **Application Notes**

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to  $abstol + \varepsilon * max(|a|,|b|)$ , where  $\varepsilon$  is the machine precision. If abstol is less than or equal to zero, then  $\varepsilon * ||T/|_1$  will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when abstol is set to twice the underflow threshold 2*?lamch('S'), not zero. If this routine returns with info > 0, indicating that some eigenvectors did not converge, try setting abstol to 2*?lamch('S').

# ?hbevx

Computes selected eigenvalues and, optionally, eigenvectors of a Hermitian band matrix.

### **Discussion**

This routine computes selected eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix *A*. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

jobz	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'. If $range = 'A'$ , the routine computes all eigenvalues. If $range = 'V'$ , the routine computes eigenvalues $\lambda_i$ in the half-open interval: $vl < \lambda_i \leq vu$ .
uplo	If <i>range</i> = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> . CHARACTER*1. Must be 'U' or 'L'. If <i>uplo</i> = 'U', <i>ab</i> stores the upper triangular part of A.
п	If $uplo = 'L'$ , <i>ab</i> stores the lower triangular part of <i>A</i> . INTEGER. The order of the matrix <i>A</i> $(n \ge 0)$ .
kd	<b>INTEGER.</b> The number of super- or sub-diagonals in $A$ ( $kd \ge 0$ ).

ab, work	COMPLEX for chbevx DOUBLE COMPLEX for zhbevx. Arrays: <i>ab</i> ( <i>ldab</i> , *) is an array containing either upper or lower triangular part of the Hermitian matrix A (as specified by <i>uplo</i> ) in band storage format. The second dimension of <i>ab</i> must be at least max(1, <i>n</i> ).
	<i>work</i> (*) is a workspace array. The dimension of <i>work</i> must be at least max(1, <i>n</i> ).
ldab	<b>INTEGER.</b> The leading dimension of $ab$ ; must be at least $kd + 1$ .
vl, vu	REAL for chbevx DOUBLE PRECISION for zhbevx. If <i>range</i> = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: <i>v</i> 1< <i>vu</i> . If <i>range</i> = 'A' or 'I', <i>v</i> 1 and <i>vu</i> are not referenced.
il, iu	INTEGER. If <i>range</i> = 'I', the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le il \le iu \le n$ , if $n > 0$ ; $il=1$ and $iu=0$ if $n = 0$ . If <i>range</i> = 'A' or 'V', <i>il</i> and <i>iu</i> are not referenced.
abstol	REAL for chbevx DOUBLE PRECISION for zhbevx. The absolute error tolerance to which each eigenvalue is required. See <i>Application notes</i> for details on error tolerance.
ldq, ldz	INTEGER. The leading dimensions of the output arrays $q$ and $z$ , respectively. Constraints: $ldq \ge 1$ , $ldz \ge 1$ ; If $jobz = 'V'$ , then $ldq \ge max(1, n)$ and $ldz \ge max(1, n)$ .

rwork	REAL for chbevx
	DOUBLE PRECISION for zhbevx
	Workspace array, DIMENSION at least $max(1, 7n)$ .
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, 5n)$ .
Output Parame	eters
m	<b>INTEGER</b> . The total number of eigenvalues found,
	$0 \le m \le n$ . If $range = 'A', m = n$ , and if $range = 'I'$ , m = iu - il + 1.
W	REAL for chbevx
	DOUBLE PRECISION for zhbevx
	Array, DIMENSION at least $max(1, n)$ .
	The first $m$ elements contain the selected eigenvalues of
	the matrix A in ascending order.
Z	COMPLEX for chbevx
	DOUBLE COMPLEX for zhbevx.
	Array $z(ldz, *)$ . The second dimension of $z$ must be
	at least $\max(1, m)$ .
	If $jobz = V'$ , then if $info = 0$ , the first m columns of z contain the orthonormal eigenvectors of the matrix A
	corresponding to the selected eigenvalues, with the <i>i</i> -th
	column of $z$ holding the eigenvector associated with
	w(i). If an eigenvector fails to converge, then that
	column of $z$ contains the latest approximation to the
	eigenvector, and the index of the eigenvector is returned
	in ifail.
	If $jobz = 'N'$ , then z is not referenced.
	Note: you must ensure that at least $max(1,m)$ columns
	are supplied in the array z; if $range = 'V'$ , the exact
	value of $m$ is not known in advance and an upper bound must be used.
ab	On exit, this array is overwritten by the values generated during the reduction to tridiagonal form. If $uplo = 'U'$ ,
	the first superdiagonal and the diagonal of the
	the mist superdiagonal and the diagonal of the

tridiagonal matrix T are returned in rows kd and kd+1 of *ab*, and if uplo = 'L', the diagonal and first subdiagonal of T are returned in the first two rows of *ab*. ifail INTEGER. Array, DIMENSION at least  $\max(1, n)$ . If jobz = V', then if info = 0, the first *m* elements of *ifail* are zero; if *info* > 0, the *ifail* contains the indices of the eigenvectors that failed to converge. If jobz = 'N', then *ifail* is not referenced. INTEGER. info If *info* = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value. If *info* = *i*, then *i* eigenvectors failed to converge; their indices are stored in the array *ifail*.

## **Application Notes**

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to  $abstol + \varepsilon * max(|a|,|b|)$ , where  $\varepsilon$  is the machine precision. If abstol is less than or equal to zero, then  $\varepsilon * ||T/|_1$  will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when abstol is set to twice the underflow threshold 2*?lamch('S'), not zero. If this routine returns with info > 0, indicating that some eigenvectors did not converge, try setting abstol to 2*?lamch('S').

# ?stev

Computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix.

```
call sstev (jobz, n, d, e, z, ldz, work, info)
call dstev (jobz, n, d, e, z, ldz, work, info)
```

## **Discussion**

This routine computes all eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix *A*.

jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then only eigenvalues are computed. If <i>jobz</i> = 'V', then eigenvalues and eigenvectors are computed.
n	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .
d, e, work	REAL for sstev DOUBLE PRECISION for dstev. Arrays: d(*) contains the <i>n</i> diagonal elements of the tridiagonal matrix <i>A</i> . The dimension of <i>d</i> must be at least max(1, <i>n</i> ).
	<ul> <li>e(*) contains the n-1 subdiagonal elements of the tridiagonal matrix A.</li> <li>The dimension of e must be at least max(1, n). The nth element of this array is used as workspace.</li> <li>work(*) is a workspace array.</li> <li>The dimension of work must be at least max(1, 2n-2).</li> <li>If jobz = 'N', work is not referenced.</li> </ul>

ldz	<b>INTEGER</b> . The leading dimension of the output array <i>z</i> ;
	$ldz \ge 1$ . If $jobz = V'$ then $ldz \ge max(1, n)$ .

# **Output Parameters**

d	On exit, if $info = 0$ , contains the eigenvalues of the matrix A in ascending order.
Ζ	<b>REAL for sstev</b> <b>DOUBLE PRECISION for dstev</b> Array, <b>DIMENSION</b> ( <i>ldz</i> , *). The second dimension of <i>z</i> must be at least max(1, <i>n</i> ). If <i>jobz</i> ='V', then if <i>info</i> = 0, <i>z</i> contains the orthonormal eigenvectors of the matrix <i>A</i> , with the <i>i</i> -th column of <i>z</i> holding the eigenvector associated with the eigenvalue returned in $d(i)$ . If <i>job</i> ='N', then <i>z</i> is not referenced.
е	On exit, this array is overwritten with intermediate results.
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = i, then the algorithm failed to converge; i elements of e did not converge to zero.</pre>

# ?stevd

Computes all eigenvalues and (optionally) all eigenvectors of a real symmetric tridiagonal matrix using divide and conquer algorithm.

call sstevd (job, n, d, e, z, ldz, work, lwork, iwork, liwork, info) call dstevd (job, n, d, e, z, ldz, work, lwork, iwork, liwork, info)

#### **Discussion**

This routine computes all the eigenvalues, and optionally all the eigenvectors, of a real symmetric tridiagonal matrix *T*. In other words, the routine can compute the spectral factorization of *T* as:  $T = Z\Lambda Z^T$ . Here  $\Lambda$  is a diagonal matrix whose diagonal elements are the eigenvalues  $\lambda_i$ , and *Z* is the orthogonal matrix whose columns are the eigenvectors  $z_i$ . Thus,

 $Tz_i = \lambda_i z_i$  for i = 1, 2, ..., n.

If the eigenvectors are requested, then this routine uses a divide and conquer algorithm to compute eigenvalues and eigenvectors. However, if only eigenvalues are required, then it uses the Pal-Walker-Kahan variant of the QL or QR algorithm.

There is no complex analogue of this routine.

job	CHARACTER*1. Must be 'N' or 'V'.
	If $job = N'$ , then only eigenvalues are computed.
	If $job = VV'$ , then eigenvalues and eigenvectors are
	computed.
n	<b>INTEGER</b> . The order of the matrix $T$ ( $n \ge 0$ ).
d, e, work	REAL for sstevd DOUBLE PRECISION for dstevd.
	Arrays:

	d(*) contains the <i>n</i> diagonal elements of the tridiagonal matrix <i>T</i> . The dimension of <i>d</i> must be at least max(1, <i>n</i> ).
	e(*) contains the <i>n</i> -1 off-diagonal elements of <i>T</i> . The dimension of $e$ must be at least max(1, <i>n</i> ). The <i>n</i> th element of this array is used as workspace.
	<ul><li>work(*) is a workspace array.</li><li>The dimension of work must be at least lwork.</li></ul>
ldz	INTEGER. The leading dimension of the output array z. Constraints: $ldz \ge 1$ if $job = 'N'$ ; $ldz \ge max(1, n)$ if $job = 'V'$ .
lwork	<b>INTEGER.</b> The dimension of the array work. Constraints: if $job = 'N'$ or $n \le 1$ , then $lwork \ge 1$ ; if $job = 'V'$ and $n > 1$ , then $lwork \ge 2n^2 + (3+2k) * n+1$ , where k is the smallest integer which satisfies $2^k \ge n$ .
iwork	INTEGER. Workspace array, DIMENSION at least <i>liwork</i> .
liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . Constraints: if $job = 'N'$ or $n \le 1$ , then $liwork \ge 1$ ; if $job = 'V'$ and $n > 1$ , then $liwork \ge 5n+2$ .

# **Output Parameters**

d	On exit, if <i>info</i> = 0, contains the eigenvalues of the matrix <i>T</i> in ascending order. See also <i>info</i> .
Ζ	REAL for sstevd DOUBLE PRECISION for dstevd Array, DIMENSION $(1dz, *)$ . The second dimension of z must be: at least 1 if $job = 'N'$ ; at least max $(1, n)$ if $job = 'V'$ .

	If $job = 'V'$ , then this array is overwritten by the orthogonal matrix Z which contains the eigenvectors of T. If $job = 'N'$ , then z is not referenced.
е	On exit, this array is overwritten with intermediate results.
work(1)	On exit, if <i>lwork</i> > 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
iwork(1)	On exit, if <i>liwork</i> > 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = i$ , then the algorithm failed to converge; <i>i</i> indicates the number of elements of an intermediate tridiagonal form which did not converge to zero. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

The computed eigenvalues and eigenvectors are exact for a matrix T + E such that  $||E||_2 = O(\varepsilon) ||T||_2$ , where  $\varepsilon$  is the machine precision.

If  $\lambda_i$  is an exact eigenvalue, and  $\mu_i$  is the corresponding computed value, then

 $|\mu_i - \lambda_i| \leq (n)\varepsilon ||T||_2$ 

where c(n) is a modestly increasing function of n.

If  $z_i$  is the corresponding exact eigenvector, and  $w_i$  is the corresponding computed vector, then the angle  $\theta(z_i, w_i)$  between them is bounded as follows:

 $\theta(z_i, w_i) \leq c(n) \varepsilon \mid |T| \mid_2 / \min_{i \neq j} |\lambda_i - \lambda_j|.$ 

Thus the accuracy of a computed eigenvector depends on the gap between its eigenvalue and all the other eigenvalues.

# ?stevx

Computes selected eigenvalues and eigenvectors of a real symmetric tridiagonal matrix.

## **Discussion**

This routine computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix A. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

jobz	CHARACTER*1. Must be 'N' or 'V'. If $job = 'N'$ , then only eigenvalues are computed. If $job = 'V'$ , then eigenvalues and eigenvectors are computed.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'. If <i>range</i> = 'A', the routine computes all eigenvalues. If <i>range</i> = 'V', the routine computes eigenvalues $\lambda_i$ in the half-open interval: $vl < \lambda_i \le vu$ . If <i>range</i> = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
d, e, work	REAL for sstevx DOUBLE PRECISION for dstevx. Arrays:

	d(*) contains the <i>n</i> diagonal elements of the tridiagonal matrix <i>A</i> . The dimension of <i>d</i> must be at least max(1, <i>n</i> ).
	$e(\star)$ contains the <i>n</i> -1 subdiagonal elements of <i>A</i> . The dimension of <i>e</i> must be at least max(1, <i>n</i> ). The <i>n</i> th element of this array is used as workspace.
	<ul><li>work(*) is a workspace array.</li><li>The dimension of work must be at least max(1, 5n).</li></ul>
vl, vu	REAL for sstevx DOUBLE PRECISION for dstevx. If range = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: vl <vu. If range = 'A' or 'I', vl and vu are not referenced.</vu. 
il, iu	INTEGER. If $range = 'I'$ , the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le il \le iu \le n$ , if $n > 0$ ; $il = 1$ and $iu = 0$ if $n = 0$ . If $range = 'A'$ or 'V', $il$ and $iu$ are not referenced.
abstol	REAL for sstevx DOUBLE PRECISION for dstevx. The absolute error tolerance to which each eigenvalue is required. See <i>Application notes</i> for details on error tolerance.
ldz	<b>INTEGER.</b> The leading dimensions of the output array $z$ ; $ldz \ge 1$ . If $jobz = 'V'$ , then $ldz \ge max(1, n)$ .
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least max(1, 5 <i>n</i> ).

# **Output Parameters**

m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', m = iu - il + 1.
W, Z	<pre>REAL for sstevx DOUBLE PRECISION for dstevx. Arrays: w(*), DIMENSION at least max(1, n). The first m elements of w contain the selected eigenvalues of the matrix A in ascending order.</pre>
	z(ldz, *). The second dimension of $z$ must be at least max $(1, m)$ . If $jobz = 'V'$ , then if $info = 0$ , the first $m$ columns of $z$ contain the orthonormal eigenvectors of the matrix $A$ corresponding to the selected eigenvalues, with the <i>i</i> -th column of $z$ holding the eigenvector associated with $w(i)$ . If an eigenvector fails to converge, then that column of $z$ contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in <i>ifail</i> . If $jobz = 'N'$ , then $z$ is not referenced. Note: you must ensure that at least max $(1,m)$ columns are supplied in the array $z$ ; if $range = 'V'$ , the exact value of $m$ is not known in advance and an upper bound must be used.
d, e	On exit, these arrays may be multiplied by a constant factor chosen to avoid overflow or underflow in computing the eigenvalues.
ifail	INTEGER. Array, DIMENSION at least max(1, n). If jobz = 'V', then if info = 0, the first m elements of ifail are zero; if info > 0, the ifail contains the indices of the eigenvectors that failed to converge.

If *jobz* = 'N', then *ifail* is not referenced.

info

INTEGER.

If *info* = 0, the execution is successful. If *info* = -*i*, the *i*th parameter had an illegal value. If *info* = *i*, then *i* eigenvectors failed to converge; their indices are stored in the array *ifail*.

#### **Application Notes**

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to  $abstol + \varepsilon * max(|a|,|b|)$ , where  $\varepsilon$  is the machine precision. If abstol is less than or equal to zero, then  $\varepsilon * ||A||_1$  will be used in its place. Eigenvalues will be computed most accurately when abstol is set to twice the underflow threshold 2*?lamch('S'), not zero. If this routine returns with info > 0, indicating that some eigenvectors did not converge, try setting abstol to 2*?lamch('S').

# ?stevr

Computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix using the Relatively Robust Representations.

## **Discussion**

This routine computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix T. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

Whenever possible, ?stevr calls <u>sstegr/dstegr</u> to compute the eigenspectrum using Relatively Robust Representations. ?stegr computes eigenvalues by the *dqds* algorithm, while orthogonal eigenvectors are computed from various "good"  $LDL^T$  representations (also known as Relatively Robust Representations). Gram-Schmidt orthogonalization is avoided as far as possible. More specifically, the various steps of the algorithm are as follows. For the i-th unreduced block of *T*,

(a) Compute  $T - \mathbf{G} = L_i D_i L_i^T$ , such that  $L_i D_i L_i^T$  is a relatively robust representation;

(b) Compute the eigenvalues,  $\lambda_j$ , of  $L_i D_i L_i^T$  to high relative accuracy by the *dqds* algorithm;

(c) If there is a cluster of close eigenvalues, "choose"  $\sigma_i$  close to the cluster, and go to step (a);

(d) Given the approximate eigenvalue  $\lambda_j$  of  $L_i D_i L_i^T$ , compute the corresponding eigenvector by forming a rank-revealing twisted factorization.

The desired accuracy of the output can be specified by the input parameter *abstol*.

The routine <code>?stevr</code> calls <code>sstegr/dstegr</code> when the full spectrum is requested on machines which conform to the IEEE-754 floating point standard. <code>?stevr</code> calls <code>sstebz/dstebz</code> and <code>sstein/dstein</code> on non-IEEE machines and when partial spectrum requests are made.

### **Input Parameters**

jobz	CHARACTER*1. Must be 'N' or 'V'.
	If $jobz = 'N'$ , then only eigenvalues are computed.
	If $jobz = V'$ , then eigenvalues and eigenvectors are computed.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'.
	If <i>range</i> = 'A', the routine computes all eigenvalues.
	If $range = V'$ , the routine computes eigenvalues $\lambda_i$ in the half-open interval: $v < \lambda_i \le v u$ .
	If <i>range</i> = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
	For range = $V'$ or $I'$ and $iu - il < n - 1$ ,
	sstebz/dstebz and sstein/dstein are called.
п	<b>INTEGER.</b> The order of the matrix $T (n \ge 0)$ .
d, e, work	REAL for sstevr
	DOUBLE PRECISION for dstevr.
	Arrays:
	d(*) contains the <i>n</i> diagonal elements of the
	tridiagonal matrix T.
	The dimension of $d$ must be at least max $(1, n)$ .
	e(*) contains the <i>n</i> -1 subdiagonal elements of <i>A</i> . The dimension of $e$ must be at least max $(1, n)$ . The <i>n</i> th
	element of this array is used as workspace.

work(lwork) is a workspace array.

vl, vu	REAL for sstevr DOUBLE PRECISION for dstevr. If <i>range</i> = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: <i>v1</i> < <i>vu</i> .
	If $range = 'A'$ or 'I', $vI$ and $vu$ are not referenced.
il, iu	INTEGER. If <i>range</i> = 'I', the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le i1 \le iu \le n$ , if $n > 0$ ; $i1=1$ and $iu=0$ if $n = 0$ .
	If $range = 'A'$ or 'V', <i>il</i> and <i>iu</i> are not referenced.
abstol	<b>REAL</b> for ssyevr <b>DOUBLE PRECISION</b> for dsyevr. The absolute error tolerance to which each eigenvalue/eigenvector is required. If $jobz = 'V'$ , the eigenvalues and eigenvectors output have residual norms bounded by <i>abstol</i> , and the dot products between different eigenvectors are bounded by <i>abstol</i> .If <i>abstol</i> < <i>n</i> $\epsilon$    <i>T</i>    ₁ ,then <i>n</i> $\epsilon$    <i>T</i>    ₁ willbeused in its place, where $\epsilon$ is the machine precision. The eigenvalues are computed to an accuracy of $\epsilon$    <i>T</i>    ₁ irrespective of <i>abstol</i> . If high relative accuracy is important, set <i>abstol</i> to ?lamch('S').
ldz	INTEGER. The leading dimension of the output array $z$ . Constraints: $ldz \ge 1$ if $jobz = 'N'$ ; $ldz \ge max(1, n)$ if $jobz = 'V'$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> . Constraint: $lwork \ge max(1, 20n)$ .
iwork	INTEGER. Workspace array, DIMENSION ( <i>liwork</i> ).
liwork	<b>INTEGER</b> . The dimension of the array <i>iwork</i> , $lwork \ge max(1, 10n)$ .

# **Output Parameters**

m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If <i>range</i> = 'A', <i>m</i> = <i>n</i> , and if <i>range</i> = 'I', m = iu - il + 1.
W, Z	<pre>REAL for sstevr DOUBLE PRECISION for dstevr. Arrays: w(*), DIMENSION at least max(1, n). The first m elements of w contain the selected eigenvalues of the matrix T in ascending order.</pre>
	<ul> <li>z(ldz,*). The second dimension of z must be at least max(1, m).</li> <li>If jobz = 'V', then if info = 0, the first m columns of z contain the orthonormal eigenvectors of the matrix T corresponding to the selected eigenvalues, with the <i>i</i>-th column of z holding the eigenvector associated with w(i).</li> <li>If jobz = 'N', then z is not referenced.</li> <li>Note: you must ensure that at least max(1,m) columns are supplied in the array z; if range = 'V', the exact value of m is not known in advance and an upper bound must be used.</li> </ul>
d, e	On exit, these arrays may be multiplied by a constant factor chosen to avoid overflow or underflow in computing the eigenvalues.
isuppz	<pre>INTEGER. Array, DIMENSION at least 2*max(1, m). The support of the eigenvectors in z, i.e., the indices indicating the nonzero elements in z. The <i>i</i>-th eigenvector is nonzero only in elements <i>isuppz</i>(2<i>i</i>-1) through <i>isuppz</i>(2<i>i</i>). Implemented only for <i>range</i> = 'A' or 'I' and <i>iu-il</i> = n-1.</pre>
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .

iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , an internal error has occurred.

# **Application Notes**

Normal execution of the routine **?stegr** may create NaNs and infinities and hence may abort due to a floating point exception in environments which do not handle NaNs and infinities in the IEEE standard default manner.

# **Nonsymmetric Eigenproblems**

This section describes LAPACK driver routines used for solving nonsymmetric eigenproblems. See also <u>computational routines</u> that can be called to solve these problems. Table 5-12 lists routines described in more detail below.

Table 5-11	Driver Routines for Solving Nonsymmetric Eigenproblems
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Routine Name	Operation performed
?gees	Computes the eigenvalues and Schur factorization of a general matrix, and orders the factorization so that selected eigenvalues are at the top left of the Schur form.
?geesx	Computes the eigenvalues and Schur factorization of a general matrix, orders the factorization and computes reciprocal condition numbers.
?geev	Computes the eigenvalues and left and right eigenvectors of a general matrix.
?geevx	Computes the eigenvalues and left and right eigenvectors of a general matrix, with preliminary matrix balancing, and computes reciprocal condition numbers for the eigenvalues and right eigenvectors.

# ?gees

Computes the eigenvalues and Schur factorization of a general matrix, and orders the factorization so that selected eigenvalues are at the top left of the Schur form.

# **Discussion**

This routine computes for an *n*-by-*n* real/complex nonsymmetric matrix *A*, the eigenvalues, the real Schur form *T*, and, optionally, the matrix of Schur vectors *Z*. This gives the Schur factorization  $A = ZTZ^{H}$ .

Optionally, it also orders the eigenvalues on the diagonal of the real-Schur/Schur form so that selected eigenvalues are at the top left. The leading columns of Z then form an orthonormal basis for the invariant subspace corresponding to the selected eigenvalues.

A real matrix is in real-Schur form if it is upper quasi-triangular with 1-by-1 and 2-by-2 blocks. 2-by-2 blocks will be standardized in the form

$$\begin{pmatrix} a & b \\ c & a \end{pmatrix}$$

where b * c < 0. The eigenvalues of such a block are  $a \pm \sqrt{bc}$ . A complex matrix is in Schur form if it is upper triangular.

jobvs	CHARACTER*1. Must be 'N' or 'V'. If <i>jobvs</i> = 'N', then Schur vectors are not computed. If <i>jobvs</i> = 'V', then Schur vectors are computed.
sort	CHARACTER*1. Must be 'N' or 'S'. Specifies whether or not to order the eigenvalues on the diagonal of the Schur form.
	If <i>sort</i> = 'N', then eigenvalues are not ordered. If <i>sort</i> = 'S', eigenvalues are ordered (see <i>select</i> ).
select	LOGICAL FUNCTION of two REAL arguments for real flavors. LOGICAL FUNCTION of one COMPLEX argument for complex flavors.
	<i>select</i> must be declared <b>EXTERNAL</b> in the calling subroutine.
	If <i>sort</i> = 'S', <i>select</i> is used to select eigenvalues to sort to the top left of the Schur form. If <i>sort</i> = 'N', <i>select</i> is not referenced.

For	real	flavors:
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For complex flavors: An eigenvalue w(j) is selected if $select(w(j))$ is true.nINTEGER. The order of the matrix $A$ ( $n \ge 0$ ).a, workREAL for sgees DOUBLE PRECISION for dgees COMPLEX for cgees DOUBLE COMPLEX for zgees. Arrays: $a(lda,*)$ is an array containing the n-by-n matrix $A$ . The second dimension of $a$ must be at least max $(1, n)$ . work (lwork) is a workspace array.ldaINTEGER. The first dimension of the array $a$ . Must be at least max $(1, n)$ .ldvsINTEGER. The leading dimension of the output array $vs$ . Constraints: ldvs $\ge 1$ ; ldvs $\ge max(1, n)$ if jobvs = 'V'.lworkINTEGER. The dimension of the array work. Constraint: lwork $\ge max(1, 2n)$ for complex flavors.rworkREAL for cgees DOUBLE PRECISION for zgees Workspace array, DIMENSION at least max $(1, n)$ . Used in complex flavors only.		An eigenvalue $wr(j) + \sqrt{-1} * wi(j)$ is selected if select(wr(j), wi(j)) is true; that is, if either one of a complex conjugate pair of eigenvalues is selected, then both complex eigenvalues are selected. Note that a selected complex eigenvalue may no longer satisfy select(wr(j), wi(j)) = .TRUE. after ordering, since ordering may change the value of complex eigenvalues (especially if the eigenvalue is ill-conditioned); in this case <i>info</i> may be set to $n+2$ (see <i>info</i> below).
nINTEGER. The order of the matrix $A$ $(n \ge 0)$ .a, workREAL for sgeesDOUBLE PRECISION for dgeesCOMPLEX for cgeesDOUBLE COMPLEX for zgees.Arrays: $a(1da, *)$ is an array containing the n-by-n matrix A.The second dimension of a must be at least max $(1, n)$ .work(lwork) is a workspace array.IdaINTEGER. The first dimension of the array a.Must be at least max $(1, n)$ .IdvsINTEGER. The leading dimension of the output array vs.Constraints:Idvs $\ge 1$ ;Idvs $\ge 1$ ;Idvs $\ge 1$ ;IworkINTEGER. The dimension of the array work.Constraint:Iwork $\ge \max(1, 3n)$ for real flavors;Iwork $\ge \max(1, 2n)$ for complex flavors.rworkREAL for cgeesDOUBLE PRECISION for zgeesWorkspace array, DIMENSION at least max $(1, n)$ . Used		* •
a, workREAL for sgees DOUBLE PRECISION for dgees COMPLEX for cgees DOUBLE COMPLEX for zgees. Arrays: $a(1da,*)$ is an array containing the <i>n</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ). work(lwork) is a workspace array.IdaINTEGER. The first dimension of the array <i>a</i> . Must be at least max(1, <i>n</i> ).IdvsINTEGER. The leading dimension of the output array <i>vs</i> . Constraints: Idvs $\geq 1$ ; Idvs $\geq max(1, n)$ if jobvs $=$ 'V'.IworkINTEGER. The dimension of the array work. Constraints: Idvs $\geq 1$ ; Idvs $\geq max(1, 3n)$ for real flavors; Iwork $\geq max(1, 2n)$ for complex flavors. <i>rwork</i> REAL for cgees DOUBLE PRECISION for zgees Workspace array, DIMENSION at least max(1, <i>n</i> ). Used	п	
IdaINTEGER. The first dimension of the array a. Must be at least $max(1, n)$ .IdvsINTEGER. The leading dimension of the output array vs. Constraints: $ldvs \ge 1$ ; $ldvs \ge 1$ ; $ldvs \ge max(1, n)$ if $jobvs = 'V'$ .IworkINTEGER. The dimension of the array work. Constraint: $lwork \ge max(1, 3n)$ for real flavors; $lwork \ge max(1, 2n)$ for complex flavors.rworkREAL for cgees DOUBLE PRECISION for zgees Workspace array, DIMENSION at least $max(1, n)$ . Used	a, work	REAL for sgees DOUBLE PRECISION for dgees COMPLEX for cgees DOUBLE COMPLEX for zgees. Arrays: a(lda,*) is an array containing the <i>n</i> -by- <i>n</i> matrix <i>A</i> .
Must be at least $max(1, n)$ .IdvsINTEGER. The leading dimension of the output array vs. Constraints: $ldvs \ge 1$ ; $ldvs \ge max(1, n)$ if $jobvs = 'V'$ .IworkINTEGER. The dimension of the array work. Constraint: $lwork \ge max(1, 3n)$ for real flavors; $lwork \ge max(1, 2n)$ for complex flavors.rworkREAL for cgees DOUBLE PRECISION for zgees Workspace array, DIMENSION at least $max(1, n)$ . Used		work(lwork) is a workspace array.
Constraints: $ldvs \ge 1$ ; $ldvs \ge max(1, n)$ if $jobvs = 'V'$ .lworkINTEGER. The dimension of the array work.Constraint: $lwork \ge max(1, 3n)$ for real flavors; $lwork \ge max(1, 2n)$ for complex flavors.rworkREAL for cgeesDOUBLE PRECISION for zgeesWorkspace array, DIMENSION at least max(1, n). Used	lda	-
Constraint: $lwork \ge max(1, 3n)$ for real flavors; $lwork \ge max(1, 2n)$ for complex flavors.rworkREAL for cgeesDOUBLE PRECISION for zgeesWorkspace array, DIMENSION at least max(1, n). Used	ldvs	Constraints: $ldvs \ge 1$ ;
DOUBLE PRECISION for zgees Workspace array, DIMENSION at least $max(1, n)$ . Used	lwork	Constraint: $lwork \ge max(1, 3n)$ for real flavors;
	rwork	DOUBLE PRECISION for zgees Workspace array, DIMENSION at least $max(1, n)$ . Used

bwork

#### LOGICAL.

Workspace array, DIMENSION at least max(1, n). Not referenced if *sort* = 'N'.

## **Output Parameters**

Output l'arameters		
a	On exit, this array is overwritten by the real-Schur/Schur form $T$ .	
sdim	INTEGER. If sort ='N', sdim=0. If sort ='S', sdim is equal to the number of eigenvalues (after sorting) for which select is true. Note that for real flavors complex conjugate pairs for which select is true for either eigenvalue count as 2.	
wr, wi	REAL for sgees DOUBLE PRECISION for dgees Arrays, DIMENSION at least max (1, <i>n</i> ) each. Contain the real and imaginary parts, respectively, of the computed eigenvalues, in the same order that they appear on the diagonal of the output real-Schur form <i>T</i> . Complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having positive imaginary part first.	
W	COMPLEX for cgees DOUBLE COMPLEX for zgees. Array, DIMENSION at least $\max(1,n)$ . Contains the computed eigenvalues. The eigenvalues are stored in the same order as they appear on the diagonal of the output Schur form <i>T</i> .	
VS	REAL for sgees DOUBLE PRECISION for dgees COMPLEX for cgees DOUBLE COMPLEX for zgees. Array vs(ldvs,*); the second dimension of vs must be at least max(1, n).	

 $\boldsymbol{v}$ 

	If $jobvs = 'V'$ , $vs$ contains the orthogonal/unitary matrix Z of Schur vectors. If $jobvs = 'N'$ , $vs$ is not referenced.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	<b>INTEGER</b> . If $info = 0$ , the execution is successful.
	If $info = -i$ , the <i>i</i> th parameter had an illegal value.
	If $info = i$ , and $i \leq n$ :
	the <i>QR</i> algorithm failed to compute all the eigenvalues; elements 1: <i>ilo</i> -1 and <i>i</i> +1: <i>n</i> of <i>wr</i> and <i>wi</i> (for real flavors) or <i>w</i> (for complex flavors) contain those eigenvalues which have converged; if <i>jobvs</i> = 'V', <i>vs</i> contains the matrix which reduces <i>A</i> to its partially converged Schur form;
	i = n+1 :
	the eigenvalues could not be reordered because some eigenvalues were too close to separate (the problem is very ill-conditioned);
	i = n+2 :
	after reordering, roundoff changed values of some complex eigenvalues so that leading eigenvalues in the Schur form no longer satisfy <i>select</i> = .TRUE This could also be caused by underflow due to

# **Application Notes**

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

scaling.

# ?geesx

Computes the eigenvalues and Schur factorization of a general matrix, orders the factorization and computes reciprocal condition numbers.

### **Discussion**

This routine computes for an *n*-by-*n* real/complex nonsymmetric matrix *A*, the eigenvalues, the real-Schur/Schur form *T*, and, optionally, the matrix of Schur vectors *Z*. This gives the Schur factorization  $A = ZTZ^{H}$ .

Optionally, it also orders the eigenvalues on the diagonal of the real-Schur/Schur form so that selected eigenvalues are at the top left; computes a reciprocal condition number for the average of the selected eigenvalues (*rconde*); and computes a reciprocal condition number for the right invariant subspace corresponding to the selected eigenvalues (*rcondv*). The leading columns of Z form an orthonormal basis for this invariant subspace.

For further explanation of the reciprocal condition numbers *rconde* and *rcondv*, see [*LUG*], Section 4.10 (where these quantities are called *s* and *sep* respectively).

A real matrix is in real-Schur form if it is upper quasi-triangular with 1-by-1 and 2-by-2 blocks. 2-by-2 blocks will be standardized in the form

```
\begin{pmatrix} a & b \\ c & a \end{pmatrix}
```

where  $b \star c < 0$ . The eigenvalues of such a block are  $a \pm \sqrt{bc}$ .

A complex matrix is in Schur form if it is upper triangular.

jobvs	CHARACTER*1. Must be 'N' or 'V'. If <i>jobvs</i> = 'N', then Schur vectors are not computed. If <i>jobvs</i> = 'V', then Schur vectors are computed.
sort	CHARACTER*1. Must be 'N' or 'S'. Specifies whether or not to order the eigenvalues on the diagonal of the Schur form.
	If <i>sort</i> = 'N', then eigenvalues are not ordered. If <i>sort</i> = 'S', eigenvalues are ordered (see <i>select</i> ).
select	LOGICAL FUNCTION of two REAL arguments for real flavors. LOGICAL FUNCTION of one COMPLEX argument for complex flavors.
	select must be declared EXTERNAL in the calling subroutine. If sort = 'S', select is used to select eigenvalues to sort to the top left of the Schur form. If sort = 'N', select is not referenced. For real flavors: An eigenvalue $wr(j) + \sqrt{-1} *wi(j)$ is selected if select( $wr(j), wi(j)$ ) is true; that is, if either one of a complex conjugate pair of eigenvalues is selected, then both complex eigenvalues are selected. Note that a selected complex eigenvalue may no longer satisfy select( $wr(j), wi(j)$ ) = .TRUE. after ordering, since ordering may change the value of complex eigenvalues (especially if the eigenvalue is ill-conditioned); in this case info may be set to $n+2$ (see info below). For complex flavors: An eigenvalue $w(j)$ is selected if select( $w(j)$ ) is true.

sense	CHARACTER*1. Must be 'N', 'E', 'V', or 'B'. Determines which reciprocal condition number are computed.
	If sense = 'N', none are computed; If sense = 'E', computed for average of selected eigenvalues only; If sense = 'V', computed for selected right invariant subspace only;
	If $sense = 'B'$ , computed for both.
	If sense is 'E', 'V', or 'B', then sort must equal 'S'.
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
a, work	REAL for sgeesx DOUBLE PRECISION for dgeesx COMPLEX for cgeesx
	DOUBLE COMPLEX for zgeesx.
	Arrays: a(1da, *) is an array containing the <i>n</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, n)$ .
ldvs	<b>INTEGER.</b> The leading dimension of the output array <i>vs</i> . Constraints: $ldvs \ge 1$ ;
	$ldvs \ge max(1, n)$ if jobvs = 'V'.
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> . Constraint: $lwork \ge max(1, 3n)$ for real flavors; $lwork \ge max(1, 2n)$ for complex flavors.
	Also, if <i>sense</i> = 'E', 'V', or 'B', then $lwork \ge n+2*sdim*(n-sdim)$ for real flavors; $lwork \ge 2*sdim*(n-sdim)$ for complex flavors;

	where <i>sdim</i> is the number of selected eigenvalues computed by this routine. Note that $2*sdim*(n-sdim) \leq n*n/2$ .
	For good performance, <i>lwork</i> must generally be larger.
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> ( <i>liwork</i> ). Used in real flavors only. Not referenced if <i>sense</i> = 'N' or 'E'.
liwork	<pre>INTEGER. The dimension of the array iwork. Used in real flavors only. Constraint: liwork ≥ 1; if sense = 'V' or 'B', liwork ≥ sdim*(n-sdim).</pre>
rwork	REAL for cgeesx DOUBLE PRECISION for zgeesx Workspace array, DIMENSION at least max(1, <i>n</i> ). Used in complex flavors only.
bwork	LOGICAL. Workspace array, DIMENSION at least $max(1, n)$ . Not referenced if <i>sort</i> = 'N'.
Output Parameters	
a	On exit, this array is overwritten by the real-Schur/Schur form $T$ .
sdim	INTEGER. If sort ='N', sdim=0. If sort ='S', sdim is equal to the number of eigenvalues (after sorting) for which select is true. Note that for real flavors complex conjugate pairs for which select is true for either eigenvalue count as 2.
wr, wi	REAL for sgeesx DOUBLE PRECISION for dgeesx Arrays, DIMENSION at least max (1, <i>n</i> ) each. Contain the real and imaginary parts, respectively, of the computed eigenvalues, in the same order that they appear on the diagonal of the output real-Schur form <i>T</i> .

Complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having positive imaginary part first.

COMPLEX for cgeesx DOUBLE COMPLEX for zgeesx.

Array, DIMENSION at least max(1,*n*).

Contains the computed eigenvalues. The eigenvalues are stored in the same order as they appear on the diagonal of the output Schur form *T*.

W

	-
VS	REAL for sgeesx
	DOUBLE PRECISION for dgeesx
	COMPLEX for cgeesx
	DOUBLE COMPLEX for zgeesx.
	Array $vs(ldvs, *)$ ; the second dimension of $vs$ must
	be at least $\max(1, n)$ .
	If $jobvs = V'$ , $vs$ contains the orthogonal/unitary matrix Z of Schur vectors.
	If $jobvs = 'N'$ , vs is not referenced.
rconde,rcondv	REAL for single precision flavors DOUBLE PRECISION for double precision flavors. If sense = 'E' or 'B', rconde contains the
	reciprocal condition number for the average of the selected eigenvalues. If $sense = 'N'$ or 'V', <i>rconde</i> is not referenced.
	If <i>sense</i> = 'V' or 'B', <i>rcondv</i> contains the reciprocal condition number for the selected right invariant subspace. If <i>sense</i> = 'N' or 'E', <i>rcondv</i> is not referenced.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful.
	If $info = -i$ , the <i>i</i> th parameter had an illegal value.

```
If info = i, and i \leq n:
```

the *QR* algorithm failed to compute all the eigenvalues; elements 1:ilo-1 and i+1:n of *wr* and *wi* (for real flavors) or *w* (for complex flavors) contain those eigenvalues which have converged; if *jobvs* = 'V', *vs* contains the transformation which reduces *A* to its partially converged Schur form;

```
i = n+1 :
```

the eigenvalues could not be reordered because some eigenvalues were too close to separate (the problem is very ill-conditioned);

```
i = n+2 :
```

after reordering, roundoff changed values of some complex eigenvalues so that leading eigenvalues in the Schur form no longer satisfy *select* = .TRUE.. This could also be caused by underflow due to scaling.

# **Application Notes**

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

# ?geev

Computes the eigenvalues and left and right eigenvectors of a general matrix.

```
call sgeev ( jobvl, jobvr, n, a, lda, wr, wi, vl, ldvl, vr, ldvr,
            work, lwork, info)
call dgeev ( jobvl, jobvr, n, a, lda, wr, wi, vl, ldvl, vr, ldvr,
            work, lwork, info)
call cgeev ( jobvl, jobvr, n, a, lda, w, vl, ldvl, vr, ldvr, work,
            lwork, rwork, info)
call zgeev ( jobvl, jobvr, n, a, lda, w, vl, ldvl, vr, ldvr, work,
            lwork, rwork, info)
```

# **Discussion**

This routine computes for an *n*-by-*n* real/complex nonsymmetric matrix *A*, the eigenvalues and, optionally, the left and/or right eigenvectors. The right eigenvector v(j) of *A* satisfies

 $A * v(j) = \lambda(j) * v(j)$ 

where  $\lambda(j)$  is its eigenvalue.

The left eigenvector u(j) of A satisfies

 $u(\mathbf{j})^H * A = \lambda(\mathbf{j}) * u(\mathbf{j})^H$ 

where  $u(j)^H$  denotes the conjugate transpose of u(j).

The computed eigenvectors are normalized to have Euclidean norm equal to 1 and largest component real.

### **Input Parameters**

jobvl

CHARACTER*1. Must be 'N' or 'V'. If jobvl = 'N', then left eigenvectors of A are not computed. If jobvl = 'V', then left eigenvectors of A are computed.

jobvr	CHARACTER*1. Must be 'N' or 'V'. If <i>jobvr</i> = 'N', then right eigenvectors of <i>A</i> are not computed. If <i>jobvr</i> = 'V', then right eigenvectors of <i>A</i> are computed.
п	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .
a, work	REAL for sgeev DOUBLE PRECISION for dgeev COMPLEX for cgeev DOUBLE COMPLEX for zgeev. Arrays: a(lda,*) is an array containing the <i>n</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of the array $a$ . Must be at least max $(1, n)$ .
ldvl, ldvr	<b>INTEGER.</b> The leading dimensions of the output arrays vl and vr, respectively. Constraints: $ldvl \ge 1$ ; $ldvr \ge 1$ . If $jobvl = 'V'$ , $ldvl \ge max(1, n)$ ; If $jobvr = 'V'$ , $ldvr \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array work. Constraint: $lwork \ge max(1, 3n)$ , and if $jobvl = 'V'$ or $jobvr = 'V'$ , $lwork \ge max(1, 4n)$ (for real flavors); $lwork \ge max(1, 2n)$ (for complex flavors). For good performance, $lwork$ must generally be larger.
rwork	REAL for cgeev DOUBLE PRECISION for zgeev Workspace array, DIMENSION at least max(1, 2n). Used in complex flavors only.

# **Output Parameters**

а	On exit, this array is overwritten by intermediate results.
wr, wi	REAL for sgeev DOUBLE PRECISION for dgeev Arrays, DIMENSION at least max (1, <i>n</i> ) each. Contain the real and imaginary parts, respectively, of the computed eigenvalues. Complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having positive imaginary part first.
W	COMPLEX for cgeev DOUBLE COMPLEX for zgeev. Array, DIMENSION at least max(1,n). Contains the computed eigenvalues.
vl, vr	REAL for sgeev DOUBLE PRECISION for dgeev COMPLEX for cgeev DOUBLE COMPLEX for zgeev. Arrays: v1(1dv1,*); the second dimension of v1 must be at least max(1, n).
	If $jobvl = 'V'$ , the left eigenvectors $u(j)$ are stored one after another in the columns of $vl$ , in the same order as their eigenvalues. If $jobvl = 'N', vl$ is not referenced. <i>For real flavors:</i> If the j-th eigenvalue is real, then $u(j) = vl(:,j)$ , the j-th column of $vl$ . If the j-th and $(j+1)$ -st eigenvalues form a complex conjugate pair, then $u(j) = vl(:,j) + i*vl(:,j+1)$ and $u(j+1) = vl(:,j) - i*vl(:,j+1)$ , where $i = \sqrt{-1}$ .
	For complex flavors: u(j) = vl(:,j), the j-th column of vl.
	vr(ldvr, *); the second dimension of $vr$ must be at least max $(1, n)$ .
	If $jobvr = V'$ , the right eigenvectors $v(j)$ are stored one

If jobvr = V', the right eigenvectors v(j) are stored one after another in the columns of vr, in the same order as their eigenvalues. If jobvr = N', vr is not referenced. For real flavors:

	If the j-th eigenvalue is real, then $v(j) = vr(:,j)$ , the j-th column of $vr$ . If the j-th and (j+1)-st eigenvalues form a complex conjugate pair, then $v(j) = vr(:,j) + i*vr(:,j+1)$ and $v(j+1) = vr(:,j) - i*vr(:,j+1)$ , where $i = \sqrt{-1}$ .
	For complex flavors: v(j) = vr(:,j), the j-th column of $vr$ .
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , the <i>QR</i> algorithm failed to compute all the eigenvalues, and no eigenvectors have been computed; elements $i+1:n$ of <i>wr</i> and <i>wi</i> (for real flavors) or <i>w</i> (for complex flavors) contain those eigenvalues which have converged.

# **Application Notes**

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

# ?geevx

Computes the eigenvalues and left and right eigenvectors of a general matrix, with preliminary matrix balancing, and computes reciprocal condition numbers for the eigenvalues and right eigenvectors.

### **Discussion**

This routine computes for an n-by-n real/complex nonsymmetric matrix A, the eigenvalues and, optionally, the left and/or right eigenvectors.

Optionally also, it computes a balancing transformation to improve the conditioning of the eigenvalues and eigenvectors (*ilo*, *ihi*, *scale*, and *abnrm*), reciprocal condition numbers for the eigenvalues (*rconde*), and reciprocal condition numbers for the right eigenvectors (*rcondv*).

The right eigenvector v(j) of A satisfies

 $A \star v(j) = \lambda(j) \star v(j)$ 

where  $\lambda(j)$  is its eigenvalue.

The left eigenvector u(j) of A satisfies

 $u(\mathbf{j})^{H} * A = \lambda(\mathbf{j}) * u(\mathbf{j})^{H}$ 

where  $u(j)^H$  denotes the conjugate transpose of u(j).

The computed eigenvectors are normalized to have Euclidean norm equal to 1 and largest component real.

Balancing a matrix means permuting the rows and columns to make it more nearly upper triangular, and applying a diagonal similarity transformation  $DAD^{-1}$ , where D is a diagonal matrix, to make its rows and columns closer in norm and the condition numbers of its eigenvalues and eigenvectors smaller. The computed reciprocal condition numbers correspond to the balanced matrix.

Permuting rows and columns will not change the condition numbers in exact arithmetic) but diagonal scaling will. For further explanation of balancing, see [*LUG*], Section 4.10.

### **Input Parameters**

```
balanc
```

CHARACTER*1. Must be 'N', 'P', 'S', or 'B'. Indicates how the input matrix should be diagonally scaled and/or permuted to improve the conditioning of its eigenvalues.

If *balanc* = 'N', do not diagonally scale or permute; If *balanc* = 'P', perform permutations to make the matrix more nearly upper triangular. Do not diagonally scale;

If *balanc* = 'S', Diagonally scale the matrix, i.e. replace A by  $D A D^{-1}$ , where D is a diagonal matrix chosen to make the rows and columns of A more equal in norm. Do not permute;

If *balanc* = 'B', both diagonally scale and permute *A*.

Computed reciprocal condition numbers will be for the matrix after balancing and/or permuting. Permuting does not change condition numbers (in exact arithmetic), but balancing does.

```
jobv1 CHARACTER*1. Must be 'N' or 'V'.
If jobv1 = 'N', left eigenvectors of A are not computed;
If jobv1 = 'V', left eigenvectors of A are computed.
If sense = 'E' or 'B', then jobv1 must be 'V'.
```

jobvr	CHARACTER*1. Must be 'N' or 'V'. If <i>jobvr</i> = 'N', right eigenvectors of <i>A</i> are not computed; If <i>jobvr</i> = 'V', right eigenvectors of <i>A</i> are computed. If <i>sense</i> = 'E' or 'B', then <i>jobvr</i> must be 'V'.
sense	CHARACTER*1. Must be 'N', 'E', 'V', or 'B'. Determines which reciprocal condition number are computed.
	If <i>sense</i> = 'N', none are computed; If <i>sense</i> = 'E', computed for eigenvalues only; If <i>sense</i> = 'V', computed for right eigenvectors only; If <i>sense</i> = 'B', computed for eigenvalues and right eigenvectors.
	If <i>sense</i> is 'E' or 'B', both left and right eigenvectors must also be computed ( <i>jobv1</i> = 'V' and <i>jobvr</i> = 'V').
п	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
a, work	REAL for sgeevx DOUBLE PRECISION for dgeevx COMPLEX for cgeevx DOUBLE COMPLEX for zgeevx. Arrays:
	a(lda,*) is an array containing the <i>n</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of the array $a$ . Must be at least max $(1, n)$ .
ldvl, ldvr	<b>INTEGER.</b> The leading dimensions of the output arrays vl and vr, respectively. Constraints: $ldvl \ge 1$ ; $ldvr \ge 1$ . If $jobvl = 'V'$ , $ldvl \ge max(1, n)$ ; If $jobvr = 'V'$ , $ldvr \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> . For real flavors: If sense = 'N' or 'E', <i>lwork</i> $\ge \max(1, 2n)$ , and

	if $jobvl = 'V'$ or $jobvr = 'V'$ , $lwork \ge 3n$ ; If $sense = 'V'$ or 'B', $lwork \ge n(n+6)$ . For good performance, $lwork$ must generally be larger.
	For complex flavors: If sense = 'N'or 'E', lwork $\ge \max(1, 2n)$ ; If sense = 'V'or 'B', lwork $\ge n^2+2n$ . For good performance, lwork must generally be larger.
rwork	REAL for cgeevx DOUBLE PRECISION for zgeevx Workspace array, DIMENSION at least max(1, 2n). Used in complex flavors only.
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least max $(1, 2n-2)$ . Used in real flavors only. Not referenced if <i>sense</i> = $'N'$ or 'E'.

a	On exit, this array is overwritten. If $jobvl = V'$ or $jobvr = V'$ , it contains the real-Schur/Schur form of the balanced version of the input matrix A.
wr, wi	REAL for sgeevx DOUBLE PRECISION for dgeevx Arrays, DIMENSION at least max (1, <i>n</i> ) each. Contain the real and imaginary parts, respectively, of the computed eigenvalues. Complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having positive imaginary part first.
W	COMPLEX for cgeevx DOUBLE COMPLEX for zgeevx. Array, DIMENSION at least $max(1,n)$ . Contains the computed eigenvalues.
vl, vr	REAL for sgeevx DOUBLE PRECISION for dgeevx COMPLEX for cgeevx DOUBLE COMPLEX for zgeevx.

Arrays:

vl(ldvl, *); the second dimension of vl must be at least max(1, n).

If jobvl = 'V', the left eigenvectors u(j) are stored one after another in the columns of vl, in the same order as their eigenvalues. If jobvl = 'N', vl is not referenced. For real flavors:

If the j-th eigenvalue is real, then u(j) = vl(:,j), the j-th column of vl. If the j-th and (j+1)-st eigenvalues form a complex conjugate pair, then u(j) = vl(:,j) + i*vl(:,j+1) and u(j+1) = vl(:,j) - i*vl(:,j+1), where  $i = \sqrt{-1}$ .

For complex flavors:

u(j) = v1(:,j), the j-th column of v1.

vr(ldvr, *); the second dimension of vr must be at least max(1, n).

If jobvr = V', the right eigenvectors v(j) are stored one after another in the columns of vr, in the same order as their eigenvalues. If jobvr = N', vr is not referenced. For real flavors:

If the j-th eigenvalue is real, then v(j) = vr(:,j), the j-th column of vr. If the j-th and (j+1)-st eigenvalues form a complex conjugate pair, then v(j) = vr(:,j) + i*vr(:,j+1) and v(j+1) = vr(:,j) - i*vr(:,j+1), where  $i = \sqrt{-1}$ .

For complex flavors: v(j) = vr(:,j), the j-th column of vr.

INTEGER.

ilo, ihi

*ilo* and *ihi* are integer values determined when A was balanced.

The balanced A(i,j) = 0 if i > j and j = 1,..., ilo-1 or i = ihi+1,..., n.

If balanc = 'N' or 'S', ilo = 1 and ihi = n.

scale

**REAL** for single-precision flavors **DOUBLE PRECISION** for double-precision flavors.

Array, **DIMENSION** at least max(1, n).

Details of the permutations and scaling factors applied

	when balancing <i>A</i> . If $P(j)$ is the index of the row and column interchanged with row and column j, and $D(j)$ is the scaling factor applied to row and column j, then
	$scale(j) = P(j), \text{ for } j = 1, \dots, ilo-1$
	= D(j),  for  j = ilo,,ihi
	$= P(\mathbf{j})  \text{for } \mathbf{j} = \mathbf{i}\mathbf{h}\mathbf{i} + 1, \dots, \mathbf{n}.$
	The order in which the interchanges are made is $n$ to $ihi+1$ , then 1 to $ilo-1$ .
abnrm	<b>REAL</b> for single-precision flavors
	DOUBLE PRECISION for double-precision flavors.
	The one-norm of the balanced matrix (the maximum of the sum of absolute values of elements of any column).
rconde,rcondv	REAL for single precision flavors DOUBLE PRECISION for double precision flavors. Arrays, DIMENSION at least max(1, n) each. <i>rconde</i> (j) is the reciprocal condition number of the j-th eigenvalue.
	<i>rcondv</i> (j) is the reciprocal condition number of the j-th right eigenvector.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , the <i>QR</i> algorithm failed to compute all the eigenvalues, and no eigenvectors or condition numbers have been computed; elements $1:ilo-1$ and $i+1:n$ of <i>wr</i> and <i>wi</i> (for real flavors) or <i>w</i> (for complex flavors) contain eigenvalues which have converged.

#### **Application Notes**

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

### **Singular Value Decomposition**

This section describes LAPACK driver routines used for solving singular value problems. See also <u>computational routines</u> that can be called to solve these problems.

Table 5-12 lists routines described in more detail below.

#### Table 5-12 Driver Routines for Singular Value Decomposition

Routine Name	Operation performed
?gesvd	Computes the singular value decomposition of a general rectangular matrix.
?gesdd	Computes the singular value decomposition of a general rectangular matrix using a divide and conquer method.
?ggsvd	Computes the generalized singular value decomposition of a pair of general rectangular matrices.

# ?gesvd

Computes the singular value decomposition of a general rectangular matrix.

call sgesvd ( jo wo	bu, jobvt, m, n rk, lwork, info	s, u,	ldu, vt,	ldvt,
call dgesvd ( <i>jo</i> wo	bu, jobvt, m, n rk, lwork, info	s, u,	ldu, vt,	ldvt,
call cgesvd ( jo wo	bu, jobvt, m, n rk, lwork, rwori	s, u,	ldu, vt,	ldvt,
call zgesvd ( <i>jo</i> wo	bu, jobvt, m, n rk, lwork, rwori	s, u,	ldu, vt,	ldvt,

#### **Discussion**

This routine computes the singular value decomposition (SVD) of a real/complex m-by-n matrix A, optionally computing the left and/or right singular vectors. The SVD is written

 $A = U \Sigma V^{H}$ 

where  $\Sigma$  is an *m*-by-*n* matrix which is zero except for its min(*m*,*n*) diagonal elements, *U* is an *m*-by-*m* orthogonal/unitary matrix, and *V* is an *n*-by-*n* orthogonal/unitary matrix. The diagonal elements of  $\Sigma$  are the singular values of *A*; they are real and non-negative, and are returned in descending order. The first min(*m*,*n*) columns of *U* and *V* are the left and right singular vectors of *A*.

Note that the routine returns  $V^H$ , not V.

jobu	CHARACTER*1. Must be 'A', 'S', 'O', or 'N'. Specifies options for computing all or part of the matrix $U$ .
	If <i>jobu</i> = 'A', all <i>m</i> columns of <i>U</i> are returned in the array <i>u</i> ; if <i>jobu</i> = 'S', the first min( <i>m</i> , <i>n</i> ) columns of <i>U</i> (the left singular vectors) are returned in the array <i>u</i> ; if <i>jobu</i> = 'O', the first min( <i>m</i> , <i>n</i> ) columns of <i>U</i> (the left singular vectors) are overwritten on the array <i>a</i> ; if <i>jobu</i> = 'N', no columns of <i>U</i> (no left singular vectors) are computed.
jobvt	CHARACTER*1. Must be 'A', 'S', 'O', or 'N'. Specifies options for computing all or part of the matrix $V^{H}$ .
	If $jobvt = 'A'$ , all <i>n</i> rows of $V^H$ are returned in the array $vt$ ; if $jobvt = 'S'$ , the first $min(m,n)$ rows of $V^H$ (the right singular vectors) are returned in the array $vt$ ; if $jobvt = 'O'$ , the first $min(m,n)$ rows of $V^H$ (the right singular vectors) are overwritten on the array <i>a</i> ; if $jobvt = 'N'$ , no rows of $V^H$ (no right singular vectors) are computed.
	jobvt and $jobu$ cannot both be 'O'.
т	<b>INTEGER.</b> The number of rows of the matrix $A \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .

a, work	REAL for sgesvd DOUBLE PRECISION for dgesvd COMPLEX for cgesvd DOUBLE COMPLEX for zgesvd. Arrays: a(lda,*) is an array containing the <i>m</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of the array $a$ . Must be at least max $(1, m)$ .
ldu, ldvt	<b>INTEGER.</b> The leading dimensions of the output arrays $u$ and $vt$ , respectively. Constraints: $ldu \ge 1$ ; $ldvt \ge 1$ . If $jobu = 'S'$ or 'A', $ldu \ge m$ ; If $jobvt = 'A'$ , $ldvt \ge n$ ; If $jobvt = 'S'$ , $ldvt \ge min(m, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> ; <i>lwork</i> $\geq$ 1. Constraints: <i>lwork</i> $\geq$ max(3*min( <i>m</i> , <i>n</i> )+max( <i>m</i> , <i>n</i> ), 5*min( <i>m</i> , <i>n</i> )) (for real flavors); <i>lwork</i> $\geq$ 2*min( <i>m</i> , <i>n</i> )+max( <i>m</i> , <i>n</i> ) (for complex flavors). For good performance, <i>lwork</i> must generally be larger.
rwork	<b>REAL for cgesvd</b> <b>DOUBLE PRECISION for zgesvd</b> Workspace array, <b>DIMENSION</b> at least max(1, 5*min(m,n)). Used in complex flavors only.

а

On exit, If jobu = '0', *a* is overwritten with the first min(m,n) columns of *U* (the left singular vectors, stored columnwise); If jobvt = '0', *a* is overwritten with the first min(m,n)

	rows of $V^H$ (the right singular vectors, stored rowwise); If $jobu \neq 0^{\circ}$ and $jobvt \neq 0^{\circ}$ , the contents of a are destroyed.
S	<b>REAL</b> for single precision flavors <b>DOUBLE PRECISION</b> for double precision flavors. Array, <b>DIMENSION</b> at least max(1, min( $m,n$ )). Contains the singular values of <i>A</i> sorted so that $s(i) \ge s(i+1)$ .
u, vt	REAL for sgesvd DOUBLE PRECISION for dgesvd COMPLEX for cgesvd DOUBLE COMPLEX for zgesvd. Arrays: u(1du, *); the second dimension of $u$ must be at least max(1, m) if $jobu = 'A'$ , and at least $max(1, min(m,n))$ if jobu = 'S'.
	If $jobu = 'A'$ , <i>u</i> contains the <i>m</i> -by- <i>m</i> orthogonal/unitary matrix <i>U</i> . If $jobu = 'S'$ , <i>u</i> contains the first $min(m,n)$ columns of <i>U</i> (the left singular vectors, stored columnwise). If $jobu = 'N' \text{ or } 'O'$ , <i>u</i> is not referenced.
	vt(ldvt, *); the second dimension of $vt$ must be at least max $(1, n)$ .
	If $jobvt = 'A'$ , $vt$ contains the <i>n</i> -by- <i>n</i> orthogonal/unitary matrix $V^H$ . If $jobvt = 'S'$ , $vt$ contains the first min( <i>m</i> , <i>n</i> ) rows of $V^H$ (the right singular vectors, stored rowwise). If $jobvt = 'N'or 'O'$ , $vt$ is not referenced.
work	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> . For real flavors: If <i>info</i> > 0, <i>work</i> (2:min( <i>m</i> , <i>n</i> )) contains the unconverged superdiagonal elements of an upper bidiagonal matrix <i>B</i> whose diagonal is in <i>s</i> (not

	necessarily sorted). <i>B</i> satisfies $A = u * B * vt$ , so it has the same singular values as <i>A</i> , and singular vectors related by <i>u</i> and <i>vt</i> .
rwork	On exit (for complex flavors), if $info > 0$ , rwork(1:min(m,n)-1) contains the unconverged superdiagonal elements of an upper bidiagonal matrix $B$ whose diagonal is in $s$ (not necessarily sorted). $B$ satisfies $A = u * B * vt$ , so it has the same singular values as $A$ , and singular vectors related by $u$ and $vt$ .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , then if ?bdsqr did not converge, <i>i</i> specifies how many superdiagonals of the intermediate bidiagonal form <i>B</i> did not converge to zero.

### **Application Notes**

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

# ?gesdd

Computes the singular value decomposition of a general rectangular matrix using a divide and conquer method.

#### **Discussion**

This routine computes the singular value decomposition (SVD) of a real/complex *m*-by-*n* matrix *A*, optionally computing the left and/or right singular vectors. If singular vectors are desired, it uses a divide and conquer algorithm.

The SVD is written

 $A = U \Sigma V^H$ 

where  $\Sigma$  is an *m*-by-*n* matrix which is zero except for its min(*m*,*n*) diagonal elements, *U* is an *m*-by-*m* orthogonal/unitary matrix, and *V* is an *n*-by-*n* orthogonal/unitary matrix. The diagonal elements of  $\Sigma$  are the singular values of *A*; they are real and non-negative, and are returned in descending order. The first min(*m*,*n*) columns of *U* and *V* are the left and right singular vectors of *A*.

Note that the routine returns  $V^H$ , not V.

#### **Input Parameters**

*jobz* CHARACTER*1. Must be 'A', 'S', 'O', or 'N'. Specifies options for computing all or part of the matrix U.

	If $jobz = 'A'$ , all <i>m</i> columns of <i>U</i> and all <i>n</i> rows of $V^T$ are returned in the arrays <i>u</i> and <i>vt</i> ; if $jobz = 'S'$ , the first min( <i>m</i> , <i>n</i> ) columns of <i>U</i> and the first min( <i>m</i> , <i>n</i> ) rows of $V^T$ are returned in the arrays <i>u</i> and <i>vt</i> ; if $jobz = 'O'$ , then if $m \ge n$ , the first <i>n</i> columns of <i>U</i> are overwritten on the array <i>a</i> and all rows of $V^T$ are returned in the
	array $vt$ ; if $m < n$ , all columns of $U$ are returned in the array $u$ and the first $m$ rows of $V^T$ are overwritten in the array $vt$ ;
	if $jobz = 'N'$ , no columns of U or rows of $V^T$ are computed.
m	<b>INTEGER.</b> The number of rows of the matrix $A (m \ge 0)$ .
п	<b>INTEGER</b> . The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgesdd DOUBLE PRECISION for dgesdd COMPLEX for cgesdd DOUBLE COMPLEX for zgesdd. Arrays: a(lda,*) is an array containing the <i>m</i> -by- <i>n</i> matrix <i>A</i> .
	The second dimension of $a$ must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, m)$ .
ldu, ldvt	INTEGER. The leading dimensions of the output arrays $u$ and $vt$ , respectively. Constraints: $ldu \ge 1$ ; $ldvt \ge 1$ . If $jobz = 'S'$ or 'A', or $jobz = 'O'$ and $m < n$ , then $ldu \ge m$ ; If $jobz = 'A'$ or $jobz = 'O'$ and $m \ge n$ , then $ldvt \ge n$ ; If $jobz = 'S'$ , $ldvt \ge \min(m, n)$ .

lwork	<b>INTEGER</b> . The dimension of the array work; $lwork \ge 1$ . See <i>Application Notes</i> for the suggested value of $lwork$ .
rwork	REAL for cgesdd
	DOUBLE PRECISION for zgesdd
	Workspace array, <b>DIMENSION</b> at least
	$\max(1, 5*\min(m,n))$ if $jobz = 'N'$ . Otherwise, the
	dimension of <i>rwork</i> must be at least $5 * (\min(m,n))^2 +$
	$7 \times \min(m,n)$ . This array is used in complex flavors only.
iwork	INTEGER. Workspace array, DIMENSION at least
	$\max(1, 8 * \min(\underline{m}, \underline{n})).$

a	On exit: If $jobz = 0^{\circ}$ , then if $m \ge n$ , <i>a</i> is overwritten with the first <i>n</i> columns of <i>U</i> (the left singular vectors, stored columnwise). If $m < n$ , <i>a</i> is overwritten with the first <i>m</i> rows of $V^T$ (the right singular vectors, stored rowwise); If $jobz \ne 0^{\circ}$ , the contents of <i>a</i> are destroyed.
S	<b>REAL</b> for single precision flavors <b>DOUBLE PRECISION</b> for double precision flavors. Array, <b>DIMENSION</b> at least max $(1, \min(m,n))$ . Contains the singular values of A sorted so that $s(i) \ge s(i+1)$ .
u, vt	REAL for sgesdd DOUBLE PRECISION for dgesdd COMPLEX for cgesdd DOUBLE COMPLEX for zgesdd. Arrays: u(ldu,*); the second dimension of $u$ must be at least max(1, m) if $jobz = 'A'$ or $jobz = '0'$ and $m < n$ . If $jobz = 'S'$ , the second dimension of $u$ must be at least $max(1, min(m,n))$ . If $jobz = 'A'$ or $jobz = '0'$ and $m < n, u$ contains the m-by- $m$ orthogonal/unitary matrix $U$ . If $jobz = 'S', u$ contains the first $min(m,n)$ columns of

	U (the left singular vectors, stored columnwise). If $jobz = 0'$ and $m \ge n$ , or $jobz = N'$ , u is not referenced.
	vt(ldvt, *); the second dimension of $vt$ must be at least max $(1, n)$ .
	If $jobz = 'A'$ or $jobz = '0'$ and $m \ge n, vt$ contains the <i>n</i> -by- <i>n</i> orthogonal/unitary matrix $V^T$ . If $jobz = 'S', vt$ contains the first min $(m,n)$ rows of $V^T$ (the right singular vectors, stored rowwise). If $jobz = '0'$ and $m < n$ , or $jobz = 'N', vt$ is not referenced.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , then ?bdsdc did not converge, updating process failed.

#### **Application Notes**

For real flavors:

For complex flavors:

If jobz = 'N',  $lwork \ge 2*min(m,n) + max(m,n)$ ; If jobz = 'O',  $lwork \ge 2*(min(m,n))^2 + max(m,n) + 2*min(m,n)$ ; If jobz = 'S' or 'A',  $lwork \ge (min(m,n))^2 + max(m,n) + 2*min(m,n)$ ;

For good performance, *lwork* should generally be larger.

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

# ?ggsvd

Computes the generalized singular value decomposition of a pair of general rectangular matrices.

#### **Discussion**

This routine computes the generalized singular value decomposition (GSVD) of an *m*-by-*n* real/complex matrix *A* and *p*-by-*n* real/complex matrix *B*:

 $U^H A Q = D_1^*(0 R), \quad V^H B Q = D_2^*(0 R),$ where U, V and Q are orthogonal/unitary matrices.

Let k+1 = the effective numerical rank of the matrix  $(A^H, B^H)^H$ , then *R* is a (k+1)-by-(k+1) nonsingular upper triangular matrix,  $D_1$  and  $D_2$  are *m*-by-(k+1) and *p*-by-(k+1) "diagonal" matrices and of the following structures, respectively:

If  $m-k-1 \geq 0$ ,

$$D_{1} = \begin{matrix} k \\ I \\ m - k - l \end{matrix} \begin{pmatrix} k & l \\ I & 0 \\ 0 & C \\ 0 & 0 \end{pmatrix}$$

$$D_2 = \frac{l}{p-l} \begin{pmatrix} k & l \\ 0 & S \\ 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} n-k-l & k & l \\ k & 0 & R_{11} & R_{12} \\ 0 & 0 & R_{22} \end{pmatrix}$$

where

$$C = \text{diag} ( alpha(k+1),...,alpha(k+1))$$
  

$$S = \text{diag} ( beta(k+1),...,beta(k+1))$$
  

$$C^{2} + S^{2} = I$$

*R* is stored in a(1:k+1, n-k-1+1:n) on exit.

If m-k-1 < 0,  $k \quad m-k \quad k+l-m$   $D_1 = \begin{array}{c} k \\ m-k \end{array} \begin{pmatrix} I & 0 & 0 \\ 0 & C & 0 \end{pmatrix}$   $k \quad m-k \quad k+l-m$ 

$$D_{2} = k + l - m \begin{pmatrix} 0 & S & 0 \\ 0 & 0 & I \\ p - l & 0 & 0 \end{pmatrix}$$

 $(0 R) = m-k \begin{pmatrix} 0 & R_{11} & R_{12} & R_{13} \\ 0 & 0 & R_{22} & R_{23} \\ k+l-m \begin{pmatrix} 0 & 0 & R_{22} & R_{23} \\ 0 & 0 & 0 & R_{33} \end{pmatrix}$ 

where

$$C = \text{diag} ( alpha(k+1),...,alpha(m)),$$
  

$$S = \text{diag} ( beta(k+1),...,beta(m)),$$
  

$$C^2 + S^2 = I$$

On exit,  $\begin{pmatrix} R_{11}R_{12}R_{13} \\ 0 & R_{22}R_{23} \end{pmatrix}$  is stored in a(1:m, n-k-1+1:n) and  $R_{33}$  is stored

in *b*(*m*-*k*+1:1, *n*+*m*-*k*-1+1:*n*).

The routine computes C, S, R, and optionally the orthogonal/unitary transformation matrices U, V and Q.

In particular, if *B* is an *n*-by-*n* nonsingular matrix, then the GSVD of *A* and *B* implicitly gives the SVD of  $AB^{-1}$ :

$$AB^{-1} = U(D_1 D_2^{-1}) V^H.$$

If  $(A^H, B^H)^H$  has orthonormal columns, then the GSVD of *A* and *B* is also equal to the CS decomposition of *A* and *B*. Furthermore, the GSVD can be used to derive the solution of the eigenvalue problem:

 $A^H A x = \lambda B^H B x.$ 

jobu	CHARACTER*1. Must be 'U' or 'N'. If $jobu = 'U'$ , orthogonal/unitary matrix U is computed. If $jobu = 'N'$ , U is not computed.
jobv	CHARACTER*1. Must be 'V' or 'N'. If $jobv = 'V'$ , orthogonal/unitary matrix V is computed. If $jobv = 'N'$ , V is not computed.
jobq	CHARACTER*1. Must be 'Q' or 'N'. If $jobq = 'Q'$ , orthogonal/unitary matrix $Q$ is computed. If $jobq = 'N'$ , $Q$ is not computed.
m	<b>INTEGER.</b> The number of rows of the matrix $A \ (m \ge 0)$ .
п	<b>INTEGER.</b> The number of columns of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
P	<b>INTEGER</b> . The number of rows of the matrix $B \ (p \ge 0)$ .
a, b, work	REAL for sggsvd DOUBLE PRECISION for dggsvd COMPLEX for cggsvd DOUBLE COMPLEX for zggsvd.

	Arrays: a(lda,*) contains the <i>m</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
	b(1db, *) contains the <i>p</i> -by- <i>n</i> matrix <i>B</i> . The second dimension of <i>b</i> must be at least max $(1, n)$ .
	work(*) is a workspace array. The dimension of work must be at least $max(3n, m, p)+n$ .
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, m)$ .
ldb	<b>INTEGER</b> . The first dimension of $b$ ; at least max $(1, p)$ .
ldu	<b>INTEGER.</b> The first dimension of the array $u$ . $ldu \ge max(1, m)$ if $jobu = 'U'$ ; $ldu \ge 1$ otherwise.
ldv	<b>INTEGER.</b> The first dimension of the array $v$ . $ldv \ge max(1, p)$ if $jobv = V'$ ; $ldv \ge 1$ otherwise.
ldq	<b>INTEGER.</b> The first dimension of the array $q$ . $ldq \ge max(1, n)$ if $jobq = 'Q'$ ; $ldq \ge 1$ otherwise.
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least $max(1, n)$ .
rwork	<b>REAL for cggsvd</b> <b>DOUBLE PRECISION for zggsvd</b> . Workspace array, <b>DIMENSION</b> at least $max(1, 2n)$ . Used in complex flavors only.

k, l	<b>INTEGER.</b> On exit, $k$ and $l$ specify the dimension of the subblocks. The sum $k+l$ is equal to the effective numerical rank of $(A^H, B^H)^H$ .
a	On exit, $a$ contains the triangular matrix $R$ or part of $R$ .
b	On exit, b contains part of the triangular matrix R if $m-k-1 < 0$ .
alpha, beta	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors. Arrays, <b>DIMENSION</b> at least $max(1,n)$ each. Contain the generalized singular value pairs of A and B:

```
alpha(1:k) = 1,
                   beta(1:k) = 0,
                   and if m-k-1 \ge 0.
                   alpha(k+1:k+1) = C,
                   beta(k+1:k+1) = S,
                   or if m-k-1 < 0,
                   alpha(k+1:m) = C, alpha(m+1:k+1) = 0
                   beta(k+1:m) = S, beta(m+1:k+1) = 1
                   and
                   alpha(k+l+1:n) = 0
                   beta(k+1+1:n) = 0.
                   REAL for sqqsvd
u, v, q
                   DOUBLE PRECISION for dggsvd
                   COMPLEX for cggsvd
                   DOUBLE COMPLEX for zggsvd.
                   Arrays:
                   u(1du, *); the second dimension of u must be at least
                   \max(1, \mathbf{m}).
                   If jobu = 'U', u contains the m-by-m orthogonal/unitary
                   matrix U.
                   If jobu = 'N', u is not referenced.
                   v(ldv, *); the second dimension of v must be at least
                   \max(1, \mathbf{p}).
                   If jobv = V', v contains the p-by-p orthogonal/unitary
                   matrix V.
                   If jobv = 'N', v is not referenced.
                   q(1dq, *); the second dimension of q must be at least
                   \max(1, \mathbf{n}).
                   If jobg = 'Q', q contains the n-by-n orthogonal/unitary
                   matrix Q.
                   If jobq = 'N', q is not referenced.
                   On exit, iwork stores the sorting information.
```

iwork

info

INTEGER.

If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value. If info = 1, the Jacobi-type procedure failed to converge. For further details, see subroutine <u>?tgsja</u>.

# **Generalized Symmetric Definite Eigenproblems**

This section describes LAPACK driver routines used for solving generalized symmetric definite eigenproblems. See also <u>computational</u> <u>routines</u> that can be called to solve these problems. <u>Table 5-13</u> lists routines described in more detail below.

# Table 5-13Driver Routines for Solving Generalized Symmetric Definite<br/>Eigenproblems

Routine Name	Operation performed
?sygv/?hegv	Computes all eigenvalues and, optionally, eigenvectors of a real / complex generalized symmetric /Hermitian definite eigenproblem.
?sygvd/?hegvd	Computes all eigenvalues and, optionally, eigenvectors of a real / complex generalized symmetric /Hermitian definite eigenproblem. If eigenvectors are desired, it uses a divide and conquer method.
<u>?sygvx</u> /?hegvx	Computes selected eigenvalues and, optionally, eigenvectors of a real / complex generalized symmetric /Hermitian definite eigenproblem.
?spgv/?hpgv	Computes all eigenvalues and, optionally, eigenvectors of a real / complex generalized symmetric /Hermitian definite eigenproblem with matrices in packed storage.
?spgvd/?hpgvd	Computes all eigenvalues and, optionally, eigenvectors of a real / complex generalized symmetric /Hermitian definite eigenproblem with matrices in packed storage. If eigenvectors are desired, it uses a divide and conquer method.
?spgvx/?hpgvx	Computes selected eigenvalues and, optionally, eigenvectors of a real / complex generalized symmetric /Hermitian definite eigenproblem with matrices in packed storage.
?sbgv/?hbgv	Computes all eigenvalues and, optionally, eigenvectors of a real / complex generalized symmetric /Hermitian definite eigenproblem with banded matrices.
?sbgvd/?hbgvd	Computes all eigenvalues and, optionally, eigenvectors of a real / complex generalized symmetric /Hermitian definite eigenproblem with banded matrices. If eigenvectors are desired, it uses a divide and conquer method.
?sbgvx/?hbgvx	Computes selected eigenvalues and, optionally, eigenvectors of a real / complex generalized symmetric /Hermitian definite eigenproblem with banded matrices.

# ?sygv

Computes all eigenvalues and, optionally, eigenvectors of a real generalized symmetric definite eigenproblem.

#### **Discussion**

This routine computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, of the form

 $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here A and B are assumed to be symmetric and B is also positive definite.

itype	<b>INTEGER.</b> Must be 1 or 2 or 3. Specifies the problem type to be solved: if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ; if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ; if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then compute eigenvalues only. If <i>jobz</i> = 'V', then compute eigenvalues and eigenvectors.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays a and b store the upper triangles of A and B; If $uplo = 'L'$ , arrays a and b store the lower triangles of A and B.
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).

a, b, work	REAL for ssygv
	DOUBLE PRECISION for dsygv.
	Arrays:
	a( <i>lda</i> , *) contains the upper or lower triangle of the symmetric matrix A, as specified by <i>uplo</i> .
	• • •
	The second dimension of a must be at least $\max(1, n)$ .
	b(1db, *) contains the upper or lower triangle of the symmetric positive definite matrix <i>B</i> , as specified by
	uplo. The second dimension of $h$ must be at least max $(1, x)$
	The second dimension of $b$ must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array work; <i>lwork</i> $\ge$ max(1, 3 <i>n</i> -1).
	See Application Notes for the suggested value of <i>lwork</i> .

a	On exit, if $jobz = V'$ , then if $info = 0$ , a contains the matrix Z of eigenvectors. The eigenvectors are normalized as follows: if $itype = 1$ or 2, $Z^{T}BZ = I$ ; if $itype = 3$ , $Z^{T}B^{-1}Z = I$ ;
	If $jobz = 'N'$ , then on exit the upper triangle (if $uplo = 'U'$ ) or the lower triangle (if $uplo = 'L'$ ) of <i>A</i> , including the diagonal, is destroyed.
b	On exit, if <i>info</i> $\leq n$ , the part of <i>b</i> containing the matrix is overwritten by the triangular factor <i>U</i> or <i>L</i> from the Cholesky factorization $B = U^{T}U$ or $B = LL^{T}$ .
W	REAL for ssygv DOUBLE PRECISION for dsygv. Array, DIMENSION at least max $(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order.

work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th argument had an illegal value. If $info > 0$ , $spotrf/dpotrf$ and $ssyev/dsyev$ returned an error code: If $info = i \le n$ , $ssyev/dsyev$ failed to converge, and <i>i</i> off-diagonal elements of an intermediate tridiagonal did not converge to zero; If $info = n + i$ , for $1 \le i \le n$ , then the leading minor of order <i>i</i> of <i>B</i> is not positive-definite. The factorization of <i>B</i> could not be completed and no eigenvalues or eigenvectors were computed.

### **Application Notes**

For optimum performance use  $lwork \ge (nb+2)*n$ , where nb is the blocksize for ssytrd/dsytrd returned by ilaenv. If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

# ?hegv

Computes all eigenvalues and, optionally, eigenvectors of a complex generalized Hermitian definite eigenproblem.

#### **Discussion**

This routine computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, of the form

 $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here A and B are assumed to be Hermitian and B is also positive definite.

itype	INTEGER. Must be 1 or 2 or 3.
	Specifies the problem type to be solved: if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ;
	if <i>itype</i> = 2, the problem type is $Ax = \lambda Bx$ , if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ;
	if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ , if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'.
	If $jobz = 'N'$ , then compute eigenvalues only.
	If $jobz = V'$ , then compute eigenvalues and
	eigenvectors.
uplo	CHARACTER*1. Must be 'U' or 'L'.
	If $uplo = 'U'$ , arrays a and b store the upper triangles
	of <i>A</i> and <i>B</i> ;
	If $uplo = 'L'$ , arrays a and b store the lower triangles
	of A and B.
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).

a, b, work	COMPLEX for chegy
	DOUBLE COMPLEX for zhegv.
	Arrays:
	a(lda,*) contains the upper or lower triangle of the
	Hermitian matrix A, as specified by uplo.
	The second dimension of $a$ must be at least max $(1, n)$ .
	b(1db, *) contains the upper or lower triangle of the Hermitian positive definite matrix <i>B</i> , as specified by
	uplo.
	The second dimension of $b$ must be at least max(1, $n$ ).
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .
lwork	<b>INTEGER</b> . The dimension of the array <i>work</i> ;
	$lwork \ge max(1, 2n-1).$
	See Application Notes for the suggested value of <i>lwork</i> .
rwork	REAL for chegv
	DOUBLE PRECISION for zhegv.
	Workspace array, DIMENSION at least $max(1, 3n-2)$ .

а

b

On exit, if $jobz = V'$ , then if $info = 0$ , a contains the matrix Z of eigenvectors. The eigenvectors are normalized as follows: if $itype = 1$ or 2, $Z^{H}BZ = I$ ; if $itype = 3$ , $Z^{H}B^{-1}Z = I$ ;
If $jobz = 'N'$ , then on exit the upper triangle (if $uplo = 'U'$ ) or the lower triangle (if $uplo = 'L'$ ) of <i>A</i> , including the diagonal, is destroyed.
On exit, if <i>info</i> $\leq n$ , the part of <i>b</i> containing the matrix is overwritten by the triangular factor <i>U</i> or <i>L</i> from the Cholesky factorization $B = U^H U$ or $B = L L^H$ .

W	<b>REAL</b> for chegv <b>DOUBLE PRECISION</b> for zhegv. Array, <b>DIMENSION</b> at least $max(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith argument had an illegal value. If info &gt; 0, cpotrf/zpotrf and cheev/zheev returned an error code:</pre>
	If $info = i \leq n$ , cheev/zheev failed to converge, and <i>i</i> off-diagonal elements of an intermediate tridiagonal did not converge to zero; If $info = n + i$ , for $1 \leq i \leq n$ , then the leading minor of order <i>i</i> of <i>B</i> is not positive-definite. The factorization of <i>B</i> could not be completed and no eigenvalues or eigenvectors were computed.

### **Application Notes**

For optimum performance use  $lwork \ge (nb+1)*n$ , where nb is the blocksize for chetrd/zhetrd returned by ilaenv. If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

# ?sygvd

Computes all eigenvalues and, optionally, eigenvectors of a real generalized symmetric definite eigenproblem. If eigenvectors are desired, it uses a divide and conquer method.

#### **Discussion**

This routine computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, of the form

 $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here A and B are assumed to be symmetric and B is also positive definite.

If eigenvectors are desired, it uses a divide and conquer algorithm.

itype	<b>INTEGER.</b> Must be 1 or 2 or 3. Specifies the problem type to be solved: if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ; if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ; if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then compute eigenvalues only. If <i>jobz</i> = 'V', then compute eigenvalues and eigenvectors.

uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays <i>a</i> and <i>b</i> store the upper triangles of <i>A</i> and <i>B</i> ;
	If $uplo = 'L'$ , arrays a and b store the lower triangles of A and B.
п	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
a, b, work	<ul> <li>REAL for ssygvd</li> <li>DOUBLE PRECISION for dsygvd.</li> <li>Arrays:</li> <li>a(lda,*) contains the upper or lower triangle of the symmetric matrix A, as specified by uplo.</li> <li>The second dimension of a must be at least max(1, n).</li> </ul>
	<ul> <li>b(ldb,*) contains the upper or lower triangle of the symmetric positive definite matrix B, as specified by uplo.</li> <li>The second dimension of b must be at least max(1, n).</li> </ul>
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> .
	Constraints: If $n \le 1$ , $lwork \ge 1$ ; If $jobz = 'N'$ and $n>1$ , $lwork \ge 2n+1$ ; If $jobz = 'V'$ and $n>1$ , $lwork \ge 2n^2+6n+1$ .
iwork	INTEGER. Workspace array, DIMENSION ( <i>liwork</i> ).
liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . Constraints: If $n \le 1$ , <i>liwork</i> $\ge 1$ ; If <i>jobz</i> = 'N' and <i>n</i> >1, <i>liwork</i> $\ge 1$ ; If <i>jobz</i> = 'V' and <i>n</i> >1, <i>liwork</i> $\ge 5n+3$ .

Output i aram	output l'alanciers		
a	On exit, if $jobz = V'$ , then if $info = 0$ , a contains the matrix Z of eigenvectors. The eigenvectors are normalized as follows: if $itype = 1$ or 2, $Z^{T}BZ = I$ ; if $itype = 3$ , $Z^{T}B^{-1}Z = I$ ;		
	If $jobz = 'N'$ , then on exit the upper triangle (if $uplo = 'U'$ ) or the lower triangle (if $uplo = 'L'$ ) of A, including the diagonal, is destroyed.		
b	On exit, if <i>info</i> $\leq n$ , the part of <i>b</i> containing the matrix is overwritten by the triangular factor <i>U</i> or <i>L</i> from the Cholesky factorization $B = U^{T}U$ or $B = L L^{T}$ .		
W	REAL for ssygvd DOUBLE PRECISION for dsygvd. Array, DIMENSION at least $max(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order.		
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .		
iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .		
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith argument had an illegal value. If info &gt; 0, spotrf/dpotrf and ssyev/dsyev returned an error code:</pre>		
	If $info = i \leq n$ , $ssyev/dsyev$ failed to converge, and <i>i</i> off-diagonal elements of an intermediate tridiagonal did not converge to zero; If $info = n + i$ , for $1 \leq i \leq n$ , then the leading minor of order <i>i</i> of <i>B</i> is not positive-definite. The factorization of <i>B</i> could not be completed and no eigenvalues or eigenvectors were computed.		

# ?hegvd

Computes all eigenvalues and, optionally, eigenvectors of a complex generalized Hermitian definite eigenproblem. If eigenvectors are desired, it uses a divide and conquer method.

#### **Discussion**

This routine computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, of the form

 $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here *A* and *B* are assumed to be Hermitian and *B* is also positive definite. If eigenvectors are desired, it uses a divide and conquer algorithm.

itype	INTEGER. Must be 1 or 2 or 3.
	Specifies the problem type to be solved:
	if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ;
	if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ;
	if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'.
	If $jobz = 'N'$ , then compute eigenvalues only.
	If $jobz = V'$ , then compute eigenvalues and
	eigenvectors.

uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays <i>a</i> and <i>b</i> store the upper triangles of <i>A</i> and <i>B</i> ; If $uplo = 'L'$ , arrays <i>a</i> and <i>b</i> store the lower triangles of <i>A</i> and <i>B</i> .
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
a, b, work	COMPLEX for chegvd DOUBLE COMPLEX for zhegvd. Arrays:
	a(lda, *) contains the upper or lower triangle of the Hermitian matrix A, as specified by uplo. The second dimension of a must be at least max(1, n).
	<b>b</b> ( <i>1db</i> , *) contains the upper or lower triangle of the Hermitian positive definite matrix <i>B</i> , as specified by uplo.
	The second dimension of $b$ must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .
lwork	<b>INTEGER</b> . The dimension of the array <i>work</i> .
	Constraints: If $n \le 1$ , $lwork \ge 1$ ; If $jobz = 'N'$ and $n>1$ , $lwork \ge n+1$ ; If $jobz = 'V'$ and $n>1$ , $lwork \ge n^2+2n$ .
rwork	REAL for chegvd DOUBLE PRECISION for zhegvd. Workspace array, DIMENSION ( <i>lrwork</i> ).
lrwork	<b>INTEGER.</b> The dimension of the array <i>rwork</i> . Constraints: If $n \le 1$ , <i>lrwork</i> $\ge 1$ ; If <i>jobz</i> = 'N' and <i>n</i> >1, <i>lrwork</i> $\ge n$ ; If <i>jobz</i> = 'V' and <i>n</i> >1, <i>lrwork</i> $\ge 2n^2+5n+1$ .
iwork	INTEGER. Workspace array, DIMENSION (liwork)

liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . Constraints: If $n \le 1$ , <i>liwork</i> $\ge 1$ ; If <i>jobz</i> = 'N ' and <i>n</i> >1, <i>liwork</i> $\ge 1$ ; If <i>jobz</i> = 'V ' and <i>n</i> >1, <i>liwork</i> $\ge 5n+3$ .
Output Parame	eters
a	On exit, if $jobz = V'$ , then if $info = 0$ , a contains the matrix Z of eigenvectors. The eigenvectors are normalized as follows: if $itype = 1$ or 2, $Z^{H}BZ = I$ ; if $itype = 3$ , $Z^{H}B^{-1}Z = I$ ;
	If $jobz = 'N'$ , then on exit the upper triangle (if $uplo = 'U'$ ) or the lower triangle (if $uplo = 'L'$ ) of <i>A</i> , including the diagonal, is destroyed.
b	On exit, if <i>info</i> $\leq n$ , the part of <i>b</i> containing the matrix is overwritten by the triangular factor <i>U</i> or <i>L</i> from the Cholesky factorization $B = U^H U$ or $B = L L^H$ .
W	REAL for chegvd DOUBLE PRECISION for zhegvd. Array, DIMENSION at least max $(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
rwork(1)	On exit, if <i>info</i> = 0, then <i>rwork(1)</i> returns the required minimal size of <i>lrwork</i> .
iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith argument had an illegal value. If info &gt; 0, cpotrf/zpotrf and cheev/zheev returned an error code:</pre>

If  $info = i \leq n$ , cheev/zheev failed to converge, and *i* off-diagonal elements of an intermediate tridiagonal did not converge to zero; If info = n + i, for  $1 \leq i \leq n$ , then the leading minor of order *i* of *B* is not positive-definite. The factorization of *B* could not be completed and no eigenvalues or eigenvectors were computed.

# ?sygvx

Computes selected eigenvalues and, optionally, eigenvectors of a real generalized symmetric definite eigenproblem.

#### **Discussion**

This routine computes selected eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, of the form

 $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here *A* and *B* are assumed to be symmetric and *B* is also positive definite. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

itype	<b>INTEGER.</b> Must be 1 or 2 or 3. Specifies the problem type to be solved: if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ; if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ; if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then compute eigenvalues only. If <i>jobz</i> = 'V', then compute eigenvalues and eigenvectors.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'.

If $range = 'A'$ , the routine computes all eigenvalues. If $range = 'V'$ , the routine computes eigenvalues $\lambda_i$ in the half-open interval: $vl < \lambda_i \leq vu$ . If $range = 'I'$ , the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays <i>a</i> and <i>b</i> store the upper triangles of <i>A</i> and <i>B</i> ; If $uplo = 'L'$ , arrays <i>a</i> and <i>b</i> store the lower triangles of <i>A</i> and <i>B</i> .
<b>INTEGER.</b> The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
REAL for ssygvx DOUBLE PRECISION for dsygvx. Arrays: a(lda, *) contains the upper or lower triangle of the symmetric matrix A, as specified by uplo. The second dimension of a must be at least max(1, n). b(ldb, *) contains the upper or lower triangle of the symmetric positive definite matrix B, as specified by uplo. The second dimension of b must be at least max(1, n). work(lwork) is a workspace array.
<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .
REAL for ssygvx DOUBLE PRECISION for dsygvx. If <i>range</i> = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: <i>v1</i> < <i>vu</i> . If <i>range</i> = 'A' or 'I', <i>v1</i> and <i>vu</i> are not referenced.

il, iu	INTEGER. If $range = 'I'$ , the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le il \le iu \le n$ , if $n > 0$ ; $il = 1$ and $iu = 0$ if $n = 0$ .
abstol	If <i>range</i> = 'A' or 'V', <i>il</i> and <i>iu</i> are not referenced. REAL for ssygvx DOUBLE PRECISION for dsygvx. The absolute error tolerance for the eigenvalues. See <i>Application Notes</i> for more information.
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ . Constraints: $ldz \ge 1$ ; if $jobz = V'$ , $ldz \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> ; <i>lwork</i> $\geq$ max(1, 8 <i>n</i> ). See Application Notes for the suggested value of <i>lwork</i> .
iwork	INTEGER. Workspace array, DIMENSION at least $max(1, 5n)$ .

a	On exit, the upper triangle (if $uplo = 'U'$ ) or the lower triangle (if $uplo = 'L'$ ) of <i>A</i> , including the diagonal, is overwritten.
b	On exit, if <i>info</i> $\leq n$ , the part of <i>b</i> containing the matrix is overwritten by the triangular factor <i>U</i> or <i>L</i> from the Cholesky factorization $B = U^{T}U$ or $B = L L^{T}$ .
m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If <i>range</i> = 'A', <i>m</i> = <i>n</i> , and if <i>range</i> = 'I', m = iu - il + 1.
W, Z	REAL for ssygvx DOUBLE PRECISION for dsygvx. Arrays:

w(*), DIMENSION at least max(1, n). The first *m* elements of *w* contain the selected eigenvalues in ascending order.

z(ldz, *). The second dimension of z must be at least max(1, m).

If jobz = 'V', then if info = 0, the first *m* columns of *z* contain the orthonormal eigenvectors of the matrix *A* corresponding to the selected eigenvalues, with the *i*-th column of *z* holding the eigenvector associated with w(i). The eigenvectors are normalized as follows:

if *itype* = 1 or 2,  $Z^T B Z = I$ ; if *itype* = 3,  $Z^T B^{-1} Z = I$ ;

If jobz = 'N', then z is not referenced.

If an eigenvector fails to converge, then that column of z contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in *ifail*. Note: you must ensure that at least max(1,*m*) columns are supplied in the array z; if *range* = 'V', the exact value of *m* is not known in advance and an upper bound must be used.

On exit, if *info* = 0, then *work(1)* returns the required minimal size of *lwork*.

ifail

work(1)

Array, DIMENSION at least max(1, n).

If jobz = 'V', then if info = 0, the first *m* elements of *ifail* are zero; if info > 0, the *ifail* contains the indices of the eigenvectors that failed to converge. If jobz = 'N', then *ifail* is not referenced.

info

INTEGER.

INTEGER.

If info = 0, the execution is successful.

If *info* = -*i*, the *i*th argument had an illegal value. If *info* > 0, spotrf/dpotrf and ssyevx/dsyevx returned an error code: If  $info = i \leq n$ , ssyevx/dsyevx failed to converge, and *i* eigenvectors failed to converge. Their indices are stored in the array *ifail*; If *info* = n + i, for  $1 \leq i \leq n$ , then the leading minor of order *i* of *B* is not positive-definite. The factorization of *B* could not be completed and no eigenvalues or eigenvectors were computed.

### **Application Notes**

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to abstol +  $\varepsilon$  * max( |a|,|b| ), where  $\varepsilon$  is the machine precision. If abstol is less than or equal to zero, then  $\varepsilon$  *|| $T/|_1$  will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when abstol is set to twice the underflow threshold 2*?lamch('S'), not zero. If this routine returns with info > 0, indicating that some eigenvectors did not converge, try setting abstol to 2*?lamch('S').

For optimum performance use  $lwork \ge (nb+3)*n$ , where nb is the blocksize for ssytrd/dsytrd returned by ilaenv.

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

# ?hegvx

Computes selected eigenvalues and, optionally, eigenvectors of a complex generalized Hermitian definite eigenproblem.

## **Discussion**

This routine computes selected eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, of the form

 $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here *A* and *B* are assumed to be Hermitian and *B* is also positive definite. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

itype	<b>INTEGER.</b> Must be 1 or 2 or 3. Specifies the problem type to be solved: if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ; if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ; if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'. If $jobz = 'N'$ , then compute eigenvalues only. If $jobz = 'V'$ , then compute eigenvalues and eigenvectors.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'.

	If <i>range</i> = 'A', the routine computes all eigenvalues. If <i>range</i> = 'V', the routine computes eigenvalues $\lambda_i$ in the half-open interval: $v1 < \lambda_i \leq vu$ . If <i>range</i> = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays <i>a</i> and <i>b</i> store the upper triangles of <i>A</i> and <i>B</i> ; If $uplo = 'L'$ , arrays <i>a</i> and <i>b</i> store the lower triangles of <i>A</i> and <i>B</i> .
п	<b>INTEGER.</b> The order of the matrices A and B ( $n \ge 0$ ).
a, b, work	COMPLEX for chegvx DOUBLE COMPLEX for zhegvx. Arrays: a(lda,*) contains the upper or lower triangle of the Hermitian matrix A, as specified by uplo.
	The second dimension of a must be at least $max(1, n)$ .
	<i>b</i> ( <i>ldb</i> , *) contains the upper or lower triangle of the Hermitian positive definite matrix <i>B</i> , as specified by <i>uplo</i> .
	The second dimension of <i>b</i> must be at least $\max(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of $b$ ; at least max $(1, n)$ .
vl, vu	REAL for chegvx DOUBLE PRECISION for zhegvx. If range = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: v1< vu. If range = 'A' or 'I', v1 and vu are not referenced.
	$\mathbf{H} = \mathbf{H} \mathbf{U} \mathbf{U} \mathbf{U} \mathbf{U} \mathbf{U} \mathbf{U} \mathbf{U} U$

il, iu	INTEGER. If <i>range</i> = 'I', the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le i1 \le iu \le n$ , if $n > 0$ ; $i1=1$ and $iu=0$ if $n = 0$ .
	If <i>range</i> = 'A' or 'V', <i>il</i> and <i>iu</i> are not referenced.
abstol	REAL for chegvx DOUBLE PRECISION for zhegvx. The absolute error tolerance for the eigenvalues. See <i>Application Notes</i> for more information.
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ . Constraints: $ldz \ge 1$ ; if $jobz = V'$ , $ldz \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> ; $lwork \ge max(1, 2n-1)$ . See Application Notes for the suggested value of <i>lwork</i> .
rwork	<b>REAL</b> for chegvx <b>DOUBLE PRECISION</b> for zhegvx. Workspace array, <b>DIMENSION</b> at least max $(1, 7n)$ .
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least $max(1, 5n)$ .

# **Output Parameters**

a	On exit, the upper triangle (if $uplo = 'U'$ ) or the lower triangle (if $uplo = 'L'$ ) of <i>A</i> , including the diagonal, is overwritten.
b	On exit, if <i>info</i> $\leq n$ , the part of <i>b</i> containing the matrix is overwritten by the triangular factor <i>U</i> or <i>L</i> from the Cholesky factorization $B = U^H U$ or $B = L L^H$ .
m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If $range =  A , m = n$ , and if $range =  I , m = iu - il + 1$ .

W	REAL for chegvx
	DOUBLE PRECISION for zhegvx.
	Array, DIMENSION at least $max(1, n)$ .
	The first $m$ elements of $w$ contain the selected
	eigenvalues in ascending order.
Z	COMPLEX for chegvx
	DOUBLE COMPLEX for zhegvx.
	Array $z(ldz, *)$ . The second dimension of $z$ must be at
	least $\max(1, m)$ .
	If $jobz = 'V'$ , then if $info = 0$ , the first <i>m</i> columns of <i>z</i> contain the orthonormal eigenvectors of the matrix <i>A</i> corresponding to the selected eigenvalues, with the <i>i</i> -th column of <i>z</i> holding the eigenvector associated with
	w(i). The eigenvectors are normalized as follows: if <i>itype</i> = 1 or 2, $Z^H B Z = I$ ; if <i>itype</i> = 3, $Z^H B^{-1} Z = I$ ;
	If $jobz = 'N'$ , then z is not referenced. If an eigenvector fails to converge, then that column of z contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in <i>ifail</i> . Note: you must ensure that at least max(1,m) columns are supplied in the array z ; if <i>range</i> = 'V', the exact value of <i>m</i> is not known in advance and an upper bound must be used.
work(1)	On exit, if $info = 0$ , then $work(1)$ returns the required minimal size of <i>lwork</i> .
ifail	<pre>INTEGER. Array, DIMENSION at least max(1, n). If jobz = 'V', then if info = 0, the first m elements of ifail are zero; if info &gt; 0, the ifail contains the indices of the eigenvectors that failed to converge.</pre>
	If $jobz = 'N'$ , then <i>ifail</i> is not referenced.

info

INTEGER.

If *info* = 0, the execution is successful. If *info* = -*i*, the *i*th argument had an illegal value. If *info* > 0, cpotrf/zpotrf and cheevx/zheevx returned an error code:

If  $info = i \leq n$ , cheevx/zheevx failed to converge, and *i* eigenvectors failed to converge. Their indices are stored in the array *ifail*; If *info* = n + i, for  $1 \leq i \leq n$ , then the leading minor of order *i* of *B* is not positive-definite. The factorization of *B* could not be completed and no eigenvalues or eigenvectors were computed.

# **Application Notes**

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to abstol +  $\varepsilon$  * max(|a|,|b|), where  $\varepsilon$  is the machine precision. If abstol is less than or equal to zero, then  $\varepsilon$  *  $||T/|_1$  will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when abstol is set to twice the underflow threshold 2*?lamch('S'), not zero. If this routine returns with info > 0, indicating that some eigenvectors did not converge, try setting abstol to 2*?lamch('S').

For optimum performance use  $lwork \ge (nb+1)*n$ , where nb is the blocksize for chetrd/zhetrd returned by ilaenv.

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

# ?spgv

Computes all eigenvalues and, optionally, eigenvectors of a real generalized symmetric definite eigenproblem with matrices in packed storage.

call sspgv ( itype, jobz, uplo, n, ap, bp, w, z, ldz, work, info )
call dspgv ( itype, jobz, uplo, n, ap, bp, w, z, ldz, work, info )

#### **Discussion**

This routine computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, of the form

 $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here *A* and *B* are assumed to be symmetric, stored in packed format, and *B* is also positive definite.

itype	<b>INTEGER.</b> Must be 1 or 2 or 3. Specifies the problem type to be solved: if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ; if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ; if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then compute eigenvalues only. If <i>jobz</i> = 'V', then compute eigenvalues and eigenvectors.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays $ap$ and $bp$ store the upper triangles of <i>A</i> and <i>B</i> ; If $uplo = 'L'$ , arrays $ap$ and $bp$ store the lower triangles of <i>A</i> and <i>B</i> .
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).

ap,	bp,	work	REAL for sspgv
			DOUBLE PRECISION for dspgv.
			Arrays:
			ap(*) contains the packed upper or lower triangle of
			the symmetric matrix A, as specified by uplo. The
			dimension of ap must be at least $\max(1, \frac{n}{(n+1)}/2)$ .
			bp(*) contains the packed upper or lower triangle of the symmetric matrix <i>B</i> , as specified by <i>uplo</i> . The dimension of <i>bp</i> must be at least max $(1, n*(n+1)/2)$ .
			<i>work(*)</i> is a workspace array, <b>DIMENSION</b> at least max(1, 3 <i>n</i> ).
ldz			<b>INTEGER.</b> The leading dimension of the output array $z$ ; $ldz \ge 1$ . If $jobz = V'$ , $ldz \ge max(1, n)$ .

# **Output Parameters**

ap	On exit, the contents of <i>ap</i> are overwritten.
bp	On exit, contains the triangular factor $U$ or $L$ from the Cholesky factorization $B = U^{T}U$ or $B = L L^{T}$ , in the same storage format as $B$ .
W, Z	<b>REAL</b> for sspgv <b>DOUBLE PRECISION</b> for dspgv. Arrays: w(*), <b>DIMENSION</b> at least max $(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order. z(1dz,*). The second dimension of $z$ must be at least max $(1, n)$ . If <i>jobz</i> ='V', then if <i>info</i> = 0, $z$ contains the matrix $Z$ of eigenvectors. The eigenvectors are normalized as follows: if <i>itype</i> = 1 or 2, $Z^T B Z = I$ ; if <i>itype</i> = 3, $Z^T B^{-1} Z = I$ ;
	If $jobz = 'N'$ , then z is not referenced.

info

INTEGER.

If *info* = 0, the execution is successful. If *info* = -*i*, the *i*th argument had an illegal value. If *info* > 0, spptrf/dpptrf and sspev/dspev returned an error code:

If  $info = i \leq n$ , sspev/dspev failed to converge, and *i* off-diagonal elements of an intermediate tridiagonal did not converge to zero; If info = n + i, for  $1 \leq i \leq n$ , then the leading minor of order *i* of *B* is not positive-definite. The factorization of *B* could not be completed and no eigenvalues or eigenvectors were computed.

# ?hpgv

Computes all eigenvalues and, optionally, eigenvectors of a complex generalized Hermitian definite eigenproblem with matrices in packed storage.

## **Discussion**

This routine computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, of the form

 $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here *A* and *B* are assumed to be Hermitian, stored in packed format, and *B* is also positive definite.

itype	<b>INTEGER.</b> Must be 1 or 2 or 3. Specifies the problem type to be solved: if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ; if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ; if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then compute eigenvalues only. If <i>jobz</i> = 'V', then compute eigenvalues and eigenvectors.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays $ap$ and $bp$ store the upper triangles of A and B; If $uplo = 'L'$ , arrays $ap$ and $bp$ store the lower triangles of A and B.

п	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
ap, bp, work	COMPLEX for chpgv DOUBLE COMPLEX for zhpgv. Arrays: ap(*) contains the packed upper or lower triangle of the Hermitian matrix A, as specified by $uplo$ . The dimension of $ap$ must be at least max $(1, n*(n+1)/2)$ .
	bp(*) contains the packed upper or lower triangle of the Hermitian matrix <i>B</i> , as specified by <i>uplo</i> . The dimension of <i>bp</i> must be at least max $(1, n*(n+1)/2)$ .
	work(*) is a workspace array, DIMENSION at least max(1, 2 <i>n</i> -1).
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ ; $ldz \ge 1$ . If $jobz = 'V'$ , $ldz \ge max(1, n)$ .
rwork	REAL for chpgv DOUBLE PRECISION for zhpgv. Workspace array, DIMENSION at least max(1, 3 <i>n</i> -2).

# **Output Parameters**

ap	On exit, the contents of <i>ap</i> are overwritten.
bp	On exit, contains the triangular factor $U$ or $L$ from the Cholesky factorization $B = U^H U$ or $B = L L^H$ , in the same storage format as $B$ .
W	REAL for chpgv DOUBLE PRECISION for zhpgv. Array, DIMENSION at least $max(1, n)$ . If $info = 0$ , contains the eigenvalues in ascending order.
Ζ	COMPLEX for chpgv DOUBLE COMPLEX for zhpgv. Array $z(ldz, *)$ . The second dimension of z must be at least max $(1, n)$ . If $jobz = 'V'$ , then if $info = 0$ , z contains the matrix Z of eigenvectors. The eigenvectors are normalized as

follows:

if *itype* = 1 or 2,  $Z^{H}BZ = I$ ; if *itype* = 3,  $Z^{H}B^{-1}Z = I$ ;

If jobz = 'N', then z is not referenced.

INTEGER.

If *info* = 0, the execution is successful. If *info* = -*i*, the *i*th argument had an illegal value. If *info* > 0, cpptrf/zpptrf and chpev/zhpev returned an error code:

If  $info = i \leq n$ , chpev/zhpev failed to converge, and *i* off-diagonal elements of an intermediate tridiagonal did not converge to zero; If info = n + i, for  $1 \leq i \leq n$ , then the leading minor of order *i* of *B* is not positive-definite. The factorization of *B* could not be completed and no eigenvalues or eigenvectors were computed.

info

# ?spgvd

Computes all eigenvalues and, optionally, eigenvectors of a real generalized symmetric definite eigenproblem with matrices in packed storage. If eigenvectors are desired, it uses a divide and conquer method.

#### **Discussion**

This routine computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, of the form

 $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here *A* and *B* are assumed to be symmetric, stored in packed format, and *B* is also positive definite. If eigenvectors are desired, it uses a divide and conquer algorithm.

itype	INTEGER. Must be 1 or 2 or 3.
	Specifies the problem type to be solved:
	if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ;
	if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ;
	if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'.
	If $jobz = 'N'$ , then compute eigenvalues only.
	If $jobz = V'$ , then compute eigenvalues and
	eigenvectors.

uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays $ap$ and $bp$ store the upper triangles of A and B; If $uplo = 'L'$ , arrays $ap$ and $bp$ store the lower triangles of A and B.
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
ap, bp, work	REAL for sspgvd DOUBLE PRECISION for dspgvd. Arrays: ap(*) contains the packed upper or lower triangle of the symmetric matrix A, as specified by $uplo$ . The dimension of $ap$ must be at least max $(1, n*(n+1)/2)$ .
	<b>bp</b> (*) contains the packed upper or lower triangle of the symmetric matrix <i>B</i> , as specified by <i>uplo</i> . The dimension of <i>bp</i> must be at least $max(1, n*(n+1)/2)$ .
	work(lwork) is a workspace array.
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ ; $ldz \ge 1$ . If $jobz = V'$ , $ldz \ge max(1, n)$ .
lwork	<b>INTEGER</b> . The dimension of the array <i>work</i> .
	Constraints: If $n \le 1$ , $lwork \ge 1$ ; If $jobz = 'N'$ and $n > 1$ , $lwork \ge 2n$ ; If $jobz = 'V'$ and $n > 1$ , $lwork \ge 2n^2 + 6n + 1$ .
iwork	INTEGER. Workspace array, DIMENSION ( <i>liwork</i> )
liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . Constraints: If $n \le 1$ , <i>liwork</i> $\ge 1$ ; If <i>jobz</i> = 'N' and <i>n</i> >1, <i>liwork</i> $\ge 1$ ; If <i>jobz</i> = 'V' and <i>n</i> >1, <i>liwork</i> $\ge 5n+3$ .

# **Output Parameters**

ap

On exit, the contents of *ap* are overwritten.

bp	On exit, contains the triangular factor $U$ or $L$ from the Cholesky factorization $B = U^T U$ or $B = L L^T$ , in the same storage format as $B$ .
W, Z	REAL for sspgv DOUBLE PRECISION for dspgv. Arrays: w(*), DIMENSION at least max $(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order. z(ldz,*). The second dimension of $z$ must be at least max $(1, n)$ . If <i>jobz</i> ='V', then if <i>info</i> = 0, $z$ contains the matrix $Z$ of eigenvectors. The eigenvectors are normalized as follows: if <i>itype</i> = 1 or 2, $Z^TBZ = I$ ; if <i>itype</i> = 3, $Z^TB^{-1}Z = I$ ;
	If $jobz = 'N'$ , then z is not referenced.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith argument had an illegal value. If info &gt; 0, spptrf/dpptrf and sspevd/dspevd returned an error code:</pre>
	If $info = i \le n$ , sspevd/dspevd failed to converge, and <i>i</i> off-diagonal elements of an intermediate tridiagonal did not converge to zero; If $info = n + i$ , for $1 \le i \le n$ , then the leading minor of order <i>i</i> of <i>B</i> is not positive-definite. The factorization of <i>B</i> could not be completed and no eigenvalues or eigenvectors were computed.

# ?hpgvd

Computes all eigenvalues and, optionally, eigenvectors of a complex generalized Hermitian definite eigenproblem with matrices in packed storage. If eigenvectors are desired, it uses a divide and conquer method.

## **Discussion**

This routine computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, of the form  $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here *A* and *B* are assumed to be Hermitian, stored in packed format, and *B* is also positive definite. If eigenvectors are desired, it uses a divide and conquer algorithm.

itype	<b>INTEGER</b> . Must be 1 or 2 or 3.
	Specifies the problem type to be solved:
	if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ;
	if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ;
	if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'.
	If $jobz = 'N'$ , then compute eigenvalues only.
	If $jobz = V'$ , then compute eigenvalues and
	eigenvectors.

uplo	CHARACTER*1. Must be 'U' or 'L'.
	If $uplo = 'U'$ , arrays $ap$ and $bp$ store the upper
	triangles of A and B;
	If $uplo = 'L'$ , arrays ap and bp store the lower
	triangles of A and B.
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
ap, bp, work	COMPLEX for chpgvd
	DOUBLE COMPLEX for zhpgvd.
	Arrays:
	ap(*) contains the packed upper or lower triangle of the Hermitian matrix A, as specified by $uplo$ . The
	dimension of ap must be at least $\max(1, \frac{n^{(n+1)}}{2})$ .
	bp(*) contains the packed upper or lower triangle of the Hermitian matrix <i>B</i> , as specified by <i>uplo</i> . The dimension of <i>bp</i> must be at least max $(1, n*(n+1)/2)$ .
	work(lwork) is a workspace array.
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ ; $ldz \ge 1$ . If $jobz = !V!$ , $ldz \ge max(1, n)$ .
lwork	<b>INTEGER</b> . The dimension of the array <i>work</i> .
	Constraints:
	If $n \leq 1$ , $lwork \geq 1$ ;
	If $jobz = N'$ and $n > 1$ , $lwork \ge n$ ;
	If $jobz = V'$ and $n > 1$ , $lwork \ge 2n$ .
rwork	REAL for chpgvd
	DOUBLE PRECISION for zhpgvd.
	Workspace array, <b>DIMENSION</b> ( <i>lrwork</i> ).
lrwork	<b>INTEGER</b> . The dimension of the array <i>rwork</i> .
	Constraints:
	If $n \leq 1$ , $lrwork \geq 1$ ;
	If $jobz = N'$ and $n > 1$ , $lrwork \ge n$ ;
	If $jobz = V'$ and $n > 1$ , $lrwork \ge 2n^2 + 5n + 1$ .
iwork	INTEGER.
	Workspace array, <b>DIMENSION</b> ( <i>liwork</i> )

liwork	<b>INTEGER.</b> The dimension of the array <i>iwork</i> . Constraints: If $n \le 1$ , <i>liwork</i> $\ge 1$ ; If <i>jobz</i> = 'N' and <i>n</i> >1, <i>liwork</i> $\ge 1$ ; If <i>jobz</i> = 'V' and <i>n</i> >1, <i>liwork</i> $\ge 5n+3$ .
Output Parame	ters
ар	On exit, the contents of <i>ap</i> are overwritten.
bp	On exit, contains the triangular factor $U$ or $L$ from the Cholesky factorization $B = U^H U$ or $B = L L^H$ , in the same storage format as $B$ .
W	REAL for chpgvd DOUBLE PRECISION for zhpgvd. Array, DIMENSION at least max $(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order.
Ζ	COMPLEX for chpgvd DOUBLE COMPLEX for zhpgvd. Array $z(ldz, *)$ . The second dimension of $z$ must be at least max $(1, n)$ . If $jobz = 'V'$ , then if $info = 0$ , $z$ contains the matrix $Z$ of eigenvectors. The eigenvectors are normalized as follows: if $itype = 1$ or 2, $Z^H B Z = I$ ; if $itype = 3$ , $Z^H B^{-1} Z = I$ ;
	If $jobz = 'N'$ , then z is not referenced.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
rwork(1)	On exit, if <i>info</i> = 0, then <i>rwork(1)</i> returns the required minimal size of <i>lrwork</i> .
iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .

info

INTEGER.

If *info* = 0, the execution is successful. If *info* = -*i*, the *i*th argument had an illegal value. If *info* > 0, cpptrf/zpptrf and chpevd/zhpevd returned an error code:

If  $info = i \leq n$ , chpevd/zhpevd failed to converge, and *i* off-diagonal elements of an intermediate tridiagonal did not converge to zero; If info = n + i, for  $1 \leq i \leq n$ , then the leading minor of order *i* of *B* is not positive-definite. The factorization of *B* could not be completed and no eigenvalues or eigenvectors were computed.

# ?spgvx

Computes selected eigenvalues and, optionally, eigenvectors of a real generalized symmetric definite eigenproblem with matrices in packed storage.

#### **Discussion**

This routine computes selected eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite eigenproblem, of the form

 $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here *A* and *B* are assumed to be symmetric, stored in packed format, and *B* is also positive definite.

Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

itype	<b>INTEGER.</b> Must be 1 or 2 or 3. Specifies the problem type to be solved: if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ; if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ; if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then compute eigenvalues only. If <i>jobz</i> = 'V', then compute eigenvalues and eigenvectors.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'.

	If $range = 'A'$ , the routine computes all eigenvalues. If $range = 'V'$ , the routine computes eigenvalues $\lambda_i$ in the half-open interval: $vl < \lambda_i \le vu$ . If $range = 'I'$ , the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays $ap$ and $bp$ store the upper triangles of A and B; If $uplo = 'L'$ , arrays $ap$ and $bp$ store the lower triangles of A and B.
n	<b>INTEGER</b> . The order of the matrices A and B ( $n \ge 0$ ).
ap, bp, work	REAL for sspgvx DOUBLE PRECISION for dspgvx. Arrays: ap(*) contains the packed upper or lower triangle of
	the symmetric matrix A, as specified by $uplo$ . The dimension of ap must be at least max $(1, n^{*}(n+1)/2)$ .
	bp(*) contains the packed upper or lower triangle of the symmetric matrix <i>B</i> , as specified by $uplo$ . The dimension of <i>bp</i> must be at least max $(1, n*(n+1)/2)$ .
	<i>work(*)</i> is a workspace array, <b>DIMENSION</b> at least max(1, 8 <i>n</i> ).
vl, vu	REAL for sspgvx DOUBLE PRECISION for dspgvx. If <i>range</i> = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: <i>v1</i> < <i>vu</i> .
	If $range = 'A'$ or 'I', $vI$ and $vu$ are not referenced.
il, iu	INTEGER. If $range = 'I'$ , the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le il \le iu \le n$ , if $n > 0$ ; $il=1$ and $iu=0$ if $n = 0$ .
	If <i>range</i> = 'A' or 'V', <i>il</i> and <i>iu</i> are not referenced.

abstol	REAL for sspgvx DOUBLE PRECISION for dspgvx. The absolute error tolerance for the eigenvalues. See <i>Application Notes</i> for more information.
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ . Constraints: $ldz \ge 1$ ; if $jobz = V'$ , $ldz \ge max(1, n)$ .
iwork	INTEGER. Workspace array, DIMENSION at least max(1, 5n).
Output Parame	eters
ар	On exit, the contents of <i>ap</i> are overwritten.
bp	On exit, contains the triangular factor $U$ or $L$ from the Cholesky factorization $B = U^T U$ or $B = L L^T$ , in the same storage format as $B$ .
m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If <i>range</i> = 'A', <i>m</i> = <i>n</i> , and if <i>range</i> = 'I', m = iu-il+1.
W, Z	REAL for sspgvx DOUBLE PRECISION for dspgvx. Arrays: w(*), DIMENSION at least max $(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order. z(ldz,*). The second dimension of z must be at least
	max(1, <i>n</i> ). If $jobz = "V"$ , then if $info = 0$ , the first <i>m</i> columns of <i>z</i> contain the orthonormal eigenvectors of the matrix <i>A</i> corresponding to the selected eigenvalues, with the <i>i</i> -th column of <i>z</i> holding the eigenvector associated with <i>w(i)</i> . The eigenvectors are normalized as follows: if <i>itype</i> = 1 or 2, $Z^TBZ = I$ ; if <i>itype</i> = 3, $Z^TB^{-1}Z = I$ ;
	If $jobz = 'N'$ , then z is not referenced. If an eigenvector fails to converge, then that column of z contains the latest approximation to the eigenvector, and

	the index of the eigenvector is returned in <i>ifail</i> . Note: you must ensure that at least $max(1,m)$ columns are supplied in the array $z$ ; if <i>range</i> = 'V', the exact value of $m$ is not known in advance and an upper bound must be used.
ifail	INTEGER. Array, DIMENSION at least max(1, n). If jobz = 'V', then if info = 0, the first m elements of if ail are zero; if info > 0, the if ail contains the indices of the eigenvectors that failed to converge. If jobz = 'N', then if ail is not referenced.
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith argument had an illegal value. If info &gt; 0, spptrf/dpptrf and sspevx/dspevx returned an error code:</pre>
	If $info = i \leq n$ , sspevx/dspevx failed to converge, and <i>i</i> eigenvectors failed to converge. Their indices are stored in the array <i>ifail</i> ; If $info = n + i$ , for $1 \leq i \leq n$ , then the leading minor of order <i>i</i> of <i>B</i> is not positive-definite. The factorization of <i>B</i> could not be completed and no eigenvalues or eigenvectors were computed.

### **Application Notes**

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to abstol +  $\varepsilon$  * max( |a|,|b| ), where  $\varepsilon$  is the machine precision. If abstol is less than or equal to zero, then  $\varepsilon$  *||T/|₁ will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when abstol is set to twice the underflow threshold 2*?lamch('S'), not zero. If this routine returns with info > 0, indicating that some eigenvectors did not converge, try setting abstol to 2*?lamch('S').

# ?hpgvx

Computes selected eigenvalues and, optionally, eigenvectors of a generalized Hermitian definite eigenproblem with matrices in packed storage.

## **Discussion**

This routine computes selected eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite eigenproblem, of the form

 $Ax = \lambda Bx$ ,  $ABx = \lambda x$ , or  $BAx = \lambda x$ .

Here *A* and *B* are assumed to be Hermitian, stored in packed format, and *B* is also positive definite.

Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

itype	<b>INTEGER.</b> Must be 1 or 2 or 3. Specifies the problem type to be solved: if <i>itype</i> = 1, the problem type is $Ax = \lambda Bx$ ; if <i>itype</i> = 2, the problem type is $ABx = \lambda x$ ; if <i>itype</i> = 3, the problem type is $BAx = \lambda x$ .
jobz	CHARACTER*1. Must be 'N' or 'V'. If $jobz = 'N'$ , then compute eigenvalues only. If $jobz = 'V'$ , then compute eigenvalues and eigenvectors.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'. If <i>range</i> = 'A', the routine computes all eigenvalues. If <i>range</i> = 'V', the routine computes eigenvalues $\lambda_i$ in the half-open interval: $v < \lambda_i \leq v u$ .

	If <i>range</i> = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays $ap$ and $bp$ store the upper triangles of A and B; If $uplo = 'L'$ , arrays $ap$ and $bp$ store the lower triangles of A and B.
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
ap, bp, work	COMPLEX for chpgvx DOUBLE COMPLEX for zhpgvx. Arrays: ap(*) contains the packed upper or lower triangle of the Hermitian matrix A, as specified by $uplo$ . The dimension of $ap$ must be at least max $(1, n*(n+1)/2)$ .
	bp(*) contains the packed upper or lower triangle of the Hermitian matrix <i>B</i> , as specified by <i>uplo</i> . The dimension of <i>bp</i> must be at least max $(1, n*(n+1)/2)$ .
	work(*) is a workspace array, DIMENSION at least $max(1, 2n)$ .
vl, vu	REAL for chpgvx DOUBLE PRECISION for zhpgvx. If <i>range</i> = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: v1< vu.
	If $range = 'A'$ or 'I', vl and vu are not referenced.
il, iu	INTEGER. If <i>range</i> = 'I', the indices in ascending order of the smallest and largest eigenvalues to be returned. Constraint: $1 \le i \le u \le n$ , if $n > 0$ ; $i \le 1 \le 1$ and $i \le 0$ if $n = 0$ .
	If <i>range</i> = 'A' or 'V', <i>il</i> and <i>iu</i> are not referenced.
abstol	REAL for chpgvx DOUBLE PRECISION for zhpgvx. The absolute error tolerance for the eigenvalues.

See Application Notes for more information.

ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ ; $ldz \ge 1$ . If $jobz = !V'$ , $ldz \ge max(1, n)$ .
rwork	REAL for chpgvx DOUBLE PRECISION for zhpgvx. Workspace array, DIMENSION at least max(1, 7n).
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least max(1, 5 <i>n</i> ).

# **Output Parameters**

•	
ap	On exit, the contents of <i>ap</i> are overwritten.
p	On exit, contains the triangular factor $U$ or $L$ from the Cholesky factorization $B = U^H U$ or $B = L L^H$ , in the same storage format as $B$ .
m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If <i>range</i> = 'A', <i>m</i> = <i>n</i> , and if <i>range</i> = 'I', m = iu-il+1.
W	<b>REAL for chpgvx</b> <b>DOUBLE PRECISION for zhpgvx.</b> Array, <b>DIMENSION</b> at least $max(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order.
Ζ	COMPLEX for chpgvx DOUBLE COMPLEX for zhpgvx. Array $z(ldz, *)$ . The second dimension of $z$ must be at least max $(1, n)$ . If $jobz = 'V'$ , then if $info = 0$ , the first $m$ columns of $z$ contain the orthonormal eigenvectors of the matrix $A$ corresponding to the selected eigenvalues, with the <i>i</i> -th column of $z$ holding the eigenvector associated with w(i). The eigenvectors are normalized as follows: if $itype = 1$ or 2, $Z^H B Z = I$ ; if $itype = 3$ , $Z^H B^{-1} Z = I$ ; If $itype = 3$ , $Z^H B^{-1} Z = I$ ;

If jobz = 'N', then z is not referenced.

	If an eigenvector fails to converge, then that column of $z$ contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in <i>ifail</i> . Note: you must ensure that at least max $(1,m)$ columns are supplied in the array $z$ ; if <i>range</i> = 'V', the exact value of $m$ is not known in advance and an upper bound must be used.
ifail	INTEGER. Array, DIMENSION at least max $(1, n)$ . If <i>jobz</i> = 'V', then if <i>info</i> = 0, the first <i>m</i> elements of <i>ifail</i> are zero; if <i>info</i> > 0, the <i>ifail</i> contains the indices of the eigenvectors that failed to converge. If <i>jobz</i> = 'N', then <i>ifail</i> is not referenced.
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith argument had an illegal value. If info &gt; 0, cpptrf/zpptrf and chpevx/zhpevx returned an error code:</pre>
	If $info = i \leq n$ , chpevx/zhpevx failed to converge, and <i>i</i> eigenvectors failed to converge. Their indices are stored in the array <i>ifail</i> ; If $info = n + i$ , for $1 \leq i \leq n$ , then the leading minor of order <i>i</i> of <i>B</i> is not positive-definite. The factorization of <i>B</i> could not be completed and no eigenvalues or eigenvectors were computed.

### **Application Notes**

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to  $abstol + \varepsilon * max(|a|,|b|)$ , where  $\varepsilon$  is the machine precision. If abstolis less than or equal to zero, then  $\varepsilon * ||T/|_1$  will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when abstol is set to twice the underflow threshold 2*?lamch('S'), not zero. If this routine returns with info > 0, indicating that some eigenvectors did not converge, try setting abstol to 2*?lamch('S').

# ?sbgv

Computes all eigenvalues and, optionally, eigenvectors of a real generalized symmetric definite eigenproblem with banded matrices.

## Discussion

This routine computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite banded eigenproblem, of the form  $Ax = \lambda Bx$ . Here *A* and *B* are assumed to be symmetric and banded, and *B* is also positive definite.

jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then compute eigenvalues only. If <i>jobz</i> = 'V', then compute eigenvalues and eigenvectors.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays <i>ab</i> and <i>bb</i> store the upper triangles of A and B; If $uplo = 'L'$ , arrays <i>ab</i> and <i>bb</i> store the lower triangles of A and B.
п	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
ka	<b>INTEGER</b> . The number of super- or sub-diagonals in $A$ ( $ka \ge 0$ ).
kb	<b>INTEGER.</b> The number of super- or sub-diagonals in $B$ ( $kb \ge 0$ ).

ab,bb,work	REAL for ssbgv
	DOUBLE PRECISION for dsbgv
	Arrays:
	ab (ldab, *) is an array containing either upper or
	lower triangular part of the symmetric matrix A (as
	specified by uplo) in band storage format.
	The second dimension of the array $ab$ must be at least max $(1, n)$ .
	bb (1dbb, *) is an array containing either upper or
	lower triangular part of the symmetric matrix B (as
	specified by <u>uplo</u> ) in band storage format.
	The second dimension of the array <i>bb</i> must be at least $max(1, n)$ .
	<pre>work(*) is a workspace array, DIMENSION at least max(1, 3n)</pre>
ldab	<b>INTEGER</b> . The first dimension of the array <i>ab</i> ; must be at least <i>ka</i> +1.
ldbb	<b>INTEGER</b> . The first dimension of the array <i>bb</i> ; must be at least <i>kb</i> +1.
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ ; $ldz \ge 1$ . If $jobz = \lor V \lor$ , $ldz \ge max(1, n)$ .

# **Output Parameters**

ab	On exit, the contents of <i>ab</i> are overwritten.
bb	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^T S$ , as returned by spbstf/dpbstf.
W, Z	<pre>REAL for ssbgv DOUBLE PRECISION for dsbgv Arrays: w(*), DIMENSION at least max(1, n). If info = 0, contains the eigenvalues in ascending order.</pre>
	<pre>z(ldz,*). The second dimension of z must be at least max(1, n). If jobz = 'V', then if info = 0, z contains the matrix Z of eigenvectors, with the i-th column of z holding the</pre>

eigenvector associated with w(i). The eigenvectors are normalized so that  $Z^T B Z = I$ . If jobz = 'N', then z is not referenced.

info

#### INTEGER.

If info = 0, the execution is successful. If info = -i, the *i*th argument had an illegal value. If info > 0, and

if  $i \leq n$ , the algorithm failed to converge, and i off-diagonal elements of an intermediate tridiagonal did not converge to zero;

if info = n + i, for  $1 \le i \le n$ , then spbstf/dpbstf returned info = i and B is not positive-definite. The factorization of B could not be completed and no eigenvalues or eigenvectors were computed.

# ?hbgv

Computes all eigenvalues and, optionally, eigenvectors of a complex generalized Hermitian definite eigenproblem with banded matrices.

#### **Discussion**

This routine computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite banded eigenproblem, of the form  $Ax = \lambda Bx$ . Here *A* and *B* are assumed to be Hermitian and banded, and *B* is also positive definite.

jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then compute eigenvalues only. If <i>jobz</i> = 'V', then compute eigenvalues and eigenvectors.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays $ab$ and $bb$ store the upper triangles of $A$ and $B$ ; If $uplo = 'L'$ , arrays $ab$ and $bb$ store the lower triangles of $A$ and $B$ .
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
ka	<b>INTEGER.</b> The number of super- or sub-diagonals in $A$ ( $ka \ge 0$ ).
kb	<b>INTEGER.</b> The number of super- or sub-diagonals in $B$ ( $kb \ge 0$ ).

ab,bb,work	COMPLEX for chbgv DOUBLE COMPLEX for zhbgv
	Arrays: <b>ab</b> ( $1dab$ , *) is an array containing either upper or lower triangular part of the Hermitian matrix A (as specified by $up1o$ ) in band storage format. The second dimension of the array <b>ab</b> must be at least max(1, n).
	bb (1dbb, *) is an array containing either upper or lower triangular part of the Hermitian matrix B (as specified by $uplo$ ) in band storage format. The second dimension of the array bb must be at least max(1, n). work(*) is a workspace array, DIMENSION at least max(1, n).
ldab	<b>INTEGER</b> . The first dimension of the array <i>ab</i> ; must be at least <i>ka</i> +1.
ldbb	<b>INTEGER</b> . The first dimension of the array <i>bb</i> ; must be at least <i>kb</i> +1.
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ ; $ldz \ge 1$ . If $jobz = V'$ , $ldz \ge max(1, n)$ .
rwork	REAL for chbgv DOUBLE PRECISION for zhbgv. Workspace array, DIMENSION at least max(1, 3n).

# **Output Parameters**

ab	On exit, the contents of <i>ab</i> are overwritten.
bb	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^H S$ , as returned by cpbstf/zpbstf.
W	REAL for chbgv
	DOUBLE PRECISION for zhbgv.
	Array, DIMENSION at least $max(1, n)$ .
	If <i>info</i> = 0, contains the eigenvalues in ascending order.

Ζ	COMPLEX for chbgv DOUBLE COMPLEX for zhbgv Array $z(ldz, *)$ . The second dimension of $z$ must be at least max $(1, n)$ . If $jobz = 'V'$ , then if $info = 0$ , $z$ contains the matrix $Z$ of eigenvectors, with the <i>i</i> -th column of $z$ holding the eigenvector associated with $w(i)$ . The eigenvectors are normalized so that $Z^H B Z = I$ . If $jobz = 'N'$ , then $z$ is not referenced.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th argument had an illegal value. If $info > 0$ , and
	if $i \leq n$ , the algorithm failed to converge, and $i$ off-diagonal elements of an intermediate tridiagonal did not converge to zero; if $info = n + i$ , for $1 \leq i \leq n$ , then cpbstf/zpbstf returned $info = i$ and $B$ is not positive-definite. The factorization of $B$ could not be completed and no eigenvalues or eigenvectors were computed.

# ?sbgvd

Computes all eigenvalues and, optionally, eigenvectors of a real generalized symmetric definite eigenproblem with banded matrices. If eigenvectors are desired, it uses a divide and conquer method.

## **Discussion**

This routine computes all the eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite banded eigenproblem, of the form  $Ax = \lambda Bx$ . Here *A* and *B* are assumed to be symmetric and banded, and *B* is also positive definite. If eigenvectors are desired, it uses a divide and conquer algorithm.

jobz	CHARACTER*1. Must be 'N' or 'V'. If $jobz = 'N'$ , then compute eigenvalues only. If $jobz = 'V'$ , then compute eigenvalues and eigenvectors.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays <i>ab</i> and <i>bb</i> store the upper triangles of <i>A</i> and <i>B</i> ; If $uplo = 'L'$ , arrays <i>ab</i> and <i>bb</i> store the lower triangles of <i>A</i> and <i>B</i> .
n	<b>INTEGER</b> . The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
ka	<b>INTEGER.</b> The number of super- or sub-diagonals in $A$ ( $ka \ge 0$ ).

kb	<b>INTEGER.</b> The number of super- or sub-diagonals in $B$ ( $kb \ge 0$ ).
ab,bb,work	<ul> <li>REAL for ssbgvd</li> <li>DOUBLE PRECISION for dsbgvd</li> <li>Arrays:</li> <li>ab (ldab, *) is an array containing either upper or lower triangular part of the symmetric matrix A (as specified by uplo) in band storage format.</li> <li>The second dimension of the array ab must be at least max(1, n).</li> </ul>
	<ul> <li>bb (1dbb, *) is an array containing either upper or lower triangular part of the symmetric matrix B (as specified by uplo) in band storage format.</li> <li>The second dimension of the array bb must be at least max(1, n).</li> </ul>
	work(lwork) is a workspace array.
ldab	<b>INTEGER.</b> The first dimension of the array <i>ab</i> ; must be at least <i>ka</i> +1.
ldbb	<b>INTEGER.</b> The first dimension of the array $bb$ ; must be at least $kb+1$ .
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ ; $ldz \ge 1$ . If $jobz = V'$ , $ldz \ge max(1, n)$ .
lwork	<b>INTEGER</b> . The dimension of the array <i>work</i> .
	Constraints: If $n \le 1$ , $lwork \ge 1$ ; If $jobz = 'N'$ and $n > 1$ , $lwork \ge 3n$ ; If $jobz = 'V'$ and $n > 1$ , $lwork \ge 2n^2 + 5n + 1$ .
iwork	INTEGER. Workspace array, DIMENSION ( <i>liwork</i> )
liwork	INTEGER. The dimension of the array <i>iwork</i> . Constraints: If $n \le 1$ , <i>liwork</i> $\ge 1$ ; If <i>jobz</i> = 'N' and $n > 1$ , <i>liwork</i> $\ge 1$ ; If <i>jobz</i> = 'V' and $n > 1$ , <i>liwork</i> $\ge 5n+3$ .

### **Output Parameters**

ab	On exit, the contents of <i>ab</i> are overwritten.
bb	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^T S$ , as returned by spbstf/dpbstf.
W, Z	<pre>REAL for ssbgvd DOUBLE PRECISION for dsbgvd Arrays: w(*), DIMENSION at least max(1, n). If info = 0, contains the eigenvalues in ascending order.</pre>
	z(ldz, *). The second dimension of $z$ must be at least max $(1, n)$ . If $jobz = 'V'$ , then if $info = 0$ , $z$ contains the matrix $Z$ of eigenvectors, with the <i>i</i> -th column of $z$ holding the eigenvector associated with $w(i)$ . The eigenvectors are normalized so that $Z^TBZ = I$ . If $jobz = 'N'$ , then $z$ is not referenced.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th argument had an illegal value. If $info > 0$ , and
	if $i \leq n$ , the algorithm failed to converge, and $i$ off-diagonal elements of an intermediate tridiagonal did not converge to zero; if $info = n + i$ , for $1 \leq i \leq n$ , then $spbstf/dpbstf$ returned $info = i$ and $B$ is not positive-definite. The factorization of $B$ could not be completed and no eigenvalues or eigenvectors were computed.

# ?hbgvd

Computes all eigenvalues and, optionally, eigenvectors of a complex generalized Hermitian definite eigenproblem with banded matrices. If eigenvectors are desired, it uses a divide and conquer method.

#### **Discussion**

This routine computes all the eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite banded eigenproblem, of the form  $Ax = \lambda Bx$ . Here *A* and *B* are assumed to be Hermitian and banded, and *B* is also positive definite. If eigenvectors are desired, it uses a divide and conquer algorithm.

jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then compute eigenvalues only. If <i>jobz</i> = 'V', then compute eigenvalues and eigenvectors.
uplo	CHARACTER*1. Must be 'U' or 'L'. If $uplo = 'U'$ , arrays $ab$ and $bb$ store the upper triangles of A and B; If $uplo = 'L'$ , arrays $ab$ and $bb$ store the lower triangles of A and B.
n	<b>INTEGER.</b> The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
ka	<b>INTEGER.</b> The number of super- or sub-diagonals in $A$ ( $ka \ge 0$ ).

kb	<b>INTEGER.</b> The number of super- or sub-diagonals in $B$ ( $kb \ge 0$ ).
ab,bb,work	<ul> <li>COMPLEX for chbgvd</li> <li>DOUBLE COMPLEX for zhbgvd</li> <li>Arrays:</li> <li>ab (ldab,*) is an array containing either upper or lower triangular part of the Hermitian matrix A (as specified by uplo) in band storage format.</li> <li>The second dimension of the array ab must be at least max(1, n).</li> </ul>
	bb (1dbb, *) is an array containing either upper or lower triangular part of the Hermitian matrix B (as specified by $uplo$ ) in band storage format. The second dimension of the array bb must be at least max(1, n).
	work(lwork) is a workspace array.
ldab	<b>INTEGER.</b> The first dimension of the array $ab$ ; must be at least $ka$ +1.
ldbb	<b>INTEGER.</b> The first dimension of the array $bb$ ; must be at least $kb+1$ .
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ ; $ldz \ge 1$ . If $jobz = V'$ , $ldz \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array <i>work</i> .
	Constraints: If $n \le 1$ , $lwork \ge 1$ ; If $jobz = 'N'$ and $n > 1$ , $lwork \ge n$ ; If $jobz = 'V'$ and $n > 1$ , $lwork \ge 2n^2$ .
rwork	REAL for chbgvd DOUBLE PRECISION for zhbgvd. Workspace array, DIMENSION ( <i>lrwork</i> ).
lrwork	<b>INTEGER</b> . The dimension of the array <i>rwork</i> .

	Constraints:
	If $n \leq 1$ , $lrwork \geq 1$ ;
	If $jobz = N'$ and $n > 1$ , $lrwork \ge n$ ;
	If $jobz = V'$ and $n > 1$ , $lrwork \ge 2n^2 + 5n + 1$ .
iwork	INTEGER.
	Workspace array, DIMENSION ( <i>liwork</i> ).
liwork	<b>INTEGER</b> . The dimension of the array <i>iwork</i> .
	Constraints:
	If $n \leq 1$ , liwork $\geq 1$ ;
	If $jobz = N'$ and $n > 1$ , $liwork \ge 1$ ;
	If $jobz = V'$ and $n > 1$ , $liwork \ge 5n+3$ .

## Output Parameters

ab	On exit, the contents of <i>ab</i> are overwritten.
bb	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^H S$ , as returned by cpbstf/zpbstf.
W	<b>REAL</b> for chbgvd DOUBLE PRECISION for zhbgvd. Array, DIMENSION at least $max(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order.
Ζ	COMPLEX for chbgvd DOUBLE COMPLEX for zhbgvd Array $z(ldz, *)$ . The second dimension of $z$ must be at least max $(1, n)$ . If $jobz = "V"$ , then if $info = 0$ , $z$ contains the matrix $Z$ of eigenvectors, with the <i>i</i> -th column of $z$ holding the eigenvector associated with $w(i)$ . The eigenvectors are normalized so that $Z^H B Z = I$ . If $jobz = "N"$ , then $z$ is not referenced.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
rwork(1)	On exit, if <i>info</i> = 0, then <i>rwork(1)</i> returns the required minimal size of <i>lrwork</i> .

iwork(1)	On exit, if <i>info</i> = 0, then <i>iwork(1)</i> returns the required minimal size of <i>liwork</i> .
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = - <i>i</i> , the <i>i</i> th argument had an illegal value. If <i>info</i> > 0, and
	if $i \leq n$ , the algorithm failed to converge, and $i$ off-diagonal elements of an intermediate tridiagonal did not converge to zero; if $info = n + i$ , for $1 \leq i \leq n$ , then cpbstf/zpbstf returned $info = i$ and $B$ is not positive-definite. The factorization of $B$ could not be completed and no eigenvalues or eigenvectors were computed.

# ?sbgvx

Computes selected eigenvalues and, optionally, eigenvectors of a real generalized symmetric definite eigenproblem with banded matrices.

#### **Discussion**

This routine computes selected eigenvalues, and optionally, the eigenvectors of a real generalized symmetric-definite banded eigenproblem, of the form  $Ax = \lambda Bx$ . Here *A* and *B* are assumed to be symmetric and banded, and *B* is also positive definite.

Eigenvalues and eigenvectors can be selected by specifying either all eigenvalues, a range of values or a range of indices for the desired eigenvalues.

jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then compute eigenvalues only. If <i>jobz</i> = 'V', then compute eigenvalues and eigenvectors.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'. If range = 'A', the routine computes all eigenvalues. If range = 'V', the routine computes eigenvalues $\lambda_i$ in the half-open interval: $vl < \lambda_i \le vu$ . If range = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
uplo	CHARACTER*1. Must be 'U' or 'L'.

	If $uplo = 'U'$ , arrays <i>ab</i> and <i>bb</i> store the upper triangles of A and B; If $uplo = 'L'$ , arrays <i>ab</i> and <i>bb</i> store the lower triangles of A and B.
п	<b>INTEGER.</b> The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
ka	<b>INTEGER.</b> The number of super- or sub-diagonals in $A$ ( $ka \ge 0$ ).
kb	<b>INTEGER.</b> The number of super- or sub-diagonals in $B$ ( $kb \ge 0$ ).
ab,bb,work	REAL for ssbgvx DOUBLE PRECISION for dsbgvx Arrays: ab (1dab, *) is an array containing either upper or
	lower triangular part of the symmetric matrix $A$ (as specified by $uplo$ ) in band storage format. The second dimension of the array $ab$ must be at least max $(1, n)$ .
	bb (1dbb, *) is an array containing either upper or lower triangular part of the symmetric matrix $B$ (as specified by $up1o$ ) in band storage format. The second dimension of the array bb must be at least max $(1, n)$ .
	work(*) is a workspace array, DIMENSION at least $max(1, 7n)$ .
ldab	<b>INTEGER.</b> The first dimension of the array $ab$ ; must be at least $ka+1$ .
ldbb	<b>INTEGER.</b> The first dimension of the array $bb$ ; must be at least $kb+1$ .
vl, vu	REAL for ssbgvx DOUBLE PRECISION for dsbgvx. If <i>range</i> = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: v1< vu.
	If $range = 'A'$ or 'I', v1 and vu are not referenced.

il, iu	INTEGER.
	If <i>range</i> = 'I', the indices in ascending order of the
	smallest and largest eigenvalues to be returned.
	Constraint: $1 \leq i \leq u \leq n$ , if $n > 0$ ; $i = 1$ and $i = 0$
	$\text{if } \mathbf{n} = 0.$
	If <i>range</i> = 'A' or 'V', <i>il</i> and <i>iu</i> are not referenced.
abstol	REAL for ssbgvx
	DOUBLE PRECISION for dsbgvx.
	The absolute error tolerance for the eigenvalues.
	See Application Notes for more information.
ldz	<b>INTEGER</b> . The leading dimension of the output array <i>z</i> ;
	$ldz \ge 1$ . If $jobz = V'$ , $ldz \ge max(1, n)$ .
ldq	<b>INTEGER.</b> The leading dimension of the output array $q$ ;
	$ldq \ge 1$ . If $jobz = V'$ , $ldq \ge max(1, n)$ .
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, 5n)$ .

### **Output Parameters**

ab	On exit, the contents of <i>ab</i> are overwritten.
bb	On exit, contains the factor S from the split Cholesky factorization $B = S^T S$ , as returned by spbstf/dpbstf.
m	<b>INTEGER.</b> The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', m = iu - il + 1.
w, z, q	<pre>REAL for ssbgvx DOUBLE PRECISION for dsbgvx Arrays: w(*), DIMENSION at least max(1, n). If info = 0, contains the eigenvalues in ascending order.</pre>
	z(ldz, *). The second dimension of $z$ must be at least max $(1, n)$ . If $jobz = 'V'$ , then if $info = 0$ , $z$ contains the matrix $Z$ of eigenvectors, with the <i>i</i> -th column of $z$ holding the eigenvector associated with $w(i)$ . The eigenvectors are

if

	normalized so that $Z^T B Z = I$ . If $jobz = 'N'$ , then z is not referenced. q(ldq, *). The second dimension of q must be at least max $(1, n)$ . If $jobz = 'V'$ , then q contains the <i>n</i> -by- <i>n</i> matrix used in the reduction of $Ax = \lambda Bx$ to standard form, that is, $Cx = \lambda x$ and consequently C to tridiagonal form. If $jobz = 'N'$ , then q is not referenced.
ifail	<pre>INTEGER. Array, DIMENSION at least max(1, n). If jobz = 'V', then if info = 0, the first m elements of ifail are zero; if info &gt; 0, the ifail contains the indices of the eigenvectors that failed to converge. If jobz = 'N', then ifail is not referenced.</pre>
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith argument had an illegal value. If info &gt; 0, and</pre>
	if $i \leq n$ , the algorithm failed to converge, and $i$ off-diagonal elements of an intermediate tridiagonal did not converge to zero; if $info = n + i$ , for $1 \leq i \leq n$ , then spbstf/dpbstf returned $info = i$ and $B$ is not positive-definite. The factorization of $B$ could not be completed and no eigenvalues or eigenvectors were computed.

#### **Application Notes**

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to  $abstol + \varepsilon * max(|a|,|b|)$ , where  $\varepsilon$  is the machine precision. If abstolis less than or equal to zero, then  $\varepsilon * ||T/|_1$  will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when *abstol* is set to twice the underflow threshold 2*?lamch('S'), not zero. If this routine returns with *info* > 0, indicating that some eigenvectors did not converge, try setting abstol to 2*?lamch('S').

# ?hbgvx

Computes selected eigenvalues and, optionally, eigenvectors of a complex generalized Hermitian definite eigenproblem with banded matrices.

#### **Discussion**

This routine computes selected eigenvalues, and optionally, the eigenvectors of a complex generalized Hermitian-definite banded eigenproblem, of the form  $Ax = \lambda Bx$ . Here *A* and *B* are assumed to be Hermitian and banded, and *B* is also positive definite.

Eigenvalues and eigenvectors can be selected by specifying either all eigenvalues, a range of values or a range of indices for the desired eigenvalues.

jobz	CHARACTER*1. Must be 'N' or 'V'. If <i>jobz</i> = 'N', then compute eigenvalues only. If <i>jobz</i> = 'V', then compute eigenvalues and eigenvectors.
range	CHARACTER*1. Must be 'A' or 'V' or 'I'. If range = 'A', the routine computes all eigenvalues. If range = 'V', the routine computes eigenvalues $\lambda_i$ in the half-open interval: $vl < \lambda_i \le vu$ . If range = 'I', the routine computes eigenvalues with indices <i>il</i> to <i>iu</i> .
uplo	CHARACTER*1. Must be 'U' or 'L'.

	If $uplo = 'U'$ , arrays <i>ab</i> and <i>bb</i> store the upper triangles of A and B; If $uplo = 'L'$ , arrays <i>ab</i> and <i>bb</i> store the lower triangles of A and B.
n	<b>INTEGER.</b> The order of the matrices <i>A</i> and <i>B</i> ( $n \ge 0$ ).
ka	<b>INTEGER.</b> The number of super- or sub-diagonals in $A$ ( $ka \ge 0$ ).
kb	<b>INTEGER.</b> The number of super- or sub-diagonals in $B$ ( $kb \ge 0$ ).
ab,bb,work	COMPLEX for chbgvx DOUBLE COMPLEX for zhbgvx Arrays:
	<ul> <li>ab (1dab, *) is an array containing either upper or lower triangular part of the Hermitian matrix A (as specified by uplo) in band storage format.</li> <li>The second dimension of the array ab must be at least max(1, n).</li> </ul>
	bb (1dbb, *) is an array containing either upper or lower triangular part of the Hermitian matrix $B$ (as specified by $up1o$ ) in band storage format. The second dimension of the array bb must be at least max(1, n).
	<pre>work(*) is a workspace array, DIMENSION at least max(1, n).</pre>
ldab	<b>INTEGER.</b> The first dimension of the array <i>ab</i> ; must be at least <i>ka</i> +1.
ldbb	<b>INTEGER.</b> The first dimension of the array $bb$ ; must be at least $kb+1$ .
vl, vu	REAL for chbgvx DOUBLE PRECISION for zhbgvx. If <i>range</i> = 'V', the lower and upper bounds of the interval to be searched for eigenvalues. Constraint: v1< vu.
	If $range = 'A'$ or 'I', vl and vu are not referenced.

il, iu	INTEGER.
	If <i>range</i> = 'I', the indices in ascending order of the
	smallest and largest eigenvalues to be returned.
	Constraint: $1 \le i1 \le iu \le n$ , if $n > 0$ ; $i1 = 1$ and $iu = 0$
	if n = 0.
	If $range = 'A'$ or 'V', <i>il</i> and <i>iu</i> are not referenced.
abstol	REAL for chbgvx
	DOUBLE PRECISION for zhbgvx.
	The absolute error tolerance for the eigenvalues. See <i>Application Notes</i> for more information.
ldz	<b>INTEGER.</b> The leading dimension of the output array $z$ ;
	$ldz \ge 1$ . If $jobz = V'$ , $ldz \ge max(1, n)$ .
ldq	<b>INTEGER</b> . The leading dimension of the output array $q$ ;
	$ldq \ge 1$ . If $jobz = 'V'$ , $ldq \ge max(1, n)$ .
rwork	REAL for chbgvx
	DOUBLE PRECISION for zhbgvx.
	Workspace array, <b>DIMENSION</b> at least $max(1, 7n)$ .
iwork	INTEGER.
	Workspace array, DIMENSION at least $max(1, 5n)$ .
Output Deven	eters
Output Parame	
ab	On exit, the contents of <i>ab</i> are overwritten.
	On exit, the contents of <i>ab</i> are overwritten. On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^H S$ , as returned by cpbstf/zpbstf.
ab	On exit, contains the factor <i>S</i> from the split Cholesky
ab bb	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^H S$ , as returned by cpbstf/zpbstf. INTEGER. The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I',
ab bb	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^H S$ , as returned by cpbstf/zpbstf. INTEGER. The total number of eigenvalues found,
ab bb	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^H S$ , as returned by cpbstf/zpbstf. INTEGER. The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', m = iu - il + 1. REAL for chbgvx
ab bb m	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^H S$ , as returned by cpbstf/zpbstf. INTEGER. The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', m = iu - il + 1. REAL for chbgvx DOUBLE PRECISION for zhbgvx.
ab bb m	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^H S$ , as returned by cpbstf/zpbstf. INTEGER. The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', m = iu - il + 1. REAL for chbgvx DOUBLE PRECISION for zhbgvx. Array w(*), DIMENSION at least max(1, $n$ ).
ab bb m	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^H S$ , as returned by cpbstf/zpbstf. INTEGER. The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', m = iu - il + 1. REAL for chbgvx DOUBLE PRECISION for zhbgvx. Array $w(*)$ , DIMENSION at least max $(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order.
ab bb m	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^H S$ , as returned by cpbstf/zpbstf. INTEGER. The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', m = iu - il + 1. REAL for chbgvx DOUBLE PRECISION for zhbgvx. Array w(*), DIMENSION at least max(1, $n$ ). If <i>info</i> = 0, contains the eigenvalues in ascending order. COMPLEX for chbgvx
ab bb m w	On exit, contains the factor <i>S</i> from the split Cholesky factorization $B = S^H S$ , as returned by cpbstf/zpbstf. INTEGER. The total number of eigenvalues found, $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', m = iu - il + 1. REAL for chbgvx DOUBLE PRECISION for zhbgvx. Array $w(*)$ , DIMENSION at least max $(1, n)$ . If <i>info</i> = 0, contains the eigenvalues in ascending order.

	z(ldz, *). The second dimension of $z$ must be at least max $(1, n)$ . If $jobz = 'V'$ , then if $info = 0$ , $z$ contains the matrix $Z$ of eigenvectors, with the <i>i</i> -th column of $z$ holding the eigenvector associated with $w(i)$ . The eigenvectors are normalized so that $Z^H B Z = I$ . If $jobz = 'N'$ , then $z$ is not referenced. q(ldq, *). The second dimension of $q$ must be at least max $(1, n)$ . If $jobz = 'V'$ , then $q$ contains the <i>n</i> -by- <i>n</i> matrix used in the reduction of $Ax = \lambda Bx$ to standard form, that is, $Cx = \lambda x$ and consequently $C$ to tridiagonal form. If $jobz = 'N'$ , then $q$ is not referenced.
ifail	<pre>INTEGER. Array, DIMENSION at least max(1, n). If jobz = 'V', then if info = 0, the first m elements of ifail are zero; if info &gt; 0, the ifail contains the indices of the eigenvectors that failed to converge. If jobz = 'N', then ifail is not referenced.</pre>
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th argument had an illegal value. If $info > 0$ , and if $i \le n$ , the algorithm failed to converge, and <i>i</i> off-diagonal elements of an intermediate tridiagonal did not converge to zero; if $info = n + i$ , for $1 \le i \le n$ , then cpbstf/zpbstf returned $info = i$ and <i>B</i> is not positive-definite. The factorization of <i>B</i> could not be completed and no eigenvalues or eigenvectors were computed.

#### **Application Notes**

An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to **abstol** +  $\varepsilon$  * max(|a|,|b|), where  $\varepsilon$  is the machine precision. If **abstol** is less than or equal to zero, then  $\varepsilon$  *  $||T/|_1$  will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when *abstol* is set to twice the underflow threshold 2*?lamch('S'), not zero. If this routine returns with *info* > 0, indicating that some eigenvectors did not converge, try setting *abstol* to 2*?lamch('S').

### **Generalized Nonsymmetric Eigenproblems**

This section describes LAPACK driver routines used for solving generalized nonsymmetric eigenproblems. See also <u>computational routines</u> that can be called to solve these problems. <u>Table 5-14</u> lists routines described in more detail below.

# Table 5-14Driver Routines for Solving Generalized Nonsymmetric<br/>Eigenproblems

Routine Name	Operation performed
?gges	Computes the generalized eigenvalues, Schur form, and the left and/or right Schur vectors for a pair of nonsymmetric matrices.
?ggesx	Computes the generalized eigenvalues, Schur form, and, optionally, the left and/or right matrices of Schur vectors .
?ggev	Computes the generalized eigenvalues, and the left and/or right generalized eigenvectors for a pair of nonsymmetric matrices.
?ggevx	Computes the generalized eigenvalues, and, optionally, the left and/or right generalized eigenvectors.

### ?gges

Computes the generalized eigenvalues, Schur form, and the left and/or right Schur vectors for a pair of nonsymmetric matrices.

#### **Discussion**

This routine computes for a pair of *n*-by-*n* real/complex nonsymmetric matrices (*A*,*B*), the generalized eigenvalues, the generalized real/complex Schur form (*S*,*T*), optionally, the left and/or right matrices of Schur vectors (*vs1* and *vsr*). This gives the generalized Schur factorization

 $(A,B) = (vsl*S*vsr^{H}, vsl*T*vsr^{H})$ 

Optionally, it also orders the eigenvalues so that a selected cluster of eigenvalues appears in the leading diagonal blocks of the upper quasi-triangular matrix *S* and the upper triangular matrix *T*. The leading columns of *vs1* and *vsr* then form an orthonormal/unitary basis for the corresponding left and right eigenspaces (deflating subspaces). (If only the generalized eigenvalues are needed, use the driver ?ggev instead, which is faster.)

A generalized eigenvalue for a pair of matrices (A,B) is a scalar *w* or a ratio *alpha / beta* = *w*, such that A - w * B is singular. It is usually represented as the pair (*alpha, beta*), as there is a reasonable interpretation for *beta*=0 or for both being zero.

A pair of matrices (S, T) is in generalized real Schur form if T is upper triangular with non-negative diagonal and S is block upper triangular with 1-by-1 and 2-by-2 blocks. 1-by-1 blocks correspond to real generalized eigenvalues, while 2-by-2 blocks of S will be "standardized" by making the corresponding elements of T have the form:

$$\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$$

and the pair of corresponding 2-by-2 blocks in *S* and *T* will have a complex conjugate pair of generalized eigenvalues.

A pair of matrices (S, T) is in generalized complex Schur form if S and T are upper triangular and, in addition, the diagonal of T are non-negative real numbers.

jobvsl	CHARACTER*1. Must be 'N' or 'V'. If <i>jobvs1</i> = 'N', then the left Schur vectors are not computed. If <i>jobvs1</i> = 'V', then the left Schur vectors are computed.
jobvsr	CHARACTER*1. Must be 'N' or 'V'. If <i>jobvsr</i> = 'N', then the right Schur vectors are not computed. If <i>jobvsr</i> = 'V', then the right Schur vectors are computed.
sort	CHARACTER*1. Must be 'N' or 'S'. Specifies whether or not to order the eigenvalues on the diagonal of the generalized Schur form.
	If <i>sort</i> = 'N', then eigenvalues are not ordered. If <i>sort</i> = 'S', eigenvalues are ordered (see <i>selctg</i> ).
selctg	LOGICAL FUNCTION of three REAL arguments for real flavors. LOGICAL FUNCTION of two COMPLEX arguments for complex flavors.
	<pre>selctg must be declared EXTERNAL in the calling subroutine. If sort = 'S', selctg is used to select eigenvalues to sort to the top left of the Schur form. If sort = 'N', selctg is not referenced.</pre>
	For real flavors: An eigenvalue (alphar(j) + alphai(j))/beta(j) is selected if selctg(alphar(j), alphai(j), beta(j)) is true; that is, if either one of a complex conjugate pair of eigenvalues is selected, then both complex eigenvalues are selected. Note that in the ill-conditioned case, a selected complex eigenvalue may no longer satisfy selctg(alphar(j), alphai(j), beta(j)) = .TRUE.
	after ordering. In this case $info$ is set to $n+2$ .

	<pre>For complex flavors: An eigenvalue alpha(j) / beta(j) is selected if selctg(alpha(j), beta(j)) is true. Note that a selected complex eigenvalue may no longer satisfy selctg(alpha(j), beta(j)) = .TRUE. after ordering, since ordering may change the value of complex eigenvalues (especially if the eigenvalue is ill-conditioned); in this case info is set to n+2 (see info below).</pre>
n	<b>INTEGER</b> . The order of the matrices $A$ , $B$ , $vsl$ , and $vsr$ $(n \ge 0)$ .
a, b, work	REAL for sgges DOUBLE PRECISION for dgges COMPLEX for cgges DOUBLE COMPLEX for zgges. Arrays: a(1da,*) is an array containing the <i>n</i> -by- <i>n</i> matrix <i>A</i> (first of the pair of matrices). The second dimension of <i>a</i> must be at least max(1, <i>n</i> ). b(1db,*) is an array containing the <i>n</i> -by- <i>n</i> matrix <i>B</i> (second of the pair of matrices). The second dimension of <i>b</i> must be at least max(1, <i>n</i> ). b(1db,*) is an array containing the <i>n</i> -by- <i>n</i> matrix <i>B</i> (second of the pair of matrices). The second dimension of <i>b</i> must be at least max(1, <i>n</i> ). work(1work) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of the array $b$ . Must be at least max $(1, n)$ .
ldvsl,ldvsr	<b>INTEGER.</b> The first dimensions of the output matrices $vsl$ and $vsr$ , respectively. Constraints: $ldvsl \ge 1$ . If $jobvsl = :V', ldvsl \ge max(1, n)$ . $ldvsr \ge 1$ . If $jobvsr = :V', ldvsr \ge max(1, n)$ .
lwork	INTEGER. The dimension of the array work.

	$lwork \ge max(1, 8n+16)$ for real flavors; $lwork \ge max(1, 2n)$ for complex flavors. For good performance, <i>lwork</i> must generally be larger.
rwork	REAL for cgges DOUBLE PRECISION for zgges Workspace array, DIMENSION at least max(1, 8n). This array is used in complex flavors only.
bwork	<b>LOGICAL</b> . Workspace array, <b>DIMENSION</b> at least $max(1, n)$ . Not referenced if <i>sort</i> = 'N'.
Output Parame	eters
а	On exit, this array has been overwritten by its generalized Schur form <i>S</i> .
b	On exit, this array has been overwritten by its generalized Schur form $T$ .
sdim	INTEGER. If sort ='N', sdim= 0. If sort ='S', sdim is equal to the number of eigenvalues (after sorting) for which selctg is true. Note that for real flavors complex conjugate pairs for which selctg is true for either eigenvalue count as 2.
alphar,alphai	REAL for sgges; DOUBLE PRECISION for dgges. Arrays, DIMENSION at least $\max(1,n)$ each. Contain values that form generalized eigenvalues in real flavors. See <i>beta</i> .
alpha	COMPLEX for cgges; DOUBLE COMPLEX for zgges. Array, DIMENSION at least $max(1,n)$ . Contain values that form generalized eigenvalues in complex flavors. See <i>beta</i> .
beta	REAL for sgges DOUBLE PRECISION for dgges

COMPLEX for cgges

	DOUBLE COMPLEX for zgges.
	Array, DIMENSION at least $\max(1,n)$ .
	For real flavors:
	On exit, $(alphar(j) + alphai(j)*i)/beta(j), j=1,,n,$
	will be the generalized eigenvalues.
	alphar(j) + alphai(j)*i and $beta(j), j=1,,n$ are the diagonals of the complex Schur form ( <i>S</i> , <i>T</i> ) that would
	result if the 2-by-2 diagonal blocks of the real
	generalized Schur form of $(A, B)$ were further reduced to
	triangular form using complex unitary transformations.
	If alphai(j) is zero, then the j-th eigenvalue is real; if
	positive, then the j-th and $(j+1)$ -st eigenvalues are a
	complex conjugate pair, with <i>alphai</i> (j+1) negative.
	For complex flavors:
	On exit, $alpha(j)/beta(j)$ , $j=1,,n$ , will be the
	generalized eigenvalues. $alpha(j), j=1,,n$ , and
	beta(j), j=1,,n, are the diagonals of the complex
	Schur form ( <i>S</i> , <i>T</i> ) output by cgges/zgges. The $beta(j)$
	will be non-negative real.
	See also Application Notes below.
vsl, vsr	REAL for sgges
	DOUBLE PRECISION for dgges
	COMPLEX for cgges
	DOUBLE COMPLEX for zgges.
	Arrays:
	vsl(ldvsl,*), the second dimension of vsl must be
	at least $\max(1, n)$ .
	If <i>jobvs1</i> = 'V', this array will contain the left Schur
	vectors.
	If $jobvsl = 'N'$ , $vsl$ is not referenced.
	vsr(ldvsr, *), the second dimension of vsr must be
	at least $\max(1, n)$ .
	If <i>jobvsr</i> = 'V', this array will contain the right Schur
	vectors.

If *jobvsr* = 'N', *vsr* is not referenced.

work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , and $i \le n$ :
	the QZ iteration failed. $(A,B)$ is not in Schur form, but alphar(j), alphai(j) (for real flavors), or alpha(j) (for complex flavors), and $beta(j)$ , $j=info+1,,n$ should be correct.
	i > n: errors that usually indicate LAPACK problems:
	i = n+1: other than $QZ$ iteration failed in ?hgeqz;
	i = n+2: after reordering, roundoff changed values of some complex eigenvalues so that leading eigenvalues in the generalized Schur form no longer satisfy selctg = .TRUE. This could also be caused due to scaling;
	i = n+3: reordering failed in ?tgsen.

#### **Application Notes**

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The quotients alphar(j)/beta(j) and alphai(j)/beta(j) may easily overor underflow, and beta(j) may even be zero. Thus, you should avoid simply computing the ratio. However, alphar and alphai will be always less than and usually comparable with norm(A) in magnitude, and beta always less than and usually comparable with norm(B).

# ?ggesx

Computes the generalized eigenvalues, Schur form, and, optionally, the left and/or right matrices of Schur vectors.

#### **Discussion**

This routine computes for a pair of *n*-by-*n* real/complex nonsymmetric matrices (*A*,*B*), the generalized eigenvalues, the generalized real/complex Schur form (*S*,*T*), optionally, the left and/or right matrices of Schur vectors (*vs1* and *vsr*). This gives the generalized Schur factorization

 $(A,B) = (vsl*S*vsr^{H}, vsl*T*vsr^{H})$ 

Optionally, it also orders the eigenvalues so that a selected cluster of eigenvalues appears in the leading diagonal blocks of the upper quasi-triangular matrix *S* and the upper triangular matrix *T*; computes a reciprocal condition number for the average of the selected eigenvalues (*rconde*); and computes a reciprocal condition number for the right and left deflating subspaces corresponding to the selected eigenvalues (*rcondv*). The leading columns of *vsl* and *vsr* then form an orthonormal/unitary basis for the corresponding left and right eigenspaces (deflating subspaces).

A generalized eigenvalue for a pair of matrices (A,B) is a scalar *w* or a ratio *alpha / beta* = *w*, such that A - w * B is singular. It is usually represented as the pair (*alpha, beta*), as there is a reasonable interpretation for *beta*=0 or for both being zero.

A pair of matrices (S, T) is in generalized real Schur form if T is upper triangular with non-negative diagonal and S is block upper triangular with 1-by-1 and 2-by-2 blocks. 1-by-1 blocks correspond to real generalized eigenvalues, while 2-by-2 blocks of S will be "standardized" by making the corresponding elements of T have the form:

```
\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}
```

and the pair of corresponding 2-by-2 blocks in *S* and *T* will have a complex conjugate pair of generalized eigenvalues.

A pair of matrices (S,T) is in generalized complex Schur form if S and T are upper triangular and, in addition, the diagonal of T are non-negative real numbers.

jobvsl	CHARACTER*1. Must be 'N' or 'V'. If <i>jobvs1</i> ='N', then the left Schur vectors are not computed. If <i>jobvs1</i> ='V', then the left Schur vectors are computed.
jobvsr	CHARACTER*1. Must be 'N' or 'V'. If <i>jobvsr</i> = 'N', then the right Schur vectors are not computed. If <i>jobvsr</i> = 'V', then the right Schur vectors are computed.
sort	CHARACTER*1. Must be 'N' or 'S'. Specifies whether or not to order the eigenvalues on the diagonal of the generalized Schur form.
	If <i>sort</i> = 'N', then eigenvalues are not ordered. If <i>sort</i> = 'S', eigenvalues are ordered (see <i>selctg</i> ).

selctg	LOGICAL FUNCTION of three REAL arguments for real flavors. LOGICAL FUNCTION of two COMPLEX arguments for complex flavors.
	<pre>selctg must be declared EXTERNAL in the calling subroutine. If sort = 'S', selctg is used to select eigenvalues to sort to the top left of the Schur form. If sort = 'N', selctg is not referenced.</pre>
	For real flavors: An eigenvalue $(alphar(j) + alphai(j))/beta(j)$ is selected if $selctg(alphar(j), alphai(j), beta(j))$ is true; that is, if either one of a complex conjugate pair of eigenvalues is selected, then both complex eigenvalues are selected. Note that in the ill-conditioned case, a selected complex eigenvalue may no longer satisfy selctg(alphar(j), alphai(j), beta(j)) = .TRUE. after ordering. In this case $info$ is set to $n+2$ .
	<pre>For complex flavors: An eigenvalue alpha(j) / beta(j) is selected if selctg(alpha(j), beta(j)) is true. Note that a selected complex eigenvalue may no longer satisfy selctg(alpha(j), beta(j)) = .TRUE. after ordering, since ordering may change the value of complex eigenvalues (especially if the eigenvalue is ill-conditioned); in this case info is set to n+2 (see info below).</pre>
sense	CHARACTER*1. Must be 'N', 'E', 'V', or 'B'. Determines which reciprocal condition number are computed.
	If sense = 'N', none are computed; If sense = 'E', computed for average of selected eigenvalues only; If sense = 'V', computed for selected deflating subspaces only;

	If $sense = 'B'$ , computed for both.
	If sense is 'E', 'V', or 'B', then sort must equal 'S'.
n	<b>INTEGER</b> . The order of the matrices $A$ , $B$ , $vsl$ , and $vsr$ $(n \ge 0)$ .
a, b, work	REAL for sggesx DOUBLE PRECISION for dggesx COMPLEX for cggesx DOUBLE COMPLEX for zggesx. Arrays: a(lda,*) is an array containing the <i>n</i> -by- <i>n</i> matrix <i>A</i> (first of the pair of matrices). The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
	b(1db, *) is an array containing the <i>n</i> -by- <i>n</i> matrix <i>B</i> (second of the pair of matrices). The second dimension of <i>b</i> must be at least max(1, <i>n</i> ).
	work(lwork) is a workspace array.
lda	<b>INTEGER</b> . The first dimension of the array <b>a</b> . Must be at least $max(1, n)$ .
ldb	<b>INTEGER</b> . The first dimension of the array $b$ . Must be at least max $(1, n)$ .
ldvsl,ldvsr	<b>INTEGER.</b> The first dimensions of the output matrices $vsl$ and $vsr$ , respectively. Constraints: $ldvsl \ge 1$ . If $jobvsl = 'V'$ , $ldvsl \ge max(1, n)$ . $ldvsr \ge 1$ . If $jobvsr = 'V'$ , $ldvsr \ge max(1, n)$ .
lwork	INTEGER. The dimension of the array work. For real flavors: $lwork \ge max(1, 8(n+1)+16);$ if sense = 'E', 'V', or 'B', then $lwork \ge max(8(n+1)+16), 2*sdim*(n-sdim)).$ For complex flavors: $lwork \ge max(1, 2n);$ if sense = 'E', 'V', or 'B', then $lwork \ge max(2n, 2*sdim*(n-sdim)).$

For good performance, *lwork* must generally be larger.

rwork	REAL for cggesx DOUBLE PRECISION for zggesx Workspace array, DIMENSION at least max(1, 8n). This array is used in complex flavors only.
iwork	INTEGER. Workspace array, DIMENSION ( <i>liwork</i> ). Not referenced if <i>sense</i> = 'N'.
liwork	<b>INTEGER</b> . The dimension of the array <i>iwork</i> .
	<i>liwork</i> ≥ $n+6$ for real flavors; <i>liwork</i> ≥ $n+2$ for complex flavors.
bwork	LOGICAL. Workspace array, DIMENSION at least $\max(1, n)$ . Not referenced if <u>sort</u> = 'N'.

### **Output Parameters**

а	On exit, this array has been overwritten by its generalized Schur form <i>S</i> .
b	On exit, this array has been overwritten by its generalized Schur form $T$ .
sdim	INTEGER. If sort ='N', sdim=0. If sort ='S', sdim is equal to the number of eigenvalues (after sorting) for which selctg is true. Note that for real flavors complex conjugate pairs for which selctg is true for either eigenvalue count as 2.
alphar,alphai	REAL for sggesx; DOUBLE PRECISION for dggesx. Arrays, DIMENSION at least $max(1,n)$ each. Contain values that form generalized eigenvalues in real flavors. See <i>beta</i> .

alpha	COMPLEX for cggesx; DOUBLE COMPLEX for zggesx. Array, DIMENSION at least $max(1,n)$ . Contain values that form generalized eigenvalues in complex flavors. See <i>beta</i> .
beta	REAL for sggesx DOUBLE PRECISION for dggesx COMPLEX for cggesx DOUBLE COMPLEX for zggesx. Array, DIMENSION at least max(1,n). For real flavors: On exit, $(alphar(j) + alphai(j)*i)/beta(j), j=1,,n,$ will be the generalized eigenvalues. alphar(j) + alphai(j)*i and $beta(j), j=1,,n$ are the diagonals of the complex Schur form $(S,T)$ that would result if the 2-by-2 diagonal blocks of the real generalized Schur form of $(A,B)$ were further reduced to triangular form using complex unitary transformations. If $alphai(j)$ is zero, then the j-th eigenvalue is real; if positive, then the j-th and $(j+1)$ -st eigenvalues are a complex conjugate pair, with $alphai(j+1)$ negative. For complex flavors: On exit, $alpha(j)/beta(j), j=1,,n$ , will be the generalized eigenvalues. $alpha(j), j=1,,n$ , and beta(j), j=1,,n, are the diagonals of the complex Schur form $(S,T)$ output by cggesx/zggesx. The beta(j) will be non-negative real.
	See also Application Notes below.
vsl, vsr	REAL for sggesx DOUBLE PRECISION for dggesx COMPLEX for cggesx DOUBLE COMPLEX for zggesx. Arrays: vsl(ldvsl,*), the second dimension of vsl must be

at least max(1, n).

	If $jobvsl = V'$ , this array will contain the left Schur vectors.
	<pre>If jobvs1 = 'N', vs1 is not referenced. vsr(ldvsr,*), the second dimension of vsr must be at least max(1, n). If jobvsr = 'V', this array will contain the right Schur vectors. If jobvsr = 'N', vsr is not referenced.</pre>
rconde,rcondv	REAL for single precision flavors DOUBLE PRECISION for double precision flavors. Arrays, DIMENSION (2) each
	If sense = 'E' or 'B', rconde(1) and rconde(2) contain the reciprocal condition numbers for the average of the selected eigenvalues. Not referenced if sense = 'N' or 'V'.
	If sense = 'V' or 'B', <i>rcondv</i> (1) and <i>rcondv</i> (2) contain the reciprocal condition numbers for the selected deflating subspaces. Not referenced if <i>sense</i> = 'N' or 'E'.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , and $i \leq n$ :
	the QZ iteration failed. $(A,B)$ is not in Schur form, but alphar(j), alphai(j) (for real flavors), or $alpha(j)$ (for complex flavors), and $beta(j), j=info+1,,n$ should be correct.
	i > n: errors that usually indicate LAPACK problems:
	i = n+1: other than QZ iteration failed in ?hgeqz;

i = n+2: after reordering, roundoff changed values of some complex eigenvalues so that leading eigenvalues in the generalized Schur form no longer satisfy selctg = .TRUE.. This could also be caused due to scaling;

i = n+3: reordering failed in ?tgsen.

#### **Application Notes**

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The quotients alphar(j)/beta(j) and alphai(j)/beta(j) may easily overor underflow, and beta(j) may even be zero. Thus, you should avoid simply computing the ratio. However, alphar and alphai will be always less than and usually comparable with norm(A) in magnitude, and beta always less than and usually comparable with norm(B).

# ?ggev

Computes the generalized eigenvalues, and the left and/or right generalized eigenvectors for a pair of nonsymmetric matrices.

#### **Discussion**

This routine computes for a pair of *n*-by-*n* real/complex nonsymmetric matrices (A, B), the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors.

A generalized eigenvalue for a pair of matrices (*A*,*B*) is a scalar  $\lambda$  or a ratio *alpha* / *beta* =  $\lambda$ , such that *A* -  $\lambda * B$  is singular. It is usually represented as the pair (*alpha*, *beta*), as there is a reasonable interpretation for *beta*=0 and even for both being zero.

The right generalized eigenvector v(j) corresponding to the generalized eigenvalue  $\lambda(j)$  of (A, B) satisfies

 $A * v(j) = \lambda(j) * B * v(j) .$ 

The left generalized eigenvector u(j) corresponding to the generalized eigenvalue  $\lambda(j)$  of (A,B) satisfies

 $u(\mathbf{j})^H * A = \lambda(\mathbf{j}) * u(\mathbf{j})^H * B$ 

where  $u(j)^H$  denotes the conjugate transpose of u(j).

jobvl	CHARACTER*1. Must be 'N' or 'V'. If <i>jobv1</i> = 'N', the left generalized eigenvectors are not computed; If <i>jobv1</i> = 'V', the left generalized eigenvectors are computed.
jobvr	CHARACTER*1. Must be 'N' or 'V'. If <i>jobvr</i> = 'N', the right generalized eigenvectors are not computed; If <i>jobvr</i> = 'V', the right generalized eigenvectors are computed.
n	<b>INTEGER.</b> The order of the matrices $A$ , $B$ , $v1$ , and $vr$ $(n \ge 0)$ .
a, b, work	<pre>REAL for sggev DOUBLE PRECISION for dggev COMPLEX for cggev DOUBLE COMPLEX for zggev. Arrays: a(lda,*) is an array containing the n-by-n matrix A (first of the pair of matrices). The second dimension of a must be at least max(1, n). b(ldb,*) is an array containing the n-by-n matrix B (second of the pair of matrices). The second dimension of b must be at least max(1, n). work(lwork) is a workspace array.</pre>
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of the array $b$ . Must be at least max $(1, n)$ .
ldvl,ldvr	<b>INTEGER.</b> The first dimensions of the output matrices v1 and vr, respectively. Constraints: $ldvl \ge 1$ . If $jobvl = 'V'$ , $ldvl \ge max(1, n)$ . $ldvr \ge 1$ . If $jobvr = 'V'$ , $ldvr \ge max(1, n)$ .
lwork	<b>INTEGER.</b> The dimension of the array work.

	$lwork \ge max(1, 8n+16)$ for real flavors; $lwork \ge max(1, 2n)$ for complex flavors.For good performance, $lwork$ must generally be larger.
rwork	REAL for cggev
	DOUBLE PRECISION for zggev
	Workspace array, DIMENSION at least $max(1, 8n)$ .
	This array is used in complex flavors only.

### **Output Parameters**

a, b	On exit, these arrays have been overwritten.
alphar,alphai	REAL for sggev; DOUBLE PRECISION for dggev. Arrays, DIMENSION at least $\max(1,n)$ each. Contain values that form generalized eigenvalues in real flavors. See <i>beta</i> .
alpha	COMPLEX for cggev; DOUBLE COMPLEX for zggev. Array, DIMENSION at least $\max(1,n)$ . Contain values that form generalized eigenvalues in complex flavors. See <i>beta</i> .
beta	REAL for sggev DOUBLE PRECISION for dggev COMPLEX for cggev DOUBLE COMPLEX for zggev. Array, DIMENSION at least max(1,n). For real flavors: On exit, (alphar(j) + alphai(j)*i)/beta(j), j=1,,n, will be the generalized eigenvalues. If alphai(j) is zero, then the j-th eigenvalue is real; if positive, then the j-th and (j+1)-st eigenvalues are a complex conjugate pair, with alphai(j+1) negative. For complex flavors: On exit, alpha(j)/beta(j), j=1,,n, will be the generalized eigenvalues. See also Application Notes below.

vl, vr

REAL for sggev DOUBLE PRECISION for dggev COMPLEX for cggev DOUBLE COMPLEX for zggev.

Arrays:

vl(ldvl, *); the second dimension of vl must be at least max(1, n).

If jobvl = 'V', the left generalized eigenvectors u(j) are stored one after another in the columns of vl, in the same order as their eigenvalues. Each eigenvector will be scaled so the largest component have abs(Re) + abs(Im) = 1. If jobvl = 'N', vl is not referenced. For real flavors:

If the j-th eigenvalue is real, then u(j) = vl(:,j), the j-th column of vl. If the j-th and (j+1)-st eigenvalues form a complex conjugate pair, then u(j) = vl(:,j) + i*vl(:,j+1) and u(j+1) = vl(:,j) - i*vl(:,j+1), where  $i = \sqrt{-1}$ .

For complex flavors:

u(j) = v1(:,j), the j-th column of v1.

vr(ldvr, *); the second dimension of vr must be at least max(1, n).

If jobvr = 'V', the right generalized eigenvectors v(j) are stored one after another in the columns of vr, in the same order as their eigenvalues. Each eigenvector will be scaled so the largest component have abs(Re) + abs(Im) = 1. If jobvr = 'N', vr is not referenced. For real flavors:

If the j-th eigenvalue is real, then v(j) = vr(:,j), the j-th column of vr. If the j-th and (j+1)-st eigenvalues form a complex conjugate pair, then v(j) = vr(:,j) + i*vr(:,j+1) and v(j+1) = vr(:,j) - i*vr(:,j+1).

For complex flavors:

v(j) = vr(:,j), the j-th column of vr.

On exit, if *info* = 0, then *work(1)* returns the required minimal size of *lwork*.

infoINTEGER.If info = 0, the execution is successful.If info = -i, the *i*th parameter had an illegal value.If info = -i, and $i \le n$ :the QZ iteration failed. No eigenvectors have beencalculated, but alphar(j), alphai(j) (for real flavors),or alpha(j) (for complex flavors), and beta(j),j=info+1,...,n should be correct.i > n: errors that usually indicate LAPACK problems:i = n+1: other than QZ iteration failed in ?hgeqz;i = n+2: error return from ?tgevc.

#### **Application Notes**

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The quotients alphar(j)/beta(j) and alphai(j)/beta(j) may easily overor underflow, and beta(j) may even be zero. Thus, you should avoid simply computing the ratio. However, alphar and alphai (for real flavors) or alpha (for complex flavors) will be always less than and usually comparable with norm(A) in magnitude, and beta always less than and usually comparable with norm(B).

### ?ggevx

Computes the generalized eigenvalues, and, optionally, the left and/or right generalized eigenvectors.

<pre>call sggevx ( balanc, jobvl, jobvr, sense, n, a, lda, b, ldb,</pre>
<pre>call dggevx ( balanc, jobvl, jobvr, sense, n, a, lda, b, ldb,</pre>
<pre>call cggevx ( balanc, jobvl, jobvr, sense, n, a, lda, b, ldb,</pre>
<pre>call zggevx ( balanc, jobvl, jobvr, sense, n, a, lda, b, ldb,</pre>

#### **Discussion**

This routine computes for a pair of *n*-by-*n* real/complex nonsymmetric matrices (A, B), the generalized eigenvalues, and optionally, the left and/or right generalized eigenvectors.

Optionally also, it computes a balancing transformation to improve the conditioning of the eigenvalues and eigenvectors (*ilo*, *ihi*, *lscale*, *rscale*, *abnrm*, and *bbnrm*), reciprocal condition numbers for the eigenvalues (*rconde*), and reciprocal condition numbers for the right eigenvectors (*rcondv*).

A generalized eigenvalue for a pair of matrices (A,B) is a scalar  $\lambda$  or a ratio *alpha / beta* =  $\lambda$ , such that  $A - \lambda * B$  is singular. It is usually represented as the pair (*alpha, beta*), as there is a reasonable interpretation for *beta*=0 and even for both being zero.

The right generalized eigenvector v(j) corresponding to the generalized eigenvalue  $\lambda(j)$  of (A, B) satisfies

 $A * v(j) = \lambda(j) * B * v(j) .$ 

The left generalized eigenvector u(j) corresponding to the generalized eigenvalue  $\lambda(j)$  of (A,B) satisfies

$$u(\mathbf{j})^H \star A = \lambda(\mathbf{j}) \star u(\mathbf{j})^H \star B$$

where  $u(j)^H$  denotes the conjugate transpose of u(j).

balanc	CHARACTER*1. Must be 'N', 'P', 'S', or 'B'. Specifies the balance option to be performed.
	If <i>balanc</i> = 'N', do not diagonally scale or permute; If <i>balanc</i> = 'P', permute only; If <i>balanc</i> = 'S', scale only; If <i>balanc</i> = 'B', both permute and scale.
	Computed reciprocal condition numbers will be for the matrices after balancing and/or permuting. Permuting does not change condition numbers (in exact arithmetic), but balancing does.
jobvl	CHARACTER*1. Must be 'N' or 'V'. If <i>jobv1</i> = 'N', the left generalized eigenvectors are not computed; If <i>jobv1</i> = 'V', the left generalized eigenvectors are computed.
jobvr	CHARACTER*1. Must be 'N' or 'V'. If <i>jobvr</i> = 'N', the right generalized eigenvectors are not computed; If <i>jobvr</i> = 'V', the right generalized eigenvectors are computed.
sense	CHARACTER*1. Must be 'N', 'E', 'V', or 'B'. Determines which reciprocal condition number are computed.

	If $sense = 'N'$ , none are computed;
	If <u>sense</u> = 'E', computed for eigenvalues only;
	If <u>sense</u> = 'V', computed for eigenvectors only;
	If $sense = 'B'$ , computed for eigenvalues and
	eigenvectors.
п	<b>INTEGER.</b> The order of the matrices $A$ , $B$ , $v1$ , and $vr$ $(n \ge 0)$ .
a, b, work	REAL for sggevx
	DOUBLE PRECISION for dggevx
	COMPLEX for cggevx
	DOUBLE COMPLEX for zggevx.
	Arrays:
	a(lda,*) is an array containing the <i>n</i> -by- <i>n</i> matrix A (first of the pair of matrices).
	The second dimension of $a$ must be at least max $(1, n)$ .
	<b>b</b> ( <i>ldb</i> , *) is an array containing the <i>n</i> -by- <i>n</i> matrix <i>B</i> (second of the pair of matrices).
	The second dimension of $b$ must be at least max $(1, n)$ .
	work(lwork) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of the array $a$ . Must be at least max $(1, n)$ .
ldb	<b>INTEGER.</b> The first dimension of the array $b$ . Must be at least max $(1, n)$ .
ldvl,ldvr	<b>INTEGER.</b> The first dimensions of the output matrices v1 and vr, respectively. Constraints: $ldvl \ge 1$ . If $jobvl = 'V'$ , $ldvl \ge max(1, n)$ . $ldvr \ge 1$ . If $jobvr = 'V'$ , $ldvr \ge max(1, n)$ .
lwork	<b>INTEGER</b> . The dimension of the array <i>work</i> .
	For real flavors:
	$lwork \geq max(1, 6n);$
	if sense = $ \mathbf{E} $ , $lwork \ge 12n$ ;
	if sense = 'V', or 'B', $lwork \ge 2n^2 + 12n + 16$ .
	For complex flavors:

	$lwork \ge max(1, 2n);$ if sense ='N', or 'E', $lwork \ge 2n;$ if sense = 'V', or 'B', $lwork \ge 2n^2 + 2n.$
rwork	<b>REAL</b> for cggevx <b>DOUBLE PRECISION</b> for zggevx Workspace array, <b>DIMENSION</b> at least max(1, 6 <i>n</i> ). This array is used in complex flavors only.
iwork	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> at least $(n+6)$ for real flavors and at least $(n+2)$ for complex flavors. Not referenced if <i>sense</i> = 'E'.
bwork	<b>LOGICAL</b> . Workspace array, <b>DIMENSION</b> at least $max(1, n)$ . Not referenced if <u>sense</u> = 'N'.

a, b	On exit, these arrays have been overwritten.
	If $jobvl = 'V'$ or $jobvr = 'V'$ or both, then a contains the first part of the real Schur form of the "balanced" versions of the input <i>A</i> and <i>B</i> , and <i>b</i> contains its second part.
alphar,alphai	REAL for sggevx; DOUBLE PRECISION for dggevx. Arrays, DIMENSION at least max(1,n) each. Contain values that form generalized eigenvalues in real flavors. See <i>beta</i> .
alpha	COMPLEX for cggevx; DOUBLE COMPLEX for zggevx. Array, DIMENSION at least max(1,n). Contain values that form generalized eigenvalues in complex flavors. See beta.
beta	REAL for sggevx DOUBLE PRECISION for dggevx COMPLEX for cggevx DOUBLE COMPLEX for zggevx.

Array, DIMENSION at least  $\max(1, n)$ . For real flavors:

On exit, (alphar(j) + alphai(j)*i)/beta(j), j=1,...,n, will be the generalized eigenvalues.

If *alphai*(j) is zero, then the j-th eigenvalue is real; if positive, then the j-th and (j+1)-st eigenvalues are a complex conjugate pair, with *alphai*(j+1) negative. *For complex flavors:* 

On exit, alpha(j)/beta(j), j=1,...,n, will be the generalized eigenvalues.

See also Application Notes below.

vl, vr

REAL for sggevx DOUBLE PRECISION for dggevx COMPLEX for cggevx DOUBLE COMPLEX for zggevx.

Arrays:

vl(ldvl, *); the second dimension of vl must be at least max(1, n).

If jobvl = 'V', the left generalized eigenvectors u(j) are stored one after another in the columns of vl, in the same order as their eigenvalues. Each eigenvector will be scaled so the largest component have abs(Re) + abs(Im) = 1. If jobvl = 'N', vl is not referenced. For real flavors:

If the j-th eigenvalue is real, then u(j) = vl(:,j), the j-th column of vl. If the j-th and (j+1)-st eigenvalues form a complex conjugate pair, then u(j) = vl(:,j) + i*vl(:,j+1) and u(j+1) = vl(:,j) - i*vl(:,j+1), where  $i = \sqrt{-1}$ .

For complex flavors: u(j) = vl(:,j), the j-th column of vl.

vr(ldvr, *); the second dimension of vr must be at least max(1, n).

If jobvr = V', the right generalized eigenvectors v(j) are stored one after another in the columns of vr, in the same order as their eigenvalues. Each eigenvector will

be scaled so the largest component have abs(Re) + abs(Im) = 1. If *jobvr* = 'N', *vr* is not referenced. For real flavors: If the j-th eigenvalue is real, then v(j) = vr(:,j), the j-th column of vr. If the j-th and (j+1)-st eigenvalues form a complex conjugate pair, then v(j) = vr(:,j) + i * vr(:,j+1)and v(j+1) = vr(:,j) - i * vr(:,j+1). For complex flavors: v(j) = vr(:,j), the j-th column of vr. ilo, ihi INTEGER. *ilo* and *ihi* are integer values such that on exit A(i,j) = 0 and B(i,j) = 0 if i > j and j = 1, ..., i lo-1 or i = *ihi*+1,..., *n*. If balanc = N' or S', ilo = 1 and ihi = n. *lscale*, *rscale* REAL for single-precision flavors **DOUBLE PRECISION** for double-precision flavors. Arrays, DIMENSION at least max(1, n) each. *lscale* contains details of the permutations and scaling factors applied to the left side of A and B. If PL(j) is the index of the row interchanged with row j, and DL(j) is the scaling factor applied to row j, then lscale(j) = PL(j), for j = 1,...,ilo-1

= DL(j), for j = ilo,...,ihi= PL(j) for j = ihi+1,...,n.

The order in which the interchanges are made is n to ihi+1, then 1 to ilo-1.

**rscale** contains details of the permutations and scaling factors applied to the right side of A and B. If PR(j) is the index of the column interchanged with column j, and DR(j) is the scaling factor applied to column j, then

$$rscale(j) = PR(j), \text{ for } j = 1,...,ilo-1$$
  
=  $DR(j), \text{ for } j = ilo,...,ihi$   
=  $PR(j)$  for  $j = ihi+1,...,n$ .

	The order in which the interchanges are made is $n$ to $ihi$ +1, then 1 to $ilo$ -1.
abnrm,bbnrm	<b>REAL</b> for single-precision flavors <b>DOUBLE PRECISION</b> for double-precision flavors.
	The one-norms of the balanced matrices <i>A</i> and <i>B</i> , respectively.
rconde,rcondv	<b>REAL</b> for single precision flavors <b>DOUBLE PRECISION</b> for double precision flavors. Arrays, <b>DIMENSION</b> at least $max(1, n)$ each.
	If <i>sense</i> = 'E', or 'B', <i>rconde</i> contains the reciprocal condition numbers of the selected eigenvalues, stored in consecutive elements of the array. For a complex conjugate pair of eigenvalues two consecutive elements of <i>rconde</i> are set to the same value. Thus <i>rconde</i> (j), <i>rcondv</i> (j), and the j-th columns of <i>v1</i> and <i>vr</i> all correspond to the same eigenpair (but not in general the j-th eigenpair, unless all eigenpairs are selected). If <i>sense</i> = 'V', <i>rconde</i> is not referenced.
	If <i>sense</i> = 'V', or 'B', <i>rcondv</i> contains the estimated reciprocal condition numbers of the selected eigenvectors, stored in consecutive elements of the array. For a complex eigenvector two consecutive elements of <i>rcondv</i> are set to the same value. If the eigenvalues cannot be reordered to compute <i>rcondv</i> (j), <i>rcondv</i> (j) is set to 0; this can only occur when the true value would be very small anyway. If <i>sense</i> = 'E', <i>rcondv</i> is not referenced.
work(1)	On exit, if <i>info</i> = 0, then <i>work(1)</i> returns the required minimal size of <i>lwork</i> .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , and $i \leq n$ :

the QZ iteration failed. No eigenvectors have been calculated, but alphar(j), alphai(j) (for real flavors), or alpha(j) (for complex flavors), and beta(j), j=info+1,...,n should be correct.

- i > n: errors that usually indicate LAPACK problems:
  - i = n+1: other than *QZ* iteration failed in ?hgeqz;
  - i = n+2: error return from ?tgevc.

### **Application Notes**

If you are in doubt how much workspace to supply for the array *work*, use a generous value of *lwork* for the first run. On exit, examine *work*(1) and use this value for subsequent runs.

The quotients alphar(j)/beta(j) and alphai(j)/beta(j) may easily overor underflow, and beta(j) may even be zero. Thus, you should avoid simply computing the ratio. However, alphar and alphai (for real flavors) or alpha (for complex flavors) will be always less than and usually comparable with norm(A) in magnitude, and beta always less than and usually comparable with norm(B).

### References

[LUG]	E. Anderson, Z. Bai et al. <i>LAPACK User's Guide</i> . Third edition, SIAM, Philadelphia, 1999.
[Golub96]	G.Golub, C. Van Loan. <i>Matrix Computations</i> . Johns Hopkins University Press, Baltimore, third edition, 1996.

# LAPACK Auxiliary Routines

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This chapter describes the Intel[®] Math Kernel Library implementation of LAPACK auxiliary routines. The library includes auxiliary routines for both real and complex data.

Routine naming conventions, mathematical notation, and matrix storage schemes used for LAPACK auxiliary routines are the same as for the driver and computational routines described in previous chapters.

Routines are listed in alphabetical order of the routine or function group name (which always begins with -?).

### ?lacgv

Conjugates a complex vector.

n x

```
call clacgv (n, x, incx)
call zlacgv (n, x, incx)
```

### **Discussion**

This routine conjugates a complex vector  $\mathbf{x}$  of length n and increment *incx* (see <u>Vector Arguments in BLAS</u> in Appendix A).

<b>INTEGER</b> . The length of the vector $\mathbf{x}$ ( $n \ge 0$ ).
COMPLEX for clacgv
COMPLEX*16 for zlacgy.
Array, dimension $(1+(n-1)* incx )$ .
Contains the vector of length $n$ to be conjugated.

*incx* INTEGER. The spacing between successive elements of *x*.

### **Output Parameters**

**x** On exit, overwritten with  $conjg(\mathbf{x})$ .

### ?lacrm

Multiplies a complex matrix by a square real matrix.

call clacrm (m, n, a, lda, b, ldb, c, ldc, rwork)
call zlacrm (m, n, a, lda, b, ldb, c, ldc, rwork)

#### **Discussion**

This routine performs a simple matrix-matrix multiplication of the form

C = A * B ,

where *A* is *m*-by-*n* and complex, *B* is *n*-by-*n* and real, *C* is *m*-by-*n* and complex.

m	<b>INTEGER.</b> The number of rows of the matrix A and of the matrix $C \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns and rows of the matrix <i>B</i> and the number of columns of the matrix <i>C</i> $(n \ge 0)$ .
a	COMPLEX for clacrm COMPLEX*16 for zlacrm
	Array, DIMENSION ( $lda, n$ ). Contains the <i>m</i> -by- <i>n</i> matrix A.
lda	<b>INTEGER.</b> The leading dimension of the array $a$ , $lda \ge max(1, m)$ .

b	REAL for clacrm DOUBLE PRECISION for zlacrm
	Array, <b>DIMENSION</b> ( <i>ldb</i> , <i>n</i> ). Contains the <i>n</i> -by- <i>n</i> matrix <i>B</i> .
ldb	<b>INTEGER.</b> The leading dimension of the array $b$ , $ldb \ge \max(1, n)$ .
ldc	<b>INTEGER.</b> The leading dimension of the output array $c$ , $ldc \ge \max(1, n)$ .
rwork	REAL for clacrm DOUBLE PRECISION for zlacrm
	Workspace array, DIMENSION $(2*m*n)$ .
Output Para	ameters
С	COMPLEX for clacrm
	COMPLEX*16 for zlacrm

Array, DIMENSION (ldc, n). Contains the *m*-by-*n* matrix *C*.

### ?lacrt

Performs a linear transformation of a pair of complex vectors.

call clacrt (n, cx, incx, cy, incy, c, s)
call zlacrt (n, cx, incx, cy, incy, c, s)

### **Discussion**

This routine performs the following transformation

$$\begin{pmatrix} c & s \\ -s & c \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \Rightarrow \begin{pmatrix} x \\ y \end{pmatrix},$$

where *c*, *s* are complex scalars and *x*, *y* are complex vectors.

### **Input Parameters**

n	<b>INTEGER.</b> The number of elements in the vectors $cx$ and $cy$ $(n \ge 0)$ .
сх, су	COMPLEX for clacrt COMPLEX*16 for zlacrt
	Arrays, dimension (n). Contain input vectors x and y, respectively.
incx	<b>INTEGER.</b> The increment between successive elements of $cx$ .
incy	<b>INTEGER.</b> The increment between successive elements of <i>cy</i> .
C, S	COMPLEX for clacrt COMPLEX*16 for zlacrt
	Complex scalars that define the transform matrix
	$\begin{bmatrix} c & s \\ -s & c \end{bmatrix}$
Output Param	eters
CX	On exit, overwritten with $c * x + s * y$ .
СУ	On exit, overwritten with $-s * x + c * y$ .

# ?laesy

Computes the eigenvalues and eigenvectors of a 2-by-2 complex symmetric matrix, and checks that the norm of the matrix of eigenvectors is larger than a threshold value.

call claesy (a, b, c, rt1, rt2, evscal, cs1, sn1)
call zlaesy (a, b, c, rt1, rt2, evscal, cs1, sn1)

### **Discussion**

This routine performs the eigendecomposition of a 2-by-2 symmetric matrix

```
ab
bc
```

provided the norm of the matrix of eigenvectors is larger than some threshold value.

rt1 is the eigenvalue of larger absolute value, and rt2 of smaller absolute
value. If the eigenvectors are computed, then on return (cs1, sn1) is the
unit eigenvector for rt1, hence

csl snl -snl csl	a b	cs1	-sn1	=	rt1	0
-snl csl	b c	sn1	cs1		0	rt2

### **Input Parameters**

a, b, c	COMPLEX for claesy
	COMPLEX*16 for zlaesy

Elements of the input matrix.

### **Output Parameters**

rt1, rt2	COMPLEX for claesy COMPLEX*16 for zlaesy
	Eigenvalues of larger and smaller modulus, respectively.
evscal	COMPLEX for claesy COMPLEX*16 for zlaesy
	The complex value by which the eigenvector matrix was scaled to make it orthonormal. If <i>evscal</i> is zero, the eigenvectors were not computed. This means one of two things: the 2-by-2 matrix could not be diagonalized, or the norm of the matrix of eigenvectors before scaling was larger than the threshold value thresh (set to 0.1E0).

csl, snl

COMPLEX for claesy COMPLEX*16 for zlaesy

If evscal is not zero, then (cs1, sn1) is the unit right eigenvector for rt1.

### ?rot

Applies a plane rotation with real cosine and complex sine to a pair of complex vectors.

call crot (n, cx, incx, cy, incy, c, s)
call zrot (n, cx, incx, cy, incy, c, s)

### **Discussion**

This routine applies a plane rotation, where the cosine (c) is real and the sine (s) is complex, and the vectors cx and cy are complex. This routine has its real equivalents in BLAS (see <u>?rot</u> in Chapter 2).

п	<b>INTEGER.</b> The number of elements in the vectors $cx$ and $cy$ .	
сх, су	COMPLEX for crot COMPLEX*16 for zrot Arrays of dimension ( <i>n</i> ), contain input vectors <i>x</i> and <i>y</i> , respectively.	
incx	<b>INTEGER.</b> The increment between successive elements of <i>cx</i> .	
incy	<b>INTEGER.</b> The increment between successive elements of <i>cy</i> .	
С	REAL for crot DOUBLE PRECISION for zrot	

COMPLEX for crot COMPLEX*16 for zrot Values that define a rotation

```
_conjg(s) c
```

where  $c^*c + s^* \operatorname{conjg}(s) = 1.0$ .

### **Output Parameters**

CX	On exit, overwritten with $c^*x + s^*y$ .	
су	On exit, overwritten with $-conjg(s) *x +$	<mark>с</mark> *у.

### ?spmv

Computes a matrix-vector product for complex vectors using a complex symmetric packed matrix.

s

call cspmv ( uplo, n, alpha, ap, x, incx, beta, y, incy )
call zspmv ( uplo, n, alpha, ap, x, incx, beta, y, incy )

### **Discussion**

These routines perform a matrix-vector operation defined as

 $y := alpha^*a^*x + beta^*y$ ,

where:

alpha and beta are complex scalars,

x and y are *n*-element complex vectors

a is an *n*-by-*n* complex symmetric matrix, supplied in packed form.

These routines have their real equivalents in BLAS (see <u>?spmv</u> in Chapter 2).

### **Input Parameters**

uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the matrix <i>a</i> is supplied in the packed array <i>ap</i> , as follows:
	If $uplo = 'U'$ or 'u', the upper triangular part of the matrix <b>a</b> is supplied in the array $ap$ . If $uplo = 'L'$ or 'l', the lower triangular part of the matrix <b>a</b> is supplied in the array $ap$ .
n	<b>INTEGER.</b> Specifies the order of the matrix $a$ . The value of $n$ must be at least zero.
alpha, beta	COMPLEX for cspmv COMPLEX*16 for zspmv
	Specify complex scalars <i>alpha</i> and <i>beta</i> . When <i>beta</i> is supplied as zero, then $y$ need not be set on input.
ap	COMPLEX for cspmv COMPLEX*16 for zspmv
	Array, DIMENSION at least $((n*(n+1))/2)$ . Before entry, with $uplo = 'U'$ or 'u', the array $ap$ must contain the upper triangular part of the symmetric matrix packed sequentially, column-by-column, so that ap(1) contains $a(1, 1)$ , $ap(2)$ and $ap(3)$ contain a(1, 2) and $a(2, 2)$ respectively, and so on. Before entry, with $uplo = 'L'$ or '1', the array $ap$ must contain the lower triangular part of the symmetric matrix packed sequentially, column-by-column, so that $ap(1)$ contains $a(1, 1)$ , $ap(2)$ and $ap(3)$ contain $a(2, 1)$ and $a(3, 1)$ respectively, and so on.
x	COMPLEX for cspmv COMPLEX*16 for zspmv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$ . Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	<b>INTEGER</b> . Specifies the increment for the elements of <b>x</b> .

**INTEGER**. Specifies the increment for the elements of **x**. The value of *incx* must not be zero.

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У	COMPLEX for cspmv COMPLEX*16 for zspmv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incy))$ . Before entry, the incremented array $y$ must contain the <i>n</i> -element vector $y$ .
incy	<b>INTEGER</b> . Specifies the increment for the elements of <i>y</i> . The value of <i>incy</i> must not be zero.
Output Parameters	

*y* Overwritten by the updated vector *y*.

### ?spr

Performs the symmetrical rank-1 update of a complex symmetric packed matrix.

call cspr( uplo, n, alpha, x, incx, ap )
call zspr( uplo, n, alpha, x, incx, ap )

### **Discussion**

The ?spr routines perform a matrix-vector operation defined as

a:= alpha*x*conjg(x') + a,

where:

alpha is a complex scalar

x is an *n*-element complex vector

a is an n-by-n complex symmetric matrix, supplied in packed form.

These routines have their real equivalents in BLAS (see <u>?spr</u> in Chapter 2).

### **Input Parameters**

*uplo* CHARACTER*1. Specifies whether the upper or lower triangular part of the matrix *a* is supplied in the packed array *ap*, as follows:

	If $uplo = 'U'$ or 'u', the upper triangular part of the matrix <i>a</i> is supplied in the array <i>ap</i> . If $uplo = 'L'$ or 'l', the lower triangular part of the matrix <i>a</i> is supplied in the array <i>ap</i> .
n	<b>INTEGER.</b> Specifies the order of the matrix $a$ . The value of $n$ must be at least zero.
alpha	COMPLEX for cspr COMPLEX*16 for zspr
	Specifies the scalar <i>alpha</i> .
x	COMPLEX for cspr COMPLEX*16 for zspr
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$ . Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	<b>INTEGER.</b> Specifies the increment for the elements of <i>x</i> . The value of <i>incx</i> must not be zero.
ар	COMPLEX for cspr COMPLEX*16 for zspr
	Array, DIMENSION at least $((n*(n+1))/2)$ . Before entry, with $uplo = 'U'$ or 'u', the array $ap$ must contain the upper triangular part of the symmetric matrix packed sequentially, column-by-column, so that ap(1) contains $a(1,1)$ , $ap(2)$ and $ap(3)$ contain a(1, 2) and $a(2, 2)$ respectively, and so on.
	Before entry, with $uplo = 'L'$ or 'l', the array $ap$ must contain the lower triangular part of the symmetric matrix packed sequentially, column-by-column, so that ap(1) contains $a(1,1)$ , $ap(2)$ and $ap(3)$ contain a(2,1) and $a(3,1)$ respectively, and so on.
	Note that the imaginary parts of the diagonal elements need not be set, they are assumed to be zero, and on exit they are set to zero.

ар

With *uplo* = 'U' or 'u', overwritten by the upper triangular part of the updated matrix. With *uplo* = 'L' or 'l', overwritten by the lower triangular part of the updated matrix.

### ?symv

Computes a matrix-vector product for a complex symmetric matrix.

call csymv ( uplo, n, alpha, a, lda, x, incx, beta, y, incy ) call zsymv ( uplo, n, alpha, a, lda, x, incx, beta, y, incy )

#### Discussion

These routines perform the matrix-vector operation defined as

 $y := alpha^*a^*x + beta^*y$ ,

where:

alpha and beta are complex scalars

x and y are *n*-element complex vectors

a is an *n*-by-*n* symmetric complex matrix.

These routines have their real equivalents in BLAS (see <u>?symv</u> in Chapter 2).

### **Input Parameters**

uplo

CHARACTER*1. Specifies whether the upper or lower triangular part of the array *a* is to be referenced, as follows:

	If $uplo = 'U'$ or 'u', the upper triangular part of the array <i>a</i> is to be referenced. If $uplo = 'L'$ or 'l', the lower triangular part of the array <i>a</i> is to be referenced.
п	<b>INTEGER.</b> Specifies the order of the matrix $a$ . The value of $n$ must be at least zero.
alpha, beta	COMPLEX for csymv COMPLEX*16 for zsymv
	Specify the scalars $alpha$ and $beta$ . When $beta$ is supplied as zero, then $y$ need not be set on input.
a	COMPLEX for csymv COMPLEX*16 for zsymv
	Array, DIMENSION $(1da, n)$ . Before entry with $uplo = 'U'$ or 'u', the leading <i>n</i> -by- <i>n</i> upper triangular part of the array <i>a</i> must contain the upper triangular part of the symmetric matrix and the strictly lower triangular part of <i>a</i> is not referenced. Before entry with $uplo = 'L'$ or 'l', the leading <i>n</i> -by- <i>n</i> lower triangular part of the array <i>a</i> must contain the lower triangular part of the symmetric matrix and the strictly upper triangular part of the symmetric matrix and the strictly upper triangular part of <i>a</i> is not referenced.
lda	<b>INTEGER.</b> Specifies the first dimension of <i>a</i> as declared in the calling (sub)program. The value of $1da$ must be at least max(1, n).
x	COMPLEX for csymv COMPLEX*16 for zsymv
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$ . Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	<b>INTEGER.</b> Specifies the increment for the elements of $x$ . The value of <i>incx</i> must not be zero.
У	COMPLEX for csymv COMPLEX*16 for zsymv

	Array, DIMENSION at least $(1 + (n - 1)*abs(incy))$ . Before entry, the incremented array y must contain the
	n-element vector $y$ .
incy	<b>INTEGER.</b> Specifies the increment for the elements of <i>y</i> . The value of <i>incy</i> must not be zero.

*y* Overwritten by the updated vector *y*.

# ?syr

Performs the symmetric rank-1 update of a complex symmetric matrix.

call csyr( uplo, n, alpha, x, incx, a, lda )
call zsyr( uplo, n, alpha, x, incx, a, lda )

### **Discussion**

These routines perform the symmetric rank 1 operation defined as

```
a := alpha^*x^*x' + a,
```

where:

alpha is a complex scalar

x is an *n*-element complex vector

a is an *n*-by-*n* complex symmetric matrix.

These routines have their real equivalents in BLAS (see <u>?syr</u> in Chapter 2).

### **Input Parameters**

*uplo* CHARACTER*1. Specifies whether the upper or lower triangular part of the array *a* is to be referenced, as follows:

	If $uplo = 'U'$ or 'u', the upper triangular part of the array a is to be referenced. If $uplo = 'L'$ or 'l', the lower triangular part of the array a is to be referenced.
п	<b>INTEGER.</b> Specifies the order of the matrix $a$ . The value of $n$ must be at least zero.
alpha	COMPLEX for csyr COMPLEX*16 for zsyr
	Specifies the scalar alpha.
x	COMPLEX for csyr COMPLEX*16 for zsyr
	Array, DIMENSION at least $(1 + (n - 1)*abs(incx))$ . Before entry, the incremented array x must contain the <i>n</i> -element vector x.
incx	<b>INTEGER.</b> Specifies the increment for the elements of $x$ . The value of <i>incx</i> must not be zero.
a	COMPLEX for csyr COMPLEX*16 for zsyr
	Array, DIMENSION $(lda, n)$ . Before entry with $uplo = 'U'$ or 'u', the leading <i>n</i> -by- <i>n</i> upper triangular part of the array <i>a</i> must contain the upper triangular part of the symmetric matrix and the strictly lower triangular part of <i>a</i> is not referenced.
	Before entry with $uplo = 'L'$ or 'l', the leading <i>n</i> -by- <i>n</i> lower triangular part of the array <i>a</i> must contain the lower triangular part of the symmetric matrix and the strictly upper triangular part of <i>a</i> is not referenced.
lda	<b>INTEGER.</b> Specifies the first dimension of <b>a</b> as declared in the calling (sub)program. The value of $1da$ must be at least max(1,n).

a With *uplo* = 'U' or 'u', the upper triangular part of the array **a** is overwritten by the upper triangular part of the updated matrix.

With uplo = 'L' or 'l', the lower triangular part of the array **a** is overwritten by the lower triangular part of the updated matrix.

### i?max1

Finds the index of the vector element whose real part has maximum absolute value.

index = icmax1 ( n, cx, incx )
index = izmax1 ( n, cx, incx )

### **Discussion**

Given a complex vector *cx*, the i?max1 functions return the index of the vector element whose real part has maximum absolute value. These functions are based on the BLAS functions icamax/izamax, but using the absolute value of the real part. They are designed for use with clacon/zlacon.

п	<b>INTEGER.</b> Specifies the number of elements in the vector $cx$ .
CX	COMPLEX for icmax1 COMPLEX*16 for izmax1
	Array, DIMENSION at least $(1+(n-1)*abs(incx))$ .
	Contains the input vector.

incx

**INTEGER**. Specifies the spacing between successive elements of *cx*.

#### **Output Parameters**

*index* **INTEGER.** Contains the index of the vector element whose real part has maximum absolute value.

### ilaenv

Environmental enquiry function which returns values for tuning algorithmic performance.

#### value = ilaenv ( ispec, name, opts, n1, n2, n3, n4 )

### **Discussion**

Enquiry function *ilaenv* is called from the LAPACK routines to choose problem-dependent parameters for the local environment. See *ispec* for a description of the parameters.

This version provides a set of parameters which should give good, but not optimal, performance on many of the currently available computers. Users are encouraged to modify this subroutine to set the tuning parameters for their particular machine using the option and problem size information in the arguments.

This routine will not function correctly if it is converted to all lower case. Converting it to all upper case is allowed.

#### **Input Parameters**

ispec INTEGER. Specifies the parameter to be returned as the value of ilaenv: = 1: the optimal blocksize; if this value is 1, an unblocked algorithm will give the best performance.

	= 2: the minimum block size for which the block routine should be used; if the usable block size is less than this value, an unblocked routine should be used.
	= 3: the crossover point (in a block routine, for $N$ less than this value, an unblocked routine should be used)
	= 4: the number of shifts, used in the nonsymmetric eigenvalue routines
	= 5: the minimum column dimension for blocking to be used; rectangular blocks must have dimension at least k by m, where k is given by ilaenv(2,) and m by ilaenv(5,)
	= 6: the crossover point for the SVD (when reducing an m by n matrix to bidiagonal form, if $max(m,n)/min(m,n)$ exceeds this value, a <i>QR</i> factorization is used first to reduce the matrix to a triangular form.)
	= 7: the number of processors
	= 8: the crossover point for the multishift $QR$ and $QZ$ methods for nonsymmetric eigenvalue problems.
	= 9: maximum size of the subproblems at the bottom of the computation tree in the divide-and-conquer algorithm (used by ?gelsd and ?gesdd)
	=10: IEEE NaN arithmetic can be trusted not to trap
	=11: infinity arithmetic can be trusted not to trap
name	CHARACTER*(*). The name of the calling subroutine, in either upper case or lower case.
opts	CHARACTER*(*). The character options to the subroutine <i>name</i> , concatenated into a single character string. For example, <i>uplo</i> = 'U', <i>trans</i> = 'T', and <i>diag</i> = 'N' for a triangular routine would be specified as <i>opts</i> = 'UTN'.
n1,n2,n3,n4	<b>INTEGER.</b> Problem dimensions for the subroutine <i>name</i> ; these may not all be required.

value

INTEGER. If  $value \ge 0$ : the value of the parameter specified by *ispec*; If value = -k < 0: the k-th argument had an illegal value.

### **Application Notes**

The following conventions have been used when calling *ilaenv* from the LAPACK routines:

1) opts is a concatenation of all of the character options to subroutine name, in the same order that they appear in the argument list for name, even if they are not used in determining the value of the parameter specified by ispec.

2) The problem dimensions n1, n2, n3, n4 are specified in the order that they appear in the argument list for name. n1 is used first, n2 second, and so on, and unused problem dimensions are passed a value of -1.

3) The parameter value returned by *ilaenv* is checked for validity in the calling subroutine. For example, *ilaenv* is used to retrieve the optimal blocksize for strtri as follows:

nb = ilaenv( 1, 'strtri', uplo // diag, n, -1, -1, -1 )
if( nb.le.1 ) nb = max( 1, n )

### Isame

*Tests two characters for equality regardless of case.* 

```
val = lsame ( ca, cb )
```

### **Discussion**

This logical function returns . TRUE. if *ca* is the same letter as *cb* regardless of case.

#### **Input Parameters**

*ca*, *cb* CHARACTER*1. Specify the single characters to be compared.

### **Output Parameters**

val LOGICAL. Result of the comparison.

### Isamen

*Tests two character strings for equality regardless of case.* 

val = lsamen ( n, ca, cb )

### Discussion

This logical function tests if the first n letters of the string ca are the same as the first n letters of cb, regardless of case. The function lsamen returns .TRUE. if ca and cb are equivalent except for case and .FALSE. otherwise. lsamen also returns .FALSE. if len(ca) or len(cb) is less than n.

#### **Input Parameters**

- *n* **INTEGER.** The number of characters in *ca* and *cb* to be compared.
- *ca*, *cb* CHARACTER*(*). Specify two character strings of length at least *n* to be compared. Only the first *n* characters of each string will be accessed.

#### **Output Parameters**

val LOGICAL. Result of the comparison.

# ?sum1

Forms the 1-norm of the complex vector using the true absolute value.

```
res = scsum1 ( n, cx, incx )
res = dzsum1 ( n, cx, incx )
```

### **Discussion**

Given a complex vector *cx*, scsum1/dzsum1 functions take the sum of the absolute values of vector elements and return a single/double precision result, respectively. These functions are based on scasum/dzasum from Level 1 BLAS, but use the true absolute value and were designed for use with clacon/zlacon.

### **Input Parameters**

n	<b>INTEGER.</b> Specifies the number of elements in the vector $cx$ .
CX	COMPLEX for scsuml COMPLEX*16 for dzsuml
	Array, DIMENSION at least (1+(n-1)*abs(incx)).
	Contains the input vector whose elements will be summed.
incx	<b>INTEGER.</b> Specifies the spacing between successive elements of $cx$ ( <i>incx</i> > 0).

### **Output Parameters**

	Contains	the sum of absolute values.
	DOUBLE	PRECISION for dzsum1
res	REAL for scsum1	

# ?gbtf2

Computes the LU factorization of a general band matrix using the unblocked version of the algorithm.

call sgbtf2 ( m, n, kl, ku, ab, ldab, ipiv, info )
call dgbtf2 ( m, n, kl, ku, ab, ldab, ipiv, info )
call cgbtf2 ( m, n, kl, ku, ab, ldab, ipiv, info )
call zgbtf2 ( m, n, kl, ku, ab, ldab, ipiv, info )

### **Discussion**

The routine forms the *LU* factorization of a general real/complex *m* by *n* band matrix *A* with *k1* sub-diagonals and *ku* super-diagonals. The routine uses partial pivoting with row interchanges and implements the unblocked version of the algorithm, calling Level 2 BLAS. See also <u>?gbtrf</u>.

m	<b>INTEGER</b> . The number of rows of the matrix $A \ (m \ge 0)$ .
п	<b>INTEGER</b> . The number of columns in $A (n \ge 0)$ .
kl	<b>INTEGER</b> . The number of sub-diagonals within the
	band of $A$ ( <i>k</i> 1 $\geq$ 0).
ku	<b>INTEGER</b> . The number of super-diagonals within the
	band of $A$ ( $ku \ge 0$ ).
ab	REAL for sgbtf2
	DOUBLE PRECISION for dgbtf2
	COMPLEX for cgbtf2
	COMPLEX*16 for zgbtf2.
	Array, DIMENSION (1dab, *).
	The array <i>ab</i> contains the matrix A in band storage
	(see Matrix Arguments).
	The second dimension of $ab$ must be at least max $(1, n)$ .
ldab	<b>INTEGER.</b> The first dimension of the array <i>ab</i> .
	$(1dab \ge 2k1 + ku + 1)$

ab	Overwritten by details of the factorization. The diagonal and $kl + ku$ super-diagonals of $U$ are stored in the first $1 + kl + ku$ rows of <i>ab</i> . The multipliers used during the factorization are stored in the next $kl$ rows.
ipiv	INTEGER. Array, DIMENSION at least max(1,min(m,n)). The pivot indices: row <i>i</i> was interchanged with row <i>ipiv(i)</i> .
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i$ , $u_{ii}$ is 0. The factorization has been completed, but <i>U</i> is exactly singular. Division by 0 will occur if you use the factor <i>U</i> for solving a system of linear equations.

# ?gebd2

Reduces a general matrix to bidiagonal form using an unblocked algorithm.

call sgebd2 ( m, n, a, lda, d, e, tauq, taup, work, info )
call dgebd2 ( m, n, a, lda, d, e, tauq, taup, work, info )
call cgebd2 ( m, n, a, lda, d, e, tauq, taup, work, info )
call zgebd2 ( m, n, a, lda, d, e, tauq, taup, work, info )

### **Discussion**

The routine reduces a general *m*-by-*n* matrix A to upper or lower bidiagonal form B by an orthogonal (unitary) transformation: Q' A P = B

If  $m \ge n$ , *B* is upper bidiagonal; if m < n, *B* is lower bidiagonal.

The routine does not form the matrices Q and P explicitly, but represents them as products of elementary reflectors. If  $m \ge n$ ,

Q = H(1)H(2)...H(n) and P = G(1)G(2)...G(n-1)

If m < n,

Q = H(1)H(2)...H(m-1) and P = G(1)G(2)...G(m)

Each H(i) and G(i) has the form

 $H(\mathbf{i}) = I - tauq * v * v'$  and  $G(\mathbf{i}) = I - taup * u * u'$ 

where *tauq* and *taup* are scalars (real for sgebd2/dgebd2, complex for cgebd2/zgebd2), and *v* and *u* are vectors (real for sgebd2/dgebd2, complex for cgebd2/zgebd2).

m	<b>INTEGER.</b> The number of rows in the matrix $A \ (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgebd2 DOUBLE PRECISION for dgebd2 COMPLEX for cgebd2 COMPLEX*16 for zgebd2.

Arrays:

a(1da, *) contains the *m*-by-*n* general matrix *A* to be reduced. The second dimension of *a* must be at least max(1, n).

work(*) is a workspace array, the dimension of work must be at least  $\max(1, m, n)$ .

1da INTEGER. The first dimension of a; at least max(1, m).

### **Output Parameters**

а

If  $m \ge n$ , the diagonal and first super-diagonal of *a* are overwritten with the upper bidiagonal matrix *B*. Elements below the diagonal, with the array *tauq*, represent the orthogonal/unitary matrix *Q* as a product of elementary reflectors, and elements above the first superdiagonal, with the array *taup*, represent the orthogonal/unitary matrix *P* as a product of elementary reflectors.

If m < n, the diagonal and first sub-diagonal of *a* are overwritten by the lower bidiagonal matrix *B*. Elements below the first subdiagonal, with the array *tauq*, represent the orthogonal/unitary matrix *Q* as a product of elementary reflectors, and elements above the diagonal, with the array *taup*, represent the orthogonal/unitary matrix *P* as a product of elementary reflectors.

**REAL** for single-precision flavors **DOUBLE PRECISION** for double-precision flavors. Array, **DIMENSION** at least  $\max(1, \min(m, n))$ . Contains the diagonal elements of the bidiagonal matrix *B*: d(i) = a(i, i).

**REAL** for single-precision flavors DOUBLE PRECISION for double-precision flavors. Array, DIMENSION at least  $\max(1, \min(m, n) - 1)$ . Contains the off-diagonal elements of the bidiagonal matrix *B*:

d

е

If  $m \ge n$ , e(i) = a(i, i+1) for i = 1, 2, ..., n-1;<br/>If m < n, e(i) = a(i+1, i) for i = 1, 2, ..., m-1.tauq, taupREAL for sgebd2<br/>DOUBLE PRECISION for dgebd2<br/>COMPLEX for cgebd2<br/>COMPLEX*16 for zgebd2.<br/>Arrays, DIMENSION at least max (1, min(m, n)).<br/>Contain scalar factors of the elementary reflectors which

represent orthogonal/unitary matrices Q and P, respectively.

info	INTEGER.
	If $info = 0$ , the execution is successful.
	If $info = -i$ , the <i>i</i> th parameter had an illegal value.

# ?gehd2

Reduces a general square matrix to upper Hessenberg form using an unblocked algorithm.

call	sgehd2	(	n,	ilo,	ihi,	a,	lda,	tau,	work,	info	)
call	dgehd2	(	n,	ilo,	ihi,	a,	lda,	tau,	work,	info	)
call	cgehd2	(	n,	ilo,	ihi,	a,	lda,	tau,	work,	info	)
call	zgehd2	(	n,	ilo,	ihi,	a,	lda,	tau,	work,	info	)

### **Discussion**

The routine reduces a real/complex general matrix A to upper Hessenberg form H by an orthogonal or unitary similarity transformation Q' A Q = H.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of *elementary reflectors*.

n	<b>INTEGER</b> . The order of the matrix $A (n \ge 0)$ .
ilo, ihi	<b>INTEGER.</b> It is assumed that <i>A</i> is already upper triangular in rows and columns $1:ilo -1$ and $ihi+1:n$ . If <i>A</i> has been output by ?gebal, then <i>ilo</i> and <i>ihi</i> must contain the values returned by that routine. Otherwise they should be set to <i>ilo</i> = 1 and <i>ihi</i> = <i>n</i> . Constraint: $1 \le ilo \le ihi \le max(1, n)$ .
a, work	REAL for sgehd2 DOUBLE PRECISION for dgehd2 COMPLEX for cgehd2 COMPLEX*16 for zgehd2. Arrays: a (1da,*) contains the <i>n</i> -by- <i>n</i> matrix <i>A</i> to be reduced. The second dimension of <i>a</i> must be at least max(1, <i>n</i> ). work ( <i>n</i> ) is a workspace array.

*lda* INTEGER. The first dimension of *a*; at least max(1, *n*).

#### **Output Parameters**

a	On exit, the upper triangle and the first subdiagonal of $A$ are overwritten with the upper Hessenberg matrix $H$ and the elements below the first subdiagonal, with the array <i>tau</i> , represent the orthogonal/unitary matrix $Q$ as a product of elementary reflectors. See <i>Application Notes</i> below.
tau	REAL for sgehd2 DOUBLE PRECISION for dgehd2 COMPLEX for cgehd2 COMPLEX*16 for zgehd2. Array, DIMENSION at least max (1, <i>n</i> -1). Contains the scalar factors of elementary reflectors. See <i>Application Notes</i> below.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

### **Application Notes**

The matrix Q is represented as a product of (ihi - ilo) elementary reflectors

 $Q = H(ilo) H(ilo + 1) \dots H(ihi - 1)$ 

Each H(i) has the form

 $H(\mathbf{i}) = I - tau * v * v'$ 

where *tau* is a real/complex scalar, and *v* is a real/complex vector with v(1:i) = 0, v(i+1) = 1 and  $v(\underline{ihi}+1:n) = 0$ .

On exit, v(i+2:ihi) is stored in a(i+2:ihi, i) and tau in tau(i).

The contents of *a* are illustrated by the following example, with n = 7, *ilo* = 2 and *ihi* = 6:

on entry	on exit
$\begin{bmatrix} a & a & a & a & a & a & a \\ a & a & a &$	$\begin{bmatrix} a & a & h & h & h & h & a \\ a & h & h & h & h & a \\ h & h & h & h & h & h \\ v_2 & h & h & h & h & h \\ v_2 & v_3 & h & h & h & h \\ v_2 & v_3 & v_4 & h & h & h \\ & & & & & & & a \end{bmatrix}$

where *a* denotes an element of the original matrix *A*, *h* denotes a modified element of the upper Hessenberg matrix *H*, and  $v_i$  denotes an element of the vector defining *H*(i).

# ?gelq2

Computes the LQ factorization of a general rectangular matrix using an unblocked algorithm.

call sgelq2 ( m, n, a, lda, tau, work, info )
call dgelq2 ( m, n, a, lda, tau, work, info )
call cgelq2 ( m, n, a, lda, tau, work, info )
call zgelq2 ( m, n, a, lda, tau, work, info )

### **Discussion**

The routine computes an LQ factorization of a real/complex *m* by *n* matrix A as A = L Q.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of  $\min(m, n)$  elementary reflectors :

 $Q = H(k) \dots H(2) H(1)$  (or  $Q = H(k)' \dots H(2)' H(1)'$  for complex flavors), where  $k = \min(m, n)$ 

Each H(i) has the form

 $H(\mathbf{i}) = I - tau * v * v'$ 

where *tau* is a real/complex scalar stored in *tau*(i), and *v* is a real/complex vector with v(1:i-1) = 0 and v(i) = 1.

On exit, v(i+1:n) is stored in a(i, i+1:n).

m	<b>INTEGER.</b> The number of rows in the matrix $A (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgelq2 DOUBLE PRECISION for dgelq2 COMPLEX for cgelq2 COMPLEX*16 for zgelq2.

	Arrays: a(1da,*) contains the <i>m</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
	<pre>work(m) is a workspace array.</pre>
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max(1, $m$ ).
Output Para	meters
a	Overwritten by the factorization data as follows:
	on exit, the elements on and below the diagonal of the array <i>a</i> contain the <i>m</i> -by-min( <i>n</i> , <i>m</i> ) lower trapezoidal matrix $L$ ( $L$ is lower triangular if $n \ge m$ ); the elements above the diagonal, with the array $tau$ , represent the orthogonal/unitary matrix $Q$ as a product of min( $n,m$ ) elementary reflectors.
tau	REAL for sgelq2 DOUBLE PRECISION for dgelq2 COMPLEX for cgelq2 COMPLEX*16 for zgelq2. Array, DIMENSION at least $max(1, min(m, n))$ . Contains scalar factors of the elementary reflectors.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

# ?geql2

Computes the QL factorization of a general rectangular matrix using an unblocked algorithm.

call sgeql2 ( m, n, a, lda, tau, work, info )
call dgeql2 ( m, n, a, lda, tau, work, info )
call cgeql2 ( m, n, a, lda, tau, work, info )
call zgeql2 ( m, n, a, lda, tau, work, info )

## **Discussion**

The routine computes a *QL* factorization of a real/complex *m* by *n* matrix *A* as A = QL.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of min(m, n) elementary reflectors :

 $Q = H(k) \dots H(2) H(1)$ , where  $k = \min(m, n)$ 

Each H(i) has the form

 $H(\mathbf{i}) = I - tau * v * v'$ 

where *tau* is a real/complex scalar stored in *tau*(i), and *v* is a real/complex vector with  $v(\mathbf{m}-\mathbf{k}+\mathbf{i}+1:\mathbf{m}) = 0$  and  $v(\mathbf{m}-\mathbf{k}+\mathbf{i}) = 1$ .

On exit, v(1:m-k+i-1) is stored in a(1:m-k+i-1, n-k+i).

m	<b>INTEGER</b> . The number of rows in the matrix $A (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgeq12 DOUBLE PRECISION for dgeq12 COMPLEX for cgeq12 COMPLEX*16 for zgeq12.

	Arrays: a(lda,*) contains the <i>m</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).
	<pre>work(m) is a workspace array.</pre>
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max(1, $m$ ).
Output Pa	rameters
а	Overwritten by the factorization data as follows:
	on exit, if $m \ge n$ , the lower triangle of the subarray a(m-n+1:m, 1:n) contains the <i>n</i> -by- <i>n</i> lower triangular matrix <i>L</i> ; if $m < n$ , the elements on and below the $(n-m)$ th
	superdiagonal contain the <i>m</i> -by- <i>n</i> lower trapezoidal matrix $L$ ; the remaining elements, with the array <i>tau</i> , represent the orthogonal/unitary matrix $Q$ as a product of elementary reflectors.
tau	REAL for sgeq12 DOUBLE PRECISION for dgeq12 COMPLEX for cgeq12 COMPLEX*16 for zgeq12. Array, DIMENSION at least max(1, min(m, n)). Contains scalar factors of the elementary reflectors.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

# ?geqr2

Computes the QR factorization of a general rectangular matrix using an unblocked algorithm.

call sgeqr2 ( m, n, a, lda, tau, work, info )
call dgeqr2 ( m, n, a, lda, tau, work, info )
call cgeqr2 ( m, n, a, lda, tau, work, info )
call zgeqr2 ( m, n, a, lda, tau, work, info )

## **Discussion**

The routine computes a *QR* factorization of a real/complex *m* by *n* matrix *A* as A = Q R.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of min(m, n) elementary reflectors :

 $Q = H(1)H(2) \dots H(k)$ , where  $k = \min(m, n)$ 

Each H(i) has the form

 $H(\mathbf{i}) = I - tau * v * v'$ 

where *tau* is a real/complex scalar stored in *tau*(i), and *v* is a real/complex vector with v(1:i-1) = 0 and v(i) = 1.

On exit, v(i+1:m) is stored in a(i+1:m, i).

m	<b>INTEGER</b> . The number of rows in the matrix $A (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgeqr2 DOUBLE PRECISION for dgeqr2 COMPLEX for cgeqr2 COMPLEX*16 for zgeqr2.

	Arrays: a(lda,*) contains the <i>m</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max $(1, n)$ .
	work(n) is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $\underline{a}$ ; at least max $(1, \underline{m})$ .
Output Para	meters
а	Overwritten by the factorization data as follows:
	on exit, the elements on and above the diagonal of the array <i>a</i> contain the min( <i>n</i> , <i>m</i> )-by- <i>n</i> upper trapezoidal matrix <i>R</i> ( <i>R</i> is upper triangular if $m \ge n$ ); the elements below the diagonal, with the array <i>tau</i> , represent the orthogonal/unitary matrix <i>Q</i> as a product of elementary reflectors.
tau	REAL for sgeqr2 DOUBLE PRECISION for dgeqr2 COMPLEX for cgeqr2 COMPLEX*16 for zgeqr2. Array, DIMENSION at least max(1, min(m, n)). Contains scalar factors of the elementary reflectors.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

# ?gerq2

Computes the RQ factorization of a general rectangular matrix using an unblocked algorithm.

call sgerq2 ( m, n, a, lda, tau, work, info )
call dgerq2 ( m, n, a, lda, tau, work, info )
call cgerq2 ( m, n, a, lda, tau, work, info )
call zgerq2 ( m, n, a, lda, tau, work, info )

### **Discussion**

The routine computes a RQ factorization of a real/complex *m* by *n* matrix *A* as A = R Q.

The routine does not form the matrix Q explicitly. Instead, Q is represented as a product of min(m, n) elementary reflectors :

 $Q = H(1)H(2) \dots H(k)$ , where  $k = \min(m, n)$ 

Each H(i) has the form

 $H(\mathbf{i}) = I - tau * v * v'$ 

where *tau* is a real/complex scalar stored in *tau*(i), and *v* is a real/complex vector with v(n-k+i+1:n) = 0 and v(n-k+i) = 1.

On exit, v(1:n-k+i-1) is stored in a(m-k+i, 1:n-k+i-1).

m	<b>INTEGER</b> . The number of rows in the matrix $A (m \ge 0)$ .
n	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
a, work	REAL for sgerq2 DOUBLE PRECISION for dgerq2 COMPLEX for cgerq2 COMPLEX*16 for zgerq2.

	Arrays: a(1da, *) contains the <i>m</i> -by- <i>n</i> matrix <i>A</i> . The second dimension of <i>a</i> must be at least max(1, <i>n</i> ). <i>work(m)</i> is a workspace array.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .
Output Pa	rameters
а	Overwritten by the factorization data as follows:
	on exit, if $m \le n$ , the upper triangle of the subarray a(1:m, n-m+1:n) contains the <i>m</i> -by- <i>m</i> upper triangular matrix <i>R</i> ; if $m > n$ , the elements on and above the $(m-n)$ th subdiagonal contain the <i>m</i> -by- <i>n</i> upper trapezoidal matrix <i>R</i> ; the remaining elements, with the array <i>tau</i> , represent the orthogonal/unitary matrix <i>Q</i> as a product of elementary reflectors.
tau	REAL for sgerq2 DOUBLE PRECISION for dgerq2 COMPLEX for cgerq2 COMPLEX*16 for zgerq2. Array, DIMENSION at least max(1, min(m, n)). Contains scalar factors of the elementary reflectors.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

# ?gesc2

Solves a system of linear equations using the LU factorization with complete pivoting computed by ?getc2.

call sgesc2 ( n, a, lda, rhs, ipiv, jpiv, scale )
call dgesc2 ( n, a, lda, rhs, ipiv, jpiv, scale )
call cgesc2 ( n, a, lda, rhs, ipiv, jpiv, scale )
call zgesc2 ( n, a, lda, rhs, ipiv, jpiv, scale )

## **Discussion**

This routine solves a system of linear equations

AX = scale * RHS

with a general n-by-n matrix A using the *LU* factorization with complete pivoting computed by ?getc2.

п	<b>INTEGER</b> . The order of the matrix <i>A</i> .
a, rhs	REAL for sgesc2 DOUBLE PRECISION for dgesc2 COMPLEX for cgesc2 COMPLEX*16 for zgesc2. Arrays: a(1da,*) contains the LU part of the factorization of the n-by-n matrix A computed by ?getc2: A = P L U Q. The second dimension of a must be at least max(1, n);
lda	rhs(n) contains on entry the right hand side vector for the system of equations. INTEGER. The first dimension of <i>a</i> ; at least max(1, <i>n</i> ).

ipiv	INTEGER. Array, DIMENSION at least $\max(1,n)$ . The pivot indices: for $1 \le i \le n$ , row i of the matrix has been interchanged with row $ipiv(i)$ .
jpiv	INTEGER. Array, DIMENSION at least max $(1,n)$ . The pivot indices: for $1 \le j \le n$ , column j of the matrix has been interchanged with column $jpiv(j)$ .
Output Pa	rameters
rhs	On exit, overwritten with the solution vector <i>X</i> .
scale	REAL for sgesc2/cgesc2 DOUBLE PRECISION for dgesc2/zgesc2 Contains the scale factor. <i>scale</i> is chosen in the range $0 \leq scale \leq 1$ to prevent overflow in the solution.

# ?getc2

Computes the LU factorization with complete pivoting of the general n-by-n matrix.

call sgetc2 ( n, a, lda, ipiv, jpiv, info )
call dgetc2 ( n, a, lda, ipiv, jpiv, info )
call cgetc2 ( n, a, lda, ipiv, jpiv, info )
call zgetc2 ( n, a, lda, ipiv, jpiv, info )

## **Discussion**

This routine computes an *LU* factorization with complete pivoting of the *n*-by-*n* matrix *A*. The factorization has the form A = P * L * U * Q, where *P* and *Q* are permutation matrices, *L* is lower triangular with unit diagonal elements and *U* is upper triangular.

### **Input Parameters**

п	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
a	REAL for sgetc2
	DOUBLE PRECISION for dgetc2 COMPLEX for cgetc2
	COMPLEX*16 for zgetc2.
	Array a (lda, *) contains the n-by-n matrix A to be
	factored.
	The second dimension of $a$ must be at least max $(1, n)$ ;
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max(1, $n$ ).

### **Output Parameters**

а

On exit, the factors L and U from the factorization A = P*L*U*Q; the unit diagonal elements of L are not stored. If U(k, k) appears to be less than smin, U(k, k) is given the value of smin, i.e., giving a nonsingular perturbed system.

ipiv	INTEGER. Array, DIMENSION at least $\max(1,n)$ . The pivot indices: for $1 \le i \le n$ , row i of the matrix has been interchanged with row $ipiv(i)$ .
jpiv	<b>INTEGER.</b> Array, <b>DIMENSION</b> at least $\max(1, n)$ . The pivot indices: for $1 \le j \le n$ , column j of the matrix has been interchanged with column $jpiv(j)$ .
info	<b>INTEGER.</b> If <i>info</i> = 0, the execution is successful. If <i>info</i> = $k > 0$ , $U(k, k)$ is likely to produce overflow if we try to solve for $x$ in $Ax = b$ . So $U$ is perturbed to avoid the overflow.

# ?getf2

Computes the LU factorization of a general m by n matrix using partial pivoting with row interchanges (unblocked algorithm).

call sgetf2 ( m, n, a, lda, ipiv, info )
call dgetf2 ( m, n, a, lda, ipiv, info )
call cgetf2 ( m, n, a, lda, ipiv, info )
call zgetf2 ( m, n, a, lda, ipiv, info )

#### **Discussion**

The routine computes the LU factorization of a general *m*-by-*n* matrix *A* using partial pivoting with row interchanges. The factorization has the form

A = PLU

where *P* is a permutation matrix, *L* is lower triangular with unit diagonal elements (lower trapezoidal if m > n) and *U* is upper triangular (upper trapezoidal if m < n).

m	<b>INTEGER.</b> The number of rows in the matrix $A \ (m \ge 0)$ .	
n	<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .	
a	REAL for sgetf2 DOUBLE PRECISION for dgetf2 COMPLEX for cgetf2 COMPLEX*16 for zgetf2. Array, DIMENSION ( <i>lda</i> , *). Contains the matrix <i>A</i> to be factored. The second dimension of <i>a</i> must be at least max(1, <i>n</i> ).	
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, m)$ .	
Output Parameters		
a	Overwritten by $L$ and $U$ . The unit diagonal elements of $L$ are not stored.	
ipiv	INTEGER. Array, DIMENSION at least $\max(1,\min(m,n))$ . The pivot indices: for $1 \le i \le n$ , row <i>i</i> was interchanged with row <i>ipiv(i)</i> .	
info	<b>INTEGER.</b> If <i>info</i> =0, the execution is successful. If <i>info</i> = $-i$ , the <i>i</i> th parameter had an illegal value. If <i>info</i> = $i > 0$ , $u_{ii}$ is 0. The factorization has been completed, but <i>U</i> is exactly singular. Division by 0 will occur if you use the factor <i>U</i> for solving a system of linear equations.	

# ?gtts2

Solves a system of linear equations with a tridiagonal matrix using the LU factorization computed by ?gttrf.

```
call sgtts2 (itrans, n, nrhs, dl, d, du, du2, ipiv, b, ldb)
call dgtts2 (itrans, n, nrhs, dl, d, du, du2, ipiv, b, ldb)
call cgtts2 (itrans, n, nrhs, dl, d, du, du2, ipiv, b, ldb)
call zgtts2 (itrans, n, nrhs, dl, d, du, du2, ipiv, b, ldb)
```

## **Discussion**

This routine solves for *X* one of the following systems of linear equations with multiple right hand sides:

AX = B  $A^TX = B$  or  $A^HX = B$  (for complex matrices only), with a tridiagonal matrix A using the *LU* factorization computed by ?gttrf.

itrans	<b>INTEGER.</b> Must be 0, 1, or 2. Indicates the form of the equations being solved: If <i>itrans</i> = 0, then $AX = B$ (no transpose). If <i>itrans</i> = 1, then $A^TX = B$ (transpose). If <i>itrans</i> = 2, then $A^HX = B$ (conjugate transpose).
n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
nrhs	<b>INTEGER.</b> The number of right-hand sides, i.e., the number of columns in $B$ ( <i>nrhs</i> $\ge$ 0).
dl,d,du,du2,b	REAL for sgtts2 DOUBLE PRECISION for dgtts2 COMPLEX for cgtts2 COMPLEX*16 for zgtts2. Arrays: dl(n - 1), d(n), du(n - 1), du2(n - 2), b(ldb, nrhs). The array dl contains the (n - 1) multipliers that define

	the matrix $L$ from the $LU$ factorization of $A$ .
	The array $d$ contains the $n$ diagonal elements of the
	upper triangular matrix $U$ from the $LU$ factorization of
	А.
	The array $du$ contains the $(n - 1)$ elements of the first
	super-diagonal of U.
	The array $du^2$ contains the $(n - 2)$ elements of the
	second super-diagonal of U.
	The array $b$ contains the matrix $B$ whose columns are
	the right-hand sides for the systems of equations.
ldb	<b>INTEGER.</b> The leading dimension of <i>b</i> ; must be
	$ldb \geq max(1, n).$
ipiv	INTEGER.
	Array, DIMENSION (n).
	The pivot indices array, as returned by <u>?gttrf</u> .
Output Parame	eters

*b* Overwritten by the solution matrix *X*.

# ?labad

Returns the square root of the underflow and overflow thresholds if the exponent-range is very large.

```
call slabad ( small, large )
call dlabad ( small, large )
```

## **Discussion**

This routine takes as input the values computed by slamch/dlamch for underflow and overflow, and returns the square root of each of these values if the log of *large* is sufficiently large. This subroutine is intended to identify machines with a large exponent range, such as the Crays, and redefine the underflow and overflow limits to be the square roots of the values computed by **?lamch**. This subroutine is needed because **?lamch** does not compensate for poor arithmetic in the upper half of the exponent range, as is found on a Cray.

# **Input Parameters**

small	REAL for slabad
	DOUBLE PRECISION for dlabad.
	The underflow threshold as computed by <b>?lamch</b> .
large	REAL for slabad
	DOUBLE PRECISION for dlabad.
	The overflow threshold as computed by ?lamch.

### **Output Parameters**

small	On exit, if log10( <i>large</i> ) is sufficiently large, the square root of <i>small</i> , otherwise unchanged.
large	On exit, if log10( <i>large</i> ) is sufficiently large, the square root of <i>large</i> , otherwise unchanged.

# ?labrd

Reduces the first nb rows and columns of a general matrix to a bidiagonal form.

call	slabrd	(	m,	n,	nb,	a,	lda,	d,	e,	tauq,	taup,	x,	ldx,	Y'	ldy	)
call	dlabrd	(	m,	n,	nb,	a,	lda,	d,	e,	tauq,	taup,	x,	ldx,	Y'	ldy	)
call	clabrd	(	m,	n,	nb,	a,	lda,	d,	e,	tauq,	taup,	x,	ldx,	Y'	ldy	)
call	zlabrd	(	m,	n,	nb,	a,	lda,	d,	e,	tauq,	taup,	х,	ldx,	у,	ldy	)

### **Discussion**

The routine reduces the first *nb* rows and columns of a general *m*-by-*n* matrix *A* to upper or lower bidiagonal form by an orthogonal/unitary transformation Q' A P, and returns the matrices *X* and *Y* which are needed to apply the transformation to the unreduced part of *A*.

If  $m \ge n$ , *A* is reduced to upper bidiagonal form; if m < n, to lower bidiagonal form.

The matrices *Q* and *P* are represented as products of elementary reflectors:  $Q = H(1) H(2) \dots H(nb)$  and  $P = G(1) G(2) \dots G(nb)$ 

Each H(i) and G(i) has the form

 $H(\mathbf{i}) = I - tauq * v * v'$  and  $G(\mathbf{i}) = I - taup * u * u'$ 

where *tauq* and *taup* are scalars, and *v* and *u* are vectors.

The elements of the vectors v and u together form the *m*-by-*nb* matrix V and the *nb*-by-*n* matrix U' which are needed, with X and Y, to apply the transformation to the unreduced part of the matrix, using a block update of the form:  $A := A - V^*Y' - X^*U'$ .

This is an auxiliary routine called by ?gebrd.

### **Input Parameters**

mINTEGER. The number of rows in the matrix  $A \ (m \ge 0)$ .nINTEGER. The number of columns in  $A \ (n \ge 0)$ .

nb	<b>INTEGER.</b> The number of leading rows and columns of $A$ to be reduced.
a	REAL for slabrd DOUBLE PRECISION for dlabrd COMPLEX for clabrd COMPLEX*16 for zlabrd.
	Array $a(1da, *)$ contains the matrix A to be reduced. The second dimension of a must be at least max $(1, n)$ .
lda	<b>INTEGER</b> . The first dimension of $a$ ; at least max $(1, m)$ .
ldx	<b>INTEGER.</b> The first dimension of the output array $x$ ; must beat least max $(1, m)$ .
ldy	<b>INTEGER.</b> The first dimension of the output array $y$ ; must beat least max $(1, n)$ .

### **Output Parameters**

а

On exit, the first *nb* rows and columns of the matrix are overwritten; the rest of the array is unchanged.

If  $m \ge n$ , elements on and below the diagonal in the first *nb* columns, with the array *tauq*, represent the orthogonal/unitary matrix *Q* as a product of elementary reflectors; and elements above the diagonal in the first *nb* rows, with the array *taup*, represent the orthogonal/unitary matrix *P* as a product of elementary reflectors.

If m < n, elements below the diagonal in the first *nb* columns, with the array *tauq*, represent the orthogonal/unitary matrix Q as a product of elementary reflectors, and elements on and above the diagonal in the first *nb* rows, with the array *taup*, represent the orthogonal/unitary matrix P as a product of elementary reflectors.

REAL for single-precision flavors DOUBLE PRECISION for double-precision flavors. Arrays, DIMENSION (*nb*) each.

d, e

	The array <i>d</i> contains the diagonal elements of the first <i>nb</i> rows and columns of the reduced matrix: d(i) = a(i,i). The array <i>e</i> contains the off-diagonal elements of the first <i>nb</i> rows and columns of the reduced matrix.
tauq,taup	REAL for slabrd DOUBLE PRECISION for dlabrd COMPLEX for clabrd COMPLEX*16 for zlabrd.
	Arrays, DIMENSION ( <i>nb</i> ) each. Contain scalar factors of the elementary reflectors which represent the orthogonal/unitary matrices <i>Q</i> and <i>P</i> , respectively.
х, у	REAL for slabrd DOUBLE PRECISION for dlabrd COMPLEX for clabrd COMPLEX*16 for zlabrd.
	Arrays, dimension $x(ldx, nb)$ , $y(ldy, nb)$ . The array $x$ contains the <i>m</i> -by- <i>nb</i> matrix $X$ required to update the unreduced part of $A$ .
	The array $y$ contains the <i>n</i> -by- <i>nb</i> matrix $Y$ required to update the unreduced part of $A$ .

### **Application Notes**

If  $m \ge n$ , then for the elementary reflectors H(i) and G(i),

v(1:i-1) = 0, v(i) = 1, and v(i:m) is stored on exit in a(i:m, i); u(1:i) = 0, u(i+1) = 1, and u(i+1:n) is stored on exit in a(i, i+1:n); tauq is stored in tauq(i) and taup in taup(i).

#### If m < n,

v(1:i) = 0, v(i+1) = 1, and v(i+1:m) is stored on exit in a(i+2:m, i); u(1:i-1) = 0, u(i) = 1, and u(i:n) is stored on exit in a(i, i+1:n); tauq is stored in tauq(i) and taup in taup(i).

The contents of a on exit are illustrated by the following examples with nb = 2:

m = 6, n = 5 (m > n)	m = 5, n = 6 (m < n)
$\begin{bmatrix} 1 & 1 & u_1 & u_1 & u_1 \\ v_1 & 1 & 1 & u_2 & u_2 \\ v_1 & v_2 & a & a & a \\ v_1 & v_2 & a & a & a \\ v_1 & v_2 & a & a & a \\ v_1 & v_2 & a & a & a \end{bmatrix}$	$\begin{bmatrix} 1 & u_1 & u_1 & u_1 & u_1 & u_1 \\ 1 & 1 & u_2 & u_2 & u_2 & u_2 \\ v_1 & 1 & a & a & a & a \\ v_1 & v_2 & a & a & a & a \\ v_1 & v_2 & a & a & a & a \end{bmatrix}$

where *a* denotes an element of the original matrix which is unchanged,  $v_i$  denotes an element of the vector defining *H*(i), and  $u_i$  an element of the vector defining *G*(i).

# ?lacon

*Estimates the 1-norm of a square matrix, using reverse communication for evaluating matrix-vector products.* 

```
call slacon ( n, v, x, isgn, est, kase )
call dlacon ( n, v, x, isgn, est, kase )
call clacon ( n, v, x, est, kase )
call zlacon ( n, v, x, est, kase )
```

#### **Discussion**

This routine estimates the 1-norm of a square, real/complex matrix *A*. Reverse communication is used for evaluating matrix-vector products.

n INTEGER.	The order of the matrix A	( <b>n</b> ≥ 1).
------------	---------------------------	------------------

V, X	REAL for slacon DOUBLE PRECISION for dlacon COMPLEX for clacon COMPLEX*16 for zlacon.
	<ul> <li>Arrays, DIMENSION (n) each.</li> <li>v is a workspace array.</li> <li>x is used as input after an intermediate return.</li> </ul>
isgn	<b>INTEGER</b> . Workspace array, <b>DIMENSION</b> $(n)$ , used with real flavors only.
kase	INTEGER. On the initial call to ?lacon, <i>kase</i> should be 0.
Output Para	meters
est	REAL for slacon/clacon DOUBLE PRECISION for dlacon/zlacon An estimate (a lower bound) for norm(A).
kase	On an intermediate return, <i>kase</i> will be 1 or 2, indicating whether $\mathbf{x}$ should be overwritten by $A * \mathbf{x}$ or $A' * \mathbf{x}$ . On the final return from ?lacon, <i>kase</i> will again be 0.
v	On the final return, $\mathbf{v} = A * \mathbf{w}$ , where <b>est</b> =

 $A * \mathbf{x}$ , if kase = 1,  $A' * \mathbf{x}$ , if kase = 2,

the other parameters unchanged.

x

On an intermediate return, **x** should be overwritten by

transpose of *A*), and **?lacon** must be re-called with all

(where for complex flavors A' is the conjugate

# ?lacpy

Copies all or part of one two-dimensional array to another.

call slacpy ( uplo, m, n, a, lda, b, ldb )
call dlacpy ( uplo, m, n, a, lda, b, ldb )
call clacpy ( uplo, m, n, a, lda, b, ldb )
call zlacpy ( uplo, m, n, a, lda, b, ldb )

## **Discussion**

This routine copies all or part of a two-dimensional matrix A to another matrix B.

CHARACTER*1.
Specifies the part of the matrix A to be copied to B.
If $uplo = 'U'$ , the upper triangular part of A is copied.
If $uplo = 'L'$ , the lower triangular part of A is copied.
Otherwise, all of the matrix A is copied.
<b>INTEGER.</b> The number of rows in the matrix $A \ (m \ge 0)$ .
<b>INTEGER.</b> The number of columns in $A (n \ge 0)$ .
REAL for slacpy
DOUBLE PRECISION for dlacpy
COMPLEX for clacpy
COMPLEX*16 for zlacpy.
Array a ( 1da, * ), contains the m-by-n matrix A.
The second dimension of a must be at least $\max(1, n)$ .
If $uplo = 'U'$ , only the upper triangle or trapezoid is
accessed; if <u>uplo</u> = 'L', only the lower triangle or
trapezoid is accessed.
<b>INTEGER</b> . The first dimension of <i>a</i> ; $1da \ge max(1, m)$ .

1db INTEGER. The first dimension of the output array b;  $1db \ge max(1, m)$ .

#### **Output Parameters**

REAL for slacpy DOUBLE PRECISION for dlacpy COMPLEX for clacpy COMPLEX*16 for zlacpy. Array b(1db, *), contains the *m*-by-*n* matrix *B*. The second dimension of *b* must be at least max(1,*n*). On exit, B = A in the locations specified by *uplo*.

# ?ladiv

Performs complex division in real arithmetic, avoiding unnecessary overflow.

b

call sladiv ( a, b, c, d, p, q )
call dladiv ( a, b, c, d, p, q )
res = cladiv ( x, y )
res = zladiv ( x, y )

### **Discussion**

The routines sladiv/dladiv perform complex division in real arithmetic

 $p + iq = \frac{a + ib}{c + id}$ 

Complex functions cladiv/zladiv compute the result as

res = x/y,

where x and y are complex. The computation of x / y will not overflow on an intermediary step unless the results overflows.

## **Input Parameters**

a, b, c, d	<b>REAL</b> for sladiv DOUBLE PRECISION for dladiv The scalars $a$ , $b$ , $c$ , and $d$ in the above expression (for real flavors only).
х, у	COMPLEX for cladiv COMPLEX*16 for zladiv The complex scalars $x$ and $y$ (for complex flavors only).

## **Output Parameters**

p, q	REAL for sladiv
	DOUBLE PRECISION for dladiv
	The scalars $p$ and $q$ in the above expression (for real
	flavors only).
res	COMPLEX for cladiv
	DOUBLE COMPLEX for zladiv
	Contains the result of division $x / y$ .

# ?lae2

Computes the eigenvalues of a 2-by-2 symmetric matrix.

call slae2 ( a, b, c, rt1, rt2 )
call dlae2 ( a, b, c, rt1, rt2 )

## **Discussion**

The routines sla2/dlae2 compute the eigenvalues of a 2-by-2 symmetric matrix

On return, rt1 is the eigenvalue of larger absolute value, and rt1 is the eigenvalue of smaller absolute value.

### **Input Parameters**

a, b, c	REAL for slae2
	DOUBLE PRECISION for dlae2
	The elements $a$ , $b$ , and $c$ of the 2-by-2 matrix above.

### **Output Parameters**

REAL for slae2
DOUBLE PRECISION for dlae2
The computed eigenvalues of larger and smaller
absolute value, respectively.

## **Application Notes**

rt1 is accurate to a few ulps barring over/underflow. rt2 may be inaccurate if there is massive cancellation in the determinant a*c-b*b; higher precision or correctly rounded or correctly truncated arithmetic would be needed to compute rt2 accurately in all cases.

Overflow is possible only if *rt1* is within a factor of 5 of overflow. Underflow is harmless if the input data is 0 or exceeds *underflow_threshold / macheps*.

# ?laebz

Computes the number of eigenvalues of a real symmetric tridiagonal matrix which are less than or equal to a given value, and performs other tasks required by the routine ?stebz.

```
call slaebz( ijob, nitmax, n, mmax, minp, nbmin, abstol,
    reltol, pivmin, d, e, e2, nval, ab, c, mout, nab,
    work, iwork, info )
call dlaebz( ijob, nitmax, n, mmax, minp, nbmin, abstol,
    reltol, pivmin, d, e, e2, nval, ab, c, mout, nab,
    work, iwork, info )
```

### Discussion

The routine **?laebz** contains the iteration loops which compute and use the function N(w), which is the count of eigenvalues of a symmetric tridiagonal matrix *T* less than or equal to its argument *w*. It performs a choice of two types of loops:

- *ijob* =1, followed by
- ijob =2: It takes as input a list of intervals and returns a list of sufficiently small intervals whose union contains the same eigenvalues as the union of the original intervals. The input intervals are (ab(j,1),ab(j,2)], j=1,...,minp. The output interval (ab(j,1),ab(j,2)] will contain eigenvalues nab(j,1)+1,...,nab(j,2), where 1 ≤ ≤mout.
- *ijob* =3: It performs a binary search in each input interval (*ab*(j,1),*ab*(j,2)] for a point *w*(j) such that *N*(*w*(j))=*nval*(j), and uses *c*(j) as the starting point of the search. If such a *w*(j) is found, then on output *ab*(j,1)=*ab*(j,2)=*w*. If no such *w*(j) is found, then on output (*ab*(j,1),*ab*(j,2)] will be a small interval containing the point where *N*(*w*) jumps through *nval*(j), unless that point lies outside the initial interval.

Note that the intervals are in all cases half-open intervals, that is, of the form (a,b], which includes b but not a.

To avoid underflow, the matrix should be scaled so that its largest element is no greater than overflow**(1/2)*underflow**(1/4) in absolute value. To assure the most accurate computation of small eigenvalues, the matrix should be scaled to be not much smaller than that, either.

Note: the arguments are, in general, **not** checked for unreasonable values.

ijob	<ul> <li>INTEGER. Specifies what is to be done:</li> <li>= 1: Compute <i>nab</i> for the initial intervals.</li> <li>= 2: Perform bisection iteration to find eigenvalues of <i>T</i>.</li> <li>= 3: Perform bisection iteration to invert <i>N(w)</i>, i.e., to find a point which has a specified number of eigenvalues of <i>T</i> to its left.</li> <li>Other values will cause ?laebz to return with <i>info</i>=-1.</li> </ul>
nitmax	INTEGER. The maximum number of "levels" of bisection to be performed, i.e., an interval of width W will not be made smaller than 2^(- <i>nitmax</i> ) * W. If not all intervals have converged after <i>nitmax</i> iterations, then <i>info</i> is set to the number of non-converged intervals.
n	INTEGER. The dimension $n$ of the tridiagonal matrix $T$ . It must be at least 1.
mmax	INTEGER. The maximum number of intervals. If more than <i>mmax</i> intervals are generated, then ?laebz will quit with <i>info=mmax</i> +1.
minp	<b>INTEGER.</b> The initial number of intervals. It may not be greater than <i>mmax</i> .

nbmin	INTEGER. The smallest number of intervals that should be processed using a vector loop. If zero, then only the scalar loop will be used.
abstol	REAL for slaebz DOUBLE PRECISION for dlaebz. The minimum (absolute) width of an interval. When an interval is narrower than <i>abstol</i> , or than <i>reltol</i> times the larger (in magnitude) endpoint, then it is considered to be sufficiently small, i.e., converged. This must be at least zero.
reltol	REAL for slaebz DOUBLE PRECISION for dlaebz. The minimum relative width of an interval. When an interval is narrower than <i>abstol</i> , or than <i>reltol</i> times the larger (in magnitude) endpoint, then it is considered to be sufficiently small, i.e., converged. Note: this should always be at least <i>radix*machine epsilon</i> .
pivmin	<b>REAL</b> for slaebz <b>DOUBLE PRECISION</b> for dlaebz. The minimum absolute value of a "pivot" in the Sturm sequence loop. This <b>must</b> be at least max $ e(j)**2  * safe_min$ and at least safe_min, where safe_min is at least the smallest number that can divide one without overflow.
d, e, e2	REAL for slaebz DOUBLE PRECISION for dlaebz. Arrays, dimension $(n)$ each. The array <i>d</i> contains the diagonal elements of the tridiagonal matrix <i>T</i> .
	The array $e$ contains the off-diagonal elements of the tridiagonal matrix $T$ in positions 1 through $n-1$ . $e(n)$ is arbitrary.
	The array $e^2$ contains the squares of the off-diagonal elements of the tridiagonal matrix <i>T</i> . $e^2(n)$ is ignored.

nval	INTEGER. Array, dimension ( <i>minp</i> ). If <i>ijob</i> =1 or 2, not referenced. If <i>ijob</i> =3, the desired values of N(w).
ab	REAL for slaebz DOUBLE PRECISION for dlaebz. Array, dimension ( $mmax$ ,2) The endpoints of the intervals. $ab(j,1)$ is $a(j)$ , the left endpoint of the j-th interval, and $ab(j,2)$ is $b(j)$ , the right endpoint of the j-th interval.
С	REAL for slaebz DOUBLE PRECISION for dlaebz. Array, dimension (mmax) If <i>ijob</i> =1, ignored. If <i>ijob</i> =2, workspace. If <i>ijob</i> =3, then on input <i>c</i> (j) should be initialized to the first search point in the binary search.
nab	INTEGER. Array, dimension (mmax,2) If $i job=2$ , then on input, $nab(i,j)$ should be set. It must satisfy the condition: $N(ab(i,1)) \leq nab(i,1) \leq nab(i,2) \leq N(ab(i,2))$ , which means that in interval i only eigenvalues nab(i,1)+1,,nab(i,2) will be considered. Usually, nab(i,j)=N(ab(i,j)), from a previous call to ?laebz with i job=1.
	If <i>ijob</i> =3, normally, <i>nab</i> should be set to some distinctive value(s) before <b>?laebz</b> is called.
work	REAL for slaebz DOUBLE PRECISION for dlaebz. Workspace array, dimension ( <i>mmax</i> ).
iwork	INTEGER. Workspace array, dimension ( <i>mmax</i> ).

## **Output Parameters**

output i aram	
nval	The elements of <i>nval</i> will be reordered to correspond with the intervals in <i>ab</i> . Thus, <i>nval</i> (j) on output will not, in general be the same as <i>nval</i> (j) on input, but it will correspond with the interval $(ab(j,1),ab(j,2)]$ on output.
ab	The input intervals will, in general, be modified, split, and reordered by the calculation.
mout	INTEGER. If <i>ijob</i> =1, the number of eigenvalues in the intervals. If <i>ijob</i> =2 or 3, the number of intervals output. If <i>ijob</i> =3, <i>mout</i> will equal <i>minp</i> .
nab	If $ijob=1$ , then on output $nab(i,j)$ will be set to $N(ab(i,j))$ . If $ijob=2$ , then on output, $nab(i,j)$ will contain $max(na(k),min(nb(k),N(ab(i,j))))$ , where k is the index of the input interval that the output interval $(ab(j,1),ab(j,2)]$ came from, and $na(k)$ and $nb(k)$ are the the input values of $nab(k,1)$ and $nab(k,2)$ . If $ijob=3$ , then on output, $nab(i,j)$ contains $N(ab(i,j))$ , unless $N(w) > nval(i)$ for all search points w, in which case $nab(i,1)$ will not be modified, i.e., the output value will be the same as the input value (modulo reorderings, see $nval$ and $ab$ ), or unless $N(w) < nval(i)$ for all search points w, in which case $nab(i,2)$ will not be modified.
info	INTEGER.0:All intervals converged.1mmax:The last info intervals did not converge.mmax+1:More than mmax intervals were generated.

# **Application Notes**

This routine is intended to be called only by other LAPACK routines, thus the interface is less user-friendly. It is intended for two purposes:

(a) finding eigenvalues. In this case, ?laebz should have one or more initial intervals set up in *ab*, and ?laebz should be called with *ijob=1*. This sets up *nab*, and also counts the eigenvalues. Intervals with no eigenvalues would usually be thrown out at this point. Also, if not all the eigenvalues in an interval i are desired, *nab*(i,1) can be increased or *nab*(i,2) decreased. For example, set *nab*(i,1)=*nab*(i,2)-1 to get the largest eigenvalue. ?laebz is then called with *ijob=2* and *mmax* no smaller than the value of *mout* returned by the call with *ijob=1*. After this (*ijob=2*) call, eigenvalues *nab*(i,1)+1 through *nab*(i,2) are approximately *ab*(i,1) (or *ab*(i,2)) to the tolerance specified by *abstol* and *reltol*.

(b) finding an interval (a',b'] containing eigenvalues w(f),...,w(l). In this case, start with a Gershgorin interval (a,b). Set up ab to contain 2 search intervals, both initially (a,b). One nval element should contain f-1 and the other should contain 1, while c should contain a and b, respectively. nab(i,1) should be -1 and nab(i,2) should be n+1, to flag an error if the desired interval does not lie in (a,b). ?laebz is then called with ijob=3. On exit, if w(f-1) < w(f), then one of the intervals -- j -- will have ab(j,1)=ab(j,2) and nab(j,1)=nab(j,2)=f-1, while if, to the specified tolerance, w(f-k)=...=w(f+r), k > 0 and  $r \ge 0$ , then the interval will have N(ab(j,1))=nab(j,1)=f-k and N(ab(j,2))=nab(j,2)=f+r. The cases w(l) < w(l+1) and w(l-r)=...=w(l+k) are handled similarly.

# ?laed0

Used by ?stedc. Computes all eigenvalues and corresponding eigenvectors of an unreduced symmetric tridiagonal matrix using the divide and conquer method.

### Discussion

Real flavors of this routine compute all eigenvalues and (optionally) corresponding eigenvectors of a symmetric tridiagonal matrix using the divide and conquer method.

Complex flavors claed0/zlaed0 compute all eigenvalues of a symmetric tridiagonal matrix which is one diagonal block of those from reducing a dense or band Hermitian matrix and corresponding eigenvectors of the dense or band matrix.

icompq	<pre>INTEGER. Used with real flavors only. If icompq = 0, compute eigenvalues only. If icompq = 1, compute eigenvectors of original dense symmetric matrix also. On entry, the array q must contain the orthogonal matrix used to reduce the original matrix to tridiagonal form. If icompq = 2, compute eigenvalues and eigenvectors of the tridiagonal matrix.</pre>
qsiz	INTEGER.

	The dimension of the orthogonal/unitary matrix used to reduce the full matrix to tridiagonal form; $qsiz \ge n$ (for real flavors, $qsiz \ge n$ if $icompq = 1$ ).
n	<b>INTEGER.</b> The dimension of the symmetric tridiagonal matrix $(n \ge 0)$ .
d, e, rwork	<ul> <li>REAL for single-precision flavors</li> <li>DOUBLE PRECISION for double-precision flavors.</li> <li>Arrays:</li> <li>d(*) contains the main diagonal of the tridiagonal matrix. The dimension of <i>d</i> must be at least max(1, <i>n</i>).</li> <li>e(*) contains the off-diagonal elements of the</li> </ul>
	tridiagonal matrix. The dimension of $e$ must be at least max $(1, n-1)$ .
	<i>rwork(*)</i> is a workspace array used in complex flavors only. The dimension of <i>rwork</i> must be at least $(1 + 3n + 2nlg(n) + 3n^2)$ , where $lg(n) =$ smallest integer k such that $2^k \ge n$ .
q, qstore	<pre>REAL for slaed0 DOUBLE PRECISION for dlaed0 COMPLEX for claed0 COMPLEX*16 for zlaed0. Arrays: q(ldq, *), qstore(ldqs, *). The second dimension of these arrays must be at least max(1, n). For real flavors: If icompq = 0, array q is not referenced. If icompq = 1, on entry, q is a subset of the columns of the orthogonal matrix used to reduce the full matrix to tridiagonal form corresponding to the subset of the full matrix which is being decomposed at this time. If icompq = 2, on entry, q will be the identity matrix. The array qstore is a workspace array referenced only when icompq = 1. Used to store parts of the eigenvector matrix when the updating matrix multiplies take place.</pre>

For complex flavors:

	On entry, <i>q</i> must contain an <i>qsiz</i> -by- <i>n</i> matrix whose columns are unitarily orthonormal. It is a part of the unitary matrix that reduces the full dense Hermitian matrix to a (reducible) symmetric tridiagonal matrix. The array <i>qstore</i> is a workspace array used to store parts of the eigenvector matrix when the updating matrix multiplies take place.
ldq	<b>INTEGER.</b> The first dimension of the array $q$ ; $ldq \ge max(1, n)$ .
ldqs	<b>INTEGER.</b> The first dimension of the array <i>qstore</i> ; $ldqs \ge max(1, n)$ .
work	<b>REAL</b> for slaed0 <b>DOUBLE PRECISION</b> for dlaed0. Workspace array, used in real flavors only. If <i>icompq</i> = 0 or 1, the dimension of <i>work</i> must be at least $(1 + 3n + 2nlg(n) + 2n^2)$ , where $lg(n) =$ smallest integer k such that $2^k \ge n$ . If <i>icompq</i> = 2, the dimension of <i>work</i> must be at least $(4n+n^2)$ .
iwork	<b>INTEGER</b> . Workspace array. For real flavors, if <i>icompq</i> = 0 or 1, and for complex flavors, the dimension of <i>iwork</i> must be at least $(6+6n+5nlg(n))$ , For real flavors, If <i>icompq</i> = 2, the dimension of <i>iwork</i> must be at least $(3+5n)$ .

# **Output Parameters**

d	On exit, contains eigenvalues in ascending order.
е	On exit, the array has been destroyed.
q	If $icompq = 2$ , on exit, q contains the eigenvectors of
	the tridiagonal matrix.

info

INTEGER.

If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value. If info = i > 0, the algorithm failed to compute an eigenvalue while working on the submatrix lying in rows and columns i/(n+1) through mod(i, n+1).

# ?laed1

Used by sstedc/dstedc. Computes the updated eigensystem of a diagonal matrix after modification by a rank-one symmetric matrix. Used when the original matrix is tridiagonal.

## **Discussion**

The routine **?laed1** computes the updated eigensystem of a diagonal matrix after modification by a rank-one symmetric matrix. This routine is used only for the eigenproblem which requires all eigenvalues and eigenvectors of a tridiagonal matrix. **?laed7** handles the case in which eigenvalues only or eigenvalues and eigenvectors of a full symmetric matrix (which was reduced to tridiagonal form) are desired.

T = Q(in) (D(in) + rho * Z*Z') Q'(in) = Q(out) * D(out) * Q'(out)

where z = Q'u, u is a vector of length n with ones in the *cutpnt* and (*cutpnt* + 1) -th elements and zeros elsewhere. The eigenvectors of the original matrix are stored in Q, and the eigenvalues are in D. The algorithm consists of three stages:

The first stage consists of deflating the size of the problem when there are multiple eigenvalues or if there is a zero in the z vector. For each such occurrence the dimension of the secular equation problem is reduced by one. This stage is performed by the routine ?laed2.

The second stage consists of calculating the updated eigenvalues. This is done by finding the roots of the secular equation via the routine <code>?laed4</code> (as called by <code>?laed3</code>). This routine also calculates the eigenvectors of the current problem.

The final stage consists of computing the updated eigenvectors directly using the updated eigenvalues. The eigenvectors for the current problem are multiplied with the eigenvectors from the overall problem.

### **Input Parameters**

n	<b>INTEGER.</b> The dimension of the symmetric tridiagonal matrix $(n \ge 0)$ .
d, q, work	REAL for slaed1 DOUBLE PRECISION for dlaed1. Arrays: d(*) contains the eigenvalues of the rank-1-perturbed matrix. The dimension of $d$ must be at least max $(1, n)$ .
	q(ldq, *) contains the eigenvectors of the rank-1-perturbed matrix. The second dimension of $q$ must be at least max $(1, n)$ .
	work (*) is a workspace array, dimension at least $(4n+n^2)$ .
ldq	<b>INTEGER.</b> The first dimension of the array $q$ ; $ldq \ge max(1, n)$ .
indxq	<b>INTEGER.</b> Array, dimension $(n)$ . On entry, the permutation which separately sorts the two subproblems in $d$ into ascending order.
rho	REAL for slaed1 DOUBLE PRECISION for dlaed1. The subdiagonal entry used to create the rank-1 modification.
cutpnt	INTEGER. The location of the last eigenvalue in the leading sub-matrix. $\min(1,n) \leq utpnt \leq n/2$ .
iwork	<b>INTEGER</b> . Workspace array, dimension (4n).
Output Parame	ters

d

On exit, contains the eigenvalues of the repaired matrix.

q	On exit, q contains the eigenvectors of the repaired tridiagonal matrix.
indxq	On exit, contains the permutation which will reintegrate the subproblems back into sorted order, that is, d(indxq(i = 1, n)) will be in ascending order.
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = 1$ , an eigenvalue did not converge.

Used by sstedc/dstedc. Merges eigenvalues and deflates secular equation. Used when the original matrix is tridiagonal.

> call slaed2( k, n, n1, d, q, ldq, indxq, rho, z, dlamda, w, q2, indx, indxc, indxp, coltyp, info) call dlaed2( k, n, n1, d, q, ldq, indxq, rho, z, dlamda, w, q2, indx, indxc, indxp, coltyp, info)

#### **Discussion**

The routine ?laed2 merges the two sets of eigenvalues together into a single sorted set. Then it tries to deflate the size of the problem. There are two ways in which deflation can occur: when two or more eigenvalues are close together or if there is a tiny entry in the z vector. For each such occurrence the order of the related secular equation problem is reduced by one.

k	<b>INTEGER.</b> The number of non-deflated eigenvalues, and the order of the related secular equation $(0 \le n)$ .
n	<b>INTEGER.</b> The dimension of the symmetric tridiagonal matrix $(n \ge 0)$ .
n1	<b>INTEGER.</b> The location of the last eigenvalue in the leading sub-matrix; $\min(1,n) \le n \le 1 \le n/2$ .
d, q, z	REAL for slaed2 DOUBLE PRECISION for dlaed2. Arrays: d(*) contains the eigenvalues of the two submatrices to be combined. The dimension of $d$ must be at least max $(1, n)$ .

q(ldq, *) contains the eigenvectors of the two submatrices in the two square blocks with corners at (1,1), (n1,n1) and $(n1+1,n1+1), (n,n)$ . The second dimension of $q$ must be at least max $(1, n)$ . z(*) contains the updating vector (the last row of the first sub-eigenvector matrix and the first row of the second sub-eigenvector matrix).
<b>INTEGER.</b> The first dimension of the array $q$ ; $ldq \ge max(1, n)$ .
<b>INTEGER.</b> Array, dimension $(n)$ . On entry, the permutation which separately sorts the two subproblems in $d$ into ascending order. Note that elements in the second half of this permutation must first have $n1$ added to their values.
REAL for slaed2 DOUBLE PRECISION for dlaed2. On entry, the off-diagonal element associated with the rank-1 cut which originally split the two submatrices which are now being recombined.
INTEGER.
Workspace arrays, dimension ( <i>n</i> ) each. Array <i>indx</i> contains the permutation used to sort the contents of <i>dlamda</i> into ascending order.
Array <i>indxp</i> contains the permutation used to place deflated values of $d$ at the end of the array. <i>indxp</i> (1:k) points to the nondeflated $d$ -values and <i>indxp</i> (k+1:n) points to the deflated eigenvalues.
<ul> <li>INTEGER. Workspace array, dimension (n).</li> <li>During execution, a label which will indicate which of the following types a column in the q2 matrix is:</li> <li>1 : non-zero in the upper half only;</li> <li>2 : dense;</li> <li>3 : non-zero in the lower half only;</li> <li>4 : deflated.</li> </ul>

d	On exit, $d$ contains the trailing $(n-k)$ updated eigenvalues (those which were deflated) sorted into increasing order.
đ	On exit, $q$ contains the trailing $(n-k)$ updated eigenvectors (those which were deflated) in its last $n-k$ columns.
indxq	Destroyed on exit.
rho	On exit, <i>rho</i> has been modified to the value required by ?laed3.
dlamda, w, q2	REAL for slaed2 DOUBLE PRECISION for dlaed2. Arrays: $dlamda(n), w(n), q2(n1^2+(n-n1)^2)$ .
	The array <i>dlamda</i> contains a copy of the first <i>k</i> eigenvalues which will be used by ?laed3 to form the secular equation.
	The array $w$ contains the first $k$ values of the final deflation-altered $z$ -vector which will be passed to ?laed3.
	The array q2 contains a copy of the first k eigenvectors which will be used by ?laed3 in a matrix multiply (sgemm/dgemm) to solve for the new eigenvectors.
indxc	INTEGER. Array, dimension $(n)$ . The permutation used to arrange the columns of the deflated $q$ matrix into three groups: the first group contains non-zero elements only at and above $n1$ , the second contains non-zero elements only below $n1$ , and the third is dense.
coltyp	On exit, <i>coltyp</i> (i) is the number of columns of type i, for i=1 to 4 only (see the definition of types in the description of <i>coltyp</i> in <i>Input Parameters</i> ).
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

Used by sstedc/dstedc. Finds the roots of the secular equation and updates the eigenvectors. Used when the original matrix is tridiagonal.

### **Discussion**

The routine ?laed3 finds the roots of the secular equation, as defined by the values in *d*, *w*, and *rho*, between 1 and *k*. It makes the appropriate calls to ?laed4 and then updates the eigenvectors by multiplying the matrix of eigenvectors of the pair of eigensystems being combined by the matrix of eigenvectors of the *k*-by-*k* system which is solved here.

This code makes very mild assumptions about floating point arithmetic. It will work on machines with a guard digit in add/subtract, or on those binary machines without guard digits which subtract like the Cray X-MP, Cray Y-MP, Cray C-90, or Cray-2. It could conceivably fail on hexadecimal or decimal machines without guard digits, but none are known.

k	<b>INTEGER.</b> The number of terms in the rational function to be solved by ?laed4 $(k \ge 0)$ .
п	<b>INTEGER</b> . The number of rows and columns in the $q$ matrix. $n \ge k$ (deflation may result in $n > k$ ).
nl	<b>INTEGER</b> . The location of the last eigenvalue in the leading sub-matrix; $\min(1,n) \le n \le n/2$ .
q	REAL for slaed3 DOUBLE PRECISION for dlaed3. Array q(ldq, *). The second dimension of q must be

	at least $\max(1, n)$ . Initially, the first $k$ columns of this array are used as workspace.
ldq	<b>INTEGER.</b> The first dimension of the array $q$ ; $ldq \ge max(1, n)$ .
rho	<b>REAL</b> for slaed3 <b>DOUBLE PRECISION</b> for dlaed3. The value of the parameter in the rank one update equation. $rho \ge 0$ required.
dlamda, q2, w	REAL for slaed3 DOUBLE PRECISION for dlaed3. Arrays: dlamda(k), q2(ldq2, *), w(k).
	The first <i>k</i> elements of the array <i>dlamda</i> contain the old roots of the deflated updating problem. These are the poles of the secular equation.
	The first $k$ columns of the array $q^2$ contain the non-deflated eigenvectors for the split problem. The second dimension of $q^2$ must be at least max $(1, n)$ .
	The first $k$ elements of the array $w$ contain the components of the deflation-adjusted updating vector.
indx	<b>INTEGER.</b> Array, dimension $(n)$ . The permutation used to arrange the columns of the deflated $q$ matrix into three groups (see ?laed2). The rows of the eigenvectors found by ?laed4 must be likewise permuted before the matrix multiply can take place.
ctot	<b>INTEGER.</b> Array, dimension (4). A count of the total number of the various types of columns in <i>q</i> , as described in <i>indx</i> . The fourth column type is any column which has been deflated.
S	REAL for slaed3 DOUBLE PRECISION for dlaed3. Workspace array, dimension (n1+1)*k.

Will contain the eigenvectors of the repaired matrix which will be multiplied by the previously accumulated eigenvectors to update the system.

d	<b>REAL for slaed3</b> <b>DOUBLE PRECISION for dlaed3</b> . Array, dimension at least max $(1, n)$ . $d(i)$ contains the updated eigenvalues for $1 \le i \le k$ .
q	On exit, the columns 1 to $k$ of $q$ contain the updated eigenvectors.
dlamda	May be changed on output by having lowest order bit set to zero on Cray X-MP, Cray Y-MP, Cray-2, or Cray C-90, as described above.
W	Destroyed on exit.
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = 1, an eigenvalue did not converge.</pre>

Used by sstedc/dstedc. Finds a single root of the secular equation.

call slaed4 ( n, i, d, z, delta, rho, dlam, info )
call dlaed4 ( n, i, d, z, delta, rho, dlam, info )

### **Discussion**

This subroutine computes the i-th updated eigenvalue of a symmetric rank-one modification to a diagonal matrix whose elements are given in the array d, and that

D(i) < D(j) for i < j

and that rho > 0. This is arranged by the calling routine, and is no loss in generality. The rank-one modified system is thus

diag(D) + **r**ho * Z * transpose(Z).

where we assume the Euclidean norm of Z is 1.

The method consists of approximating the rational functions in the secular equation by simpler interpolating rational functions.

n	<b>INTEGER.</b> The length of all arrays.
i	<b>INTEGER.</b> The index of the eigenvalue to be computed; $1 \le i \le n$ .
d, z	<b>REAL</b> for slaed4 <b>DOUBLE PRECISION</b> for dlaed4 Arrays, dimension ( <i>n</i> ) each. The array <i>d</i> contains the original eigenvalues. It is assumed that they are in order, $d(i) < d(j)$ for $i < j$ .
	The array $z$ contains the components of the updating vector $Z$ .

rho REAL for slaed4 DOUBLE PRECISION for dlaed4 The scalar in the symmetric updating formula.

## **Output Parameters**

delta	REAL for slaed4 DOUBLE PRECISION for dlaed4 Array, dimension (n). If $n \neq 1$ , delta contains (d(j) - lambda_i) in its j-th component. If $n = 1$ , then delta(1) = 1. The vector delta contains the information necessary to construct the eigenvectors.
dlam	REAL for slaed4 DOUBLE PRECISION for dlaed4 The computed <i>lambda_i</i> , the <i>i</i> -th updated eigenvalue.
info	INTEGER. If <i>info</i> = 0, the execution is successful. If <i>info</i> = 1, the updating process failed.

# ?laed5

Used by sstedc/dstedc. Solves the 2-by-2 secular equation.

call slaed5 ( i, d, z, delta, rho, dlam )
call dlaed5 ( i, d, z, delta, rho, dlam )

#### **Discussion**

This subroutine computes the i-th eigenvalue of a symmetric rank-one modification of a 2-by-2 diagonal matrix

diag(D) + **rho** * Z * transpose(Z).

The diagonal elements in the array D are assumed to satisfy

D(i) < D(j) for i < j.

We also assume rho > 0 and that the Euclidean norm of the vector *Z* is one.

## **Input Parameters**

· · · · ·		
i	<b>INTEGER</b> . The index of the eigenvalue to be computed; $1 \le i \le 2$ .	
d, z	<b>REAL</b> for slaed5 <b>DOUBLE PRECISION</b> for dlaed5 Arrays, dimension (2) each. The array <i>d</i> contains the original eigenvalues. It is assumed that $d(1) < d(2)$ .	
	The array $z$ contains the components of the updating vector.	
rho	REAL for slaed5 DOUBLE PRECISION for dlaed5 The scalar in the symmetric updating formula.	
Output Parameters		
delta	REAL for slaed5 DOUBLE PRECISION for dlaed5 Array, dimension (2). The vector <i>delta</i> contains the information necessary to construct the eigenvectors.	
dlam	REAL for slaed5 DOUBLE PRECISION for dlaed5 The computed <i>lambda_i</i> , the <i>i</i> -th updated eigenvalue.	

# ?laed6

Used by sstedc/dstedc. Computes one Newton step in solution of the secular equation.

call slaed6(kniter, orgati, rho, d, z, finit, tau, info)

#### call dlaed6(kniter, orgati, rho, d, z, finit, tau, info)

#### **Discussion**

This routine computes the positive or negative root (closest to the origin) of

$$f(x) = rho + \frac{z(1)}{d(1) - x} + \frac{z(2)}{d(2) - x} + \frac{z(3)}{d(3) - x}$$

It is assumed that if orgati = .TRUE. the root is between d(2) and d(3); otherwise it is between d(1) and d(2)

This routine will be called by **?laed4** when necessary. In most cases, the root sought is the smallest in magnitude, though it might not be in some extremely rare situations.

kniter	INTEGER. Refer to ?laed4 for its significance.
orgati	LOGICAL. If $orgati = .TRUE.$ , the needed root is between $d(2)$ and $d(3)$ ; otherwise it is between $d(1)$ and $d(2)$ . See ?laed4 for further details.
rho	<b>REAL for slaed6</b> <b>DOUBLE PRECISION for dlaed6</b> <b>Refer to the equation for</b> $f(x)$ <b>above.</b>
d, z	REAL for slaed6 DOUBLE PRECISION for dlaed6 Arrays, dimension (3) each.
	The array $d$ satisfies $d(1) < d(2) < d(3)$ .
	Each of the elements in the array $z$ must be positive.
finit	<b>REAL</b> for slaed6 <b>DOUBLE PRECISION</b> for dlaed6 The value of $f(x)$ at 0. It is more accurate than the one evaluated inside this routine (if someone wants to do so).

tau	REAL for slaed6
	DOUBLE PRECISION for dlaed6
	The root of the equation for $f(x)$ .
info	INTEGER.
	If <i>info</i> = 0, the execution is successful.
	If $info = 1$ , failure to converge.

Used by ?stedc. Computes the updated eigensystem of a diagonal matrix after modification by a rank-one symmetric matrix. Used when the original matrix is dense.

### **Discussion**

The routine **?laed7** computes the updated eigensystem of a diagonal matrix after modification by a rank-one symmetric matrix. This routine is used only for the eigenproblem which requires all eigenvalues and optionally eigenvectors of a dense symmetric/Hermitian matrix that has been reduced to tridiagonal form. For real flavors, **slaed1/dlaed1** handles the case in which all eigenvalues and eigenvectors of a symmetric tridiagonal matrix are desired.

T = Q(in) (D(in) + rho * Z*Z') Q'(in) = Q(out) * D(out) * Q'(out)

where z = Q'u, *u* is a vector of length *n* with ones in the *cutpnt* and (*cutpnt* + 1) -th elements and zeros elsewhere. The eigenvectors of the original matrix are stored in *Q*, and the eigenvalues are in *D*. The algorithm consists of three stages:

The first stage consists of deflating the size of the problem when there are multiple eigenvalues or if there is a zero in the z vector. For each such occurrence the dimension of the secular equation problem is reduced by one. This stage is performed by the routine slaed8/dlaed8 (for real flavors) or by the routine slaed2/dlaed2 (for complex flavors).

The second stage consists of calculating the updated eigenvalues. This is done by finding the roots of the secular equation via the routine ?laed4 (as called by ?laed9 or ?laed3). This routine also calculates the eigenvectors of the current problem.

The final stage consists of computing the updated eigenvectors directly using the updated eigenvalues. The eigenvectors for the current problem are multiplied with the eigenvectors from the overall problem.

icompq	INTEGER. Used with real flavors only.
	If $icompq = 0$ , compute eigenvalues only. If $icompq = 1$ , compute eigenvectors of original dense symmetric matrix also. On entry, the array $q$ must contain the orthogonal matrix used to reduce the original matrix to tridiagonal form.
п	<b>INTEGER</b> . The dimension of the symmetric tridiagonal matrix $(n \ge 0)$ .
cutpnt	<b>INTEGER.</b> The location of the last eigenvalue in the leading sub-matrix. $\min(1,n) \leq output \leq n$ .
qsiz	<b>INTEGER.</b> The dimension of the orthogonal/unitary matrix used to reduce the full matrix to tridiagonal form; $qsiz \ge n$ (for real flavors, $qsiz \ge n$ if $icompq = 1$ ).
tlvls	<b>INTEGER.</b> The total number of merging levels in the overall divide and conquer tree.
curlvl	<b>INTEGER.</b> The current level in the overall merge routine, $0 \leq curlvl \leq lvls$ .
curpbm	<b>INTEGER.</b> The current problem in the current level in the overall merge routine (counting from upper left to lower right).

d	REAL for slaed7/claed7 DOUBLE PRECISION for dlaed7/zlaed7.
	Array, dimension at least $max(1, n)$ . Array $d(*)$ contains the eigenvalues of the rank-1-perturbed matrix.
q, work	REAL for slaed7 DOUBLE PRECISION for dlaed7 COMPLEX for claed7 COMPLEX*16 for zlaed7. Arrays: q(ldq, *) contains the the eigenvectors of the rank-1-perturbed matrix. The second dimension of $q$ must be at least max(1, $n$ ).
	work(*) is a workspace array, dimension at least $(3n+qsiz*n)$ for real flavors and at least $(qsiz*n)$ for complex flavors.
ldq	<b>INTEGER.</b> The first dimension of the array $q$ ; $ldq \ge max(1, n)$ .
rho	REAL for slaed7/claed7 DOUBLE PRECISION for dlaed7/zlaed7. The subdiagonal element used to create the rank-1 modification.
qstore	REAL for slaed7/claed7 DOUBLE PRECISION for dlaed7/zlaed7. Array, dimension $(n^2+1)$ . Serves also as output parameter. Stores eigenvectors of submatrices encountered during divide and conquer, packed together. <i>qptr</i> points to beginning of the submatrices.
qptr	<b>INTEGER.</b> Array, dimension $(n+2)$ . Serves also as output parameter. List of indices pointing to beginning of submatrices stored in <i>qstore</i> . The submatrices are numbered starting at the bottom left of the divide and conquer tree, from left to right and bottom to top.

prmptr,	perm,	
givptr		<b>INTEGER.</b> Arrays, dimension $(n \lg n)$ each.
		The array prmptr(*) contains a list of pointers which indicate where in perm a level's permutation is stored. prmptr(i+1) - prmptr(i) indicates the size of the permutation and also the size of the full, non-deflated problem.
		The array <i>perm</i> (*) contains the permutations (from deflation and sorting) to be applied to each eigenblock.
		The array <i>givptr</i> (*) contains a list of pointers which indicate where in <i>givcol</i> a level's Givens rotations are stored. <i>givptr</i> (i+1) - <i>givptr</i> (i) indicates the number of Givens rotations.
givcol		<b>INTEGER.</b> Array, dimension $(2, n \lg n)$ . Each pair of numbers indicates a pair of columns to take place in a Givens rotation.
givnum		REAL for slaed7/claed7 DOUBLE PRECISION for dlaed7/zlaed7. Array, dimension $(2, n \lg n)$ . Each number indicates the <i>S</i> value to be used in the corresponding Givens rotation.
iwork		INTEGER. Workspace array, dimension (4n).
rwork		REAL for claed7 DOUBLE PRECISION for zlaed7. Workspace array, dimension $(3n+2qsiz*n)$ . Used in complex flavors only.

d	On exit, contains the eigenvalues of the repaired matrix.
q	On exit, $q$ contains the eigenvectors of the repaired
	tridiagonal matrix.

indxq	<b>INTEGER.</b> Array, dimension $(n)$ . Contains the permutation which will reintegrate the subproblems back into sorted order, that is, d(indxq(i=1, n)) will be in ascending order.
info	<pre>INTEGER. If info = 0, the execution is successful. If info = -i, the ith parameter had an illegal value. If info = 1, an eigenvalue did not converge.</pre>

Used by ?stedc. Merges eigenvalues and deflates secular equation. Used when the original matrix is dense.

#### **Discussion**

This routine merges the two sets of eigenvalues together into a single sorted set. Then it tries to deflate the size of the problem. There are two ways in which deflation can occur: when two or more eigenvalues are close together or if there is a tiny element in the z vector. For each such occurrence the order of the related secular equation problem is reduced by one.

icompq	<pre>INTEGER. Used with real flavors only. If icompq = 0, compute eigenvalues only. If icompq = 1, compute eigenvectors of original dense symmetric matrix also. On entry, the array q must contain the orthogonal matrix used to reduce the original</pre>
	matrix to tridiagonal form.
n	<b>INTEGER.</b> The dimension of the symmetric tridiagonal matrix $(n \ge 0)$ .

cutpnt	<b>INTEGER.</b> The location of the last eigenvalue in the leading sub-matrix. $\min(1,n) \leq utpnt \leq n$ .
qsiz	<b>INTEGER.</b> The dimension of the orthogonal/unitary matrix used to reduce the full matrix to tridiagonal form; $qsiz \ge n$ (for real flavors, $qsiz \ge n$ if $icompq = 1$ ).
d, z	<ul> <li>REAL for slaed8/claed8</li> <li>DOUBLE PRECISION for dlaed8/zlaed8.</li> <li>Arrays, dimension at least max(1, n) each.</li> <li>The array d(*) contains the eigenvalues of the two submatrices to be combined.</li> <li>On entry, z(*) contains the updating vector (the last row of the first sub-eigenvector matrix and the first row of the second sub-eigenvector matrix). The contents of z are destroyed by the updating process.</li> </ul>
đ	<ul> <li>REAL for slaed8</li> <li>DOUBLE PRECISION for dlaed8</li> <li>COMPLEX for claed8</li> <li>COMPLEX*16 for zlaed8.</li> <li>Array q(ldq, *). The second dimension of q must be at least max(1, n). On entry, q contains the eigenvectors of the partially solved system which has been previously updated in matrix multiplies with other partially solved eigensystems.</li> <li>For real flavors, if icompq = 0, q is not referenced.</li> </ul>
ldq	<b>INTEGER.</b> The first dimension of the array $q$ ; $ldq \ge max(1, n)$ .
ldq2	<b>INTEGER.</b> The first dimension of the output array $q_2$ ; $ldq_2 \ge max(1, n)$ .
indxq	<b>INTEGER.</b> Array, dimension ( <i>n</i> ). The permutation which separately sorts the two sub-problems in <i>d</i> into ascending order. Note that elements in the second half of this permutation must first have <i>cutpnt</i> added to their values in order to be accurate.

rho	REAL for slaed8/claed8 DOUBLE PRECISION for dlaed8/zlaed8. On entry, the off-diagonal element associated with the rank-1 cut which originally split the two submatrices which are now being recombined.
Output Param	eters
k	<b>INTEGER</b> . The number of non-deflated eigenvalues, and the order of the related secular equation.
d	On exit, contains the trailing ( <i>n-k</i> ) updated eigenvalues (those which were deflated) sorted into increasing order.
đ	On exit, $q$ contains the trailing $(n-k)$ updated eigenvectors (those which were deflated) in its last $(n-k)$ columns.
rho	On exit, <i>rho</i> has been modified to the value required by <b>?laed3</b> .
dlamda, w	REAL for slaed8/claed8 DOUBLE PRECISION for dlaed8/zlaed8. Arrays, dimension ( <i>n</i> ) each. The array <i>dlamda</i> (*) contains a copy of the first <i>k</i> eigenvalues which will be used by ?laed3 to form the secular equation.
	The array $w(*)$ will hold the first $k$ values of the final deflation-altered z-vector and will be passed to ?laed3.
q2	REAL for slaed8 DOUBLE PRECISION for dlaed8 COMPLEX for claed8 COMPLEX*16 for zlaed8. Array $q2(ldq2, *)$ . The second dimension of $q2$ must be at least max(1, n). Contains a copy of the first k eigenvectors which will be used by slaed7/dlaed7 in a matrix multiply (sgemm/dgemm) to update the new eigenvectors. For real flavors, if <i>icompq</i> = 0, $q2$ is not referenced.
indxp, indx	<b>INTEGER</b> . Workspace arrays, dimension ( <i>n</i> ) each.

	The array $indxp(*)$ will contain the permutation used to place deflated values of $d$ at the end of the array. On output, $indxp(1:k)$ points to the nondeflated $d$ -values and $indxp(k+1:n)$ points to the deflated eigenvalues.
	The array $indx(*)$ will contain the permutation used to sort the contents of $d$ into ascending order.
perm	<b>INTEGER.</b> Array, dimension ( <i>n</i> ). Contains the permutations (from deflation and sorting) to be applied to each eigenblock.
givptr	<b>INTEGER</b> . Contains the number of Givens rotations which took place in this subproblem.
givcol	<b>INTEGER.</b> Array, dimension $(2, n)$ . Each pair of numbers indicates a pair of columns to take place in a Givens rotation.
givnum	REAL for slaed8/claed8 DOUBLE PRECISION for dlaed8/zlaed8. Array, dimension (2, <i>n</i> ). Each number indicates the <i>S</i> value to be used in the corresponding Givens rotation.
info	<b>INTEGER</b> . If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

Used by sstedc/dstedc. Finds the roots of the secular equation and updates the eigenvectors. Used when the original matrix is dense.

#### **Discussion**

This routine finds the roots of the secular equation, as defined by the values in *d*, *z*, and *rho*, between *kstart* and *kstop*. It makes the appropriate calls to slaed4/dlaed4 and then stores the new matrix of eigenvectors for use in calculating the next level of z vectors.

k	<b>INTEGER.</b> The number of terms in the rational function to be solved by slaed4/dlaed4 ( $k \ge 0$ ).
kstart, kstop	<b>INTEGER.</b> The updated eigenvalues <i>lambda</i> (i), <i>kstart</i> $\leq$ i $\leq$ <i>kstop</i> are to be computed. 1 $\leq$ <i>kstart</i> $\leq$ <i>kstop</i> $\leq$ <i>k</i> .
п	<b>INTEGER.</b> The number of rows and columns in the <i>Q</i> matrix. $n \ge k$ (deflation may result in $n > k$ ).
q	REAL for slaed9 DOUBLE PRECISION for dlaed9. Workspace array, dimension $(ldq, *)$ . The second dimension of $q$ must be at least max $(1, n)$ .
ldq	<b>INTEGER.</b> The first dimension of the array $q$ ; $ldq \ge max(1, n)$ .

rho	<b>REAL</b> for slaed9 <b>DOUBLE PRECISION</b> for dlaed9 The value of the parameter in the rank one update equation. $rho \ge 0$ required.
dlamda, w	REAL for slaed9 DOUBLE PRECISION for dlaed9 Arrays, dimension (k) each. The first k elements of the array dlamda(*) contain the old roots of the deflated updating problem. These are the poles of the secular equation.
lds	The first $k$ elements of the array $w(*)$ contain the components of the deflation-adjusted updating vector. INTEGER. The first dimension of the output array $s$ ;
105	$lds \ge max(1, k)$ .

d	<b>REAL for slaed9</b> <b>DOUBLE PRECISION for dlaed9</b> Array, dimension ( <i>n</i> ). <i>d</i> (i) contains the updated eigenvalues for $kstart \leq i \leq kstop$ .
S	<ul> <li>REAL for slaed9</li> <li>DOUBLE PRECISION for dlaed9.</li> <li>Array, dimension (<i>lds</i>, *). The second dimension of <i>s</i> must be at least max(1, <i>k</i>).</li> <li>Will contain the eigenvectors of the repaired matrix which will be stored for subsequent Z vector calculation and multiplied by the previously accumulated eigenvectors to update the system.</li> </ul>
info	<b>INTEGER.</b> If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value.

If info = -i, the *i*th parameter had an illegal value If info = 1, the eigenvalue did not converge.

Used by ?stedc. Computes the Z vector determining the rank-one modification of the diagonal matrix. Used when the original matrix is dense.

```
call slaeda( n, tlvls, curlvl, curpbm, prmptr, perm, givptr, givcol,
      givnum, q, qptr, z, ztemp, info )
call dlaeda( n, tlvls, curlvl, curpbm, prmptr, perm, givptr, givcol,
      givnum, q, qptr, z, ztemp, info )
```

#### **Discussion**

The routine ?laeda computes the z vector corresponding to the merge step in the *curlvl*-th step of the merge process with *tlvls* steps for the *curpbm*-th problem.

п	<b>INTEGER.</b> The dimension of the symmetric tridiagonal matrix $(n \ge 0)$ .
tlvls	<b>INTEGER.</b> The total number of merging levels in the overall divide and conquer tree.
curlvl	<b>INTEGER.</b> The current level in the overall merge routine, $0 \leq curlvl \leq lvls$ .
curpbm	<b>INTEGER.</b> The current problem in the current level in the overall merge routine (counting from upper left to lower right).
prmptr, perm,	
givptr	<b>INTEGER.</b> Arrays, dimension $(n \lg n)$ each.
	The array prmptr(*) contains a list of pointers which indicate where in perm a level's permutation is stored. prmptr(i+1) - prmptr(i) indicates the size of the permutation and also the size of the full, non-deflated problem.

	The array <i>perm</i> (*) contains the permutations (from deflation and sorting) to be applied to each eigenblock.
	The array <i>givptr</i> (*) contains a list of pointers which indicate where in <i>givcol</i> a level's Givens rotations are stored. <i>givptr</i> (i+1) - <i>givptr</i> (i) indicates the number of Givens rotations.
givcol	<b>INTEGER.</b> Array, dimension $(2, n \lg n)$ . Each pair of numbers indicates a pair of columns to take place in a Givens rotation.
givnum	REAL for slaeda DOUBLE PRECISION for dlaeda. Array, dimension (2, <i>n</i> lg <i>n</i> ). Each number indicates the <i>S</i> value to be used in the corresponding Givens rotation.
đ	REAL for slaeda DOUBLE PRECISION for dlaeda. Array, dimension $(n^2)$ . Contains the square eigenblocks from previous levels, the starting positions for blocks are given by <i>qptr</i> .
qptr	<b>INTEGER.</b> Array, dimension $(n+2)$ . Contains a list of pointers which indicate where in $q$ an eigenblock is stored. $sqrt(qptr(i+1) - qptr(i))$ indicates the size of the block.
ztemp	REAL for slaeda DOUBLE PRECISION for dlaeda. Workspace array, dimension ( <i>n</i> ).

Z	REAL for slaeda
	DOUBLE PRECISION for dlaeda.
	Array, dimension ( <i>n</i> ). Contains the updating vector (the
	last row of the first sub-eigenvector matrix and the first
	row of the second sub-eigenvector matrix).

info

INTEGER.

If info = 0, the execution is successful. If info = -i, the *i*th parameter had an illegal value.

# ?laein

Computes a specified right or left eigenvector of an upper Hessenberg matrix by inverse iteration.

```
call slaein( rightv, noinit, n, h, ldh, wr, wi, vr, vi, b, ldb,
        work, eps3, smlnum, bignum, info )
call dlaein( rightv, noinit, n, h, ldh, wr, wi, vr, vi, b, ldb,
        work, eps3, smlnum, bignum, info )
call claein( rightv, noinit, n, h, ldh, w, v, b, ldb,
        rwork, eps3, smlnum, info )
call zlaein( rightv, noinit, n, h, ldh, w, v, b, ldb,
        rwork, eps3, smlnum, info )
```

### **Discussion**

The routine ?laein uses inverse iteration to find a right or left eigenvector corresponding to the eigenvalue (wr,wi) of a real upper Hessenberg matrix H (for real flavors slaein/dlaein) or to the eigenvalue w of a complex upper Hessenberg matrix H (for complex flavors claein/zlaein).

rightv	LOGICAL. If <i>rightv</i> = .TRUE., compute right eigenvector; if <i>rightv</i> = .FALSE., compute left eigenvector.
noinit	LOGICAL. If <i>noinit</i> = .TRUE., no initial vector is supplied in ( <i>vr,vi</i> ) or in <i>v</i> (for complex flavors); if <i>noinit</i> = .FALSE., initial vector is supplied in ( <i>vr,vi</i> ) or in <i>v</i> (for complex flavors).
n	<b>INTEGER.</b> The order of the matrix $H$ ( $n \ge 0$ ).

h	<pre>REAL for slaein DOUBLE PRECISION for dlaein COMPLEX for claein COMPLEX*16 for zlaein. Array h(ldh, *). The second dimension of h must be at least max(1, n). Contains the upper Hessenberg matrix H.</pre>
ldh	<b>INTEGER.</b> The first dimension of the array $h$ ; $ldh \ge max(1, n)$ .
wr, wi	REAL for slaein DOUBLE PRECISION for dlaein. The real and imaginary parts of the eigenvalue of <i>H</i> whose corresponding right or left eigenvector is to be computed (for real flavors of the routine).
W	COMPLEX for claein COMPLEX*16 for zlaein. The eigenvalue of <i>H</i> whose corresponding right or left eigenvector is to be computed (for complex flavors of the routine).
vr, vi	REAL for slaein DOUBLE PRECISION for dlaein. Arrays, dimension $(n)$ each. Used for real flavors only. On entry, if <i>noinit</i> = .FALSE. and <i>wi</i> = 0.0, <i>vr</i> must contain a real starting vector for inverse iteration using the real eigenvalue <i>wr</i> ; if <i>noinit</i> = .FALSE. and <i>wi</i> $\neq$ 0.0, <i>vr</i> and <i>vi</i> must contain the real and imaginary parts of a complex starting vector for inverse iteration using the complex eigenvalue ( <i>wr</i> , <i>wi</i> ); otherwise <i>vr</i> and <i>vi</i> need not be set.
V	COMPLEX for claein COMPLEX*16 for zlaein. Array, dimension ( <i>n</i> ). Used for complex flavors only. On entry, if <i>noinit</i> = .FALSE., <i>v</i> must contain a starting vector for inverse iteration; otherwise <i>v</i> need not be set.

Ъ	<pre>REAL for slaein DOUBLE PRECISION for dlaein COMPLEX for claein COMPLEX*16 for zlaein. Workspace array b(ldb, *). The second dimension of b must be at least max(1, n).</pre>
ldb	<b>INTEGER.</b> The first dimension of the array b; $ldb \ge n+1$ for real flavors; $ldb \ge max(1, n)$ for complex flavors.
work	REAL for slaein DOUBLE PRECISION for dlaein. Workspace array, dimension ( <i>n</i> ). Used for real flavors only.
rwork	REAL for claein DOUBLE PRECISION for zlaein. Workspace array, dimension ( <i>n</i> ). Used for complex flavors only.
eps3, smlnum	REAL for slaein/claein DOUBLE PRECISION for dlaein/zlaein. eps3 is a small machine-dependent value which is used to perturb close eigenvalues, and to replace zero pivots. smlnum is a machine-dependent value close to underflow threshold.
bignum	REAL for slaein DOUBLE PRECISION for dlaein. <i>bignum</i> is a machine-dependent value close to overflow threshold. Used for real flavors only.

vr, viOn exit, if wi = 0.0 (real eigenvalue), vr contains the<br/>computed real eigenvector; if  $wi \neq 0.0$  (complex<br/>eigenvalue), vr and vi contain the real and imaginary<br/>parts of the computed complex eigenvector. The<br/>eigenvector is normalized so that the component of

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	largest magnitude has magnitude 1; here the magnitude of a complex number $(x,y)$ is taken to be $ x  +  y $ . <i>vi</i> is not referenced if <i>wi</i> = 0.0.
v	On exit, $\mathbf{v}$ contains the computed eigenvector, normalized so that the component of largest magnitude has magnitude 1; here the magnitude of a complex number ( <i>x</i> , <i>y</i> ) is taken to be $ x  +  y $ .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = 1$ , inverse iteration did not converge. For real flavors, $vr$ is set to the last iterate, and so is $vi$ if $wi \neq 0.0$ . For complex flavors, $v$ is set to the last iterate.

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# ?laev2

Computes the eigenvalues and eigenvectors of a 2-by-2 symmetric/Hermitian matrix.

call	slaev2	(a,	b,	C,	rt1,	rt2,	csl,	sn1)
call	dlaev2	(a,	b,	с,	rt1,	rt2,	cs1,	sn1)
call	claev2	(a,	b,	с,	rt1,	rt2,	cs1,	sn1)
call	zlaev2	(a,	b,	c,	rt1,	rt2,	cs1,	sn1)

### **Discussion**

This routine performs the eigendecomposition of a 2-by-2 symmetric matrix

$$\begin{bmatrix} a & b \\ b & c \end{bmatrix}$$
 (for slaev2/dlaev2) or Hermitian matrix 
$$\begin{bmatrix} a & b \\ conjg(b) & c \end{bmatrix}$$

#### (for claev2/zlaev2).

On return, rt1 is the eigenvalue of larger absolute value, rt2 of smaller absolute value, and (cs1, sn1) is the unit right eigenvector for rt1, giving the decomposition

$$\begin{bmatrix} cs1 \ sn1 \\ -sn1 \ cs1 \end{bmatrix} \cdot \begin{bmatrix} a \ b \\ b \ c \end{bmatrix} \cdot \begin{bmatrix} cs1 \ -sn1 \\ sn1 \ cs1 \end{bmatrix} = \begin{bmatrix} rt1 \ 0 \\ 0 \ rt2 \end{bmatrix}$$
(for slaev2/dlaev2),  
or
$$\begin{bmatrix} cs1 \ conjg(sn1) \\ -sn1 \ cs1 \end{bmatrix} \cdot \begin{bmatrix} a \ b \\ conjg(b) \ c \end{bmatrix} \cdot \begin{bmatrix} cs1 \ -conjg(sn1) \\ sn1 \ cs1 \end{bmatrix} = \begin{bmatrix} rt1 \ 0 \\ 0 \ rt2 \end{bmatrix}$$

(for claev2/zlaev2).

## **Input Parameters**

a, b, c	REAL for slaev2
	DOUBLE PRECISION for dlaev2
	COMPLEX for claev2
	COMPLEX*16 for zlaev2.
	Elements of the input matrix.

rt1, rt2	REAL for slaev2/claev2 DOUBLE PRECISION for dlaev2/zlaev2. Eigenvalues of larger and smaller absolute value, respectively.
cs1	REAL for slaev2/claev2 DOUBLE PRECISION for dlaev2/zlaev2.
snl	REAL for slaev2 DOUBLE PRECISION for dlaev2 COMPLEX for claev2 COMPLEX*16 for zlaev2. The vector ( <i>cs1</i> , <i>sn1</i> ) is the unit right eigenvector for <i>rt1</i> .

### **Application Notes**

**rt1** is accurate to a few ulps barring over/underflow. **rt2** may be inaccurate if there is massive cancellation in the determinant a*c-b*b; higher precision or correctly rounded or correctly truncated arithmetic would be needed to compute **rt2** accurately in all cases. **cs1** and **sn1** are accurate to a few ulps barring over/underflow. Overflow is possible only if **rt1** is within a factor of 5 of overflow. Underflow is harmless if the input data is 0 or exceeds underflow_threshold / macheps.

# ?laexc

Swaps adjacent diagonal blocks of a real upper quasi-triangular matrix in Schur canonical form, by an orthogonal similarity transformation.

call slaexc ( wantq, n, t, ldt, q, ldq, j1, n1, n2, work, info )
call dlaexc ( wantq, n, t, ldt, q, ldq, j1, n1, n2, work, info )

### **Discussion**

This routine swaps adjacent diagonal blocks  $T_{11}$  and  $T_{22}$  of order 1 or 2 in an upper quasi-triangular matrix *T* by an orthogonal similarity transformation.

*T* must be in Schur canonical form, that is, block upper triangular with 1-by-1 and 2-by-2 diagonal blocks; each 2-by-2 diagonal block has its diagonal elements equal and its off-diagonal elements of opposite sign.

wantq	LOGICAL.
	If wantq = . TRUE ., accumulate the transformation in
	the matrix $Q$ ;
	If $wantq = .FALSE.$ , do not accumulate the
	transformation.
n	<b>INTEGER.</b> The order of the matrix $T (n \ge 0)$ .
t, q	REAL for slaexc
	DOUBLE PRECISION for dlaexc
	Arrays:
	t(ldt, *) contains on entry the upper quasi-triangular
	matrix <i>T</i> , in Schur canonical form.
	The second dimension of $t$ must be at least max $(1, n)$ .

	q(ldq, *) contains on entry, if want $q = .TRUE.$ , the orthogonal matrix $Q$ . If want $q = .FALSE.$ , $q$ is not referenced. The second dimension of $q$ must be at least max $(1, n)$ .
ldt	<b>INTEGER.</b> The first dimension of $t$ ; at least max $(1, n)$ .
ldq	<b>INTEGER.</b> The first dimension of $q$ ; If want $q = .FALSE.$ , then $ldq \ge 1$ . If want $q = .TRUE.$ , then $ldq \ge max(1,n)$ .
jl	<b>INTEGER.</b> The index of the first row of the first block $T_{11}$ .
nl	<b>INTEGER.</b> The order of the first block $T_{11}$ ( <i>n</i> 1 = 0, 1, or 2).
n2	<b>INTEGER.</b> The order of the second block $T_{22}$ ( <i>n2</i> = 0, 1, or 2).
work	REAL for slaexc; DOUBLE PRECISION for dlaexc. Workspace array, DIMENSION (n).

t	On exit, the updated matrix <i>T</i> , again in Schur canonical form.
q	On exit, if $wantq = .TRUE$ , the updated matrix $Q$ .
info	INTEGER. If $info = 0$ , the execution is successful. If $info = 1$ , the transformed matrix <i>T</i> would be too far from Schur form; the blocks are not swapped and <i>T</i> and <i>Q</i> are unchanged.

# ?lag2

Computes the eigenvalues of a 2-by-2 generalized eigenvalue problem, with scaling as necessary to avoid over-/underflow.

call slag2 ( a, lda, b, ldb, safmin, scale1, scale2, wr1, wr2, wi )
call dlag2 ( a, lda, b, ldb, safmin, scale1, scale2, wr1, wr2, wi )

#### **Discussion**

This routine computes the eigenvalues of a  $2 \ge 2$  generalized eigenvalue problem A - w B, with scaling as necessary to avoid over-/underflow. The scaling factor, *s*, results in a modified eigenvalue equation

sA - wB,

a, b

lda

where s is a non-negative scaling factor chosen so that w, w B, and s A do not overflow and, if possible, do not underflow, either.

REAL for slag2
DOUBLE PRECISION for dlag2
Arrays:
a(lda,2) contains, on entry, the 2 x 2 matrix A. It is assumed that its 1-norm is less than 1/safmin. Entries less than sqrt(safmin)*norm(A) are subject to being treated as zero.
b(1db, 2) contains, on entry, the 2 x 2 upper triangular matrix B. It is assumed that the one-norm of B is less than $1/safmin$ . The diagonals should be at least sqrt(safmin) times the largest element of B (in absolute value); if a diagonal is smaller than that, then +/- sqrt(safmin) will be used instead of that diagonal.
INTEGER. The first dimension of $a: 1da > 2$ .

ldb	<b>INTEGER</b> . The first dimension of <i>b</i> ; $1db \ge 2$ .
safmin	REAL for slag2; DOUBLE PRECISION for dlag2. The smallest positive number such that 1/safmin does not overflow. (This should always be ?lamch('S') - it is an argument in order to avoid having to call ?lamch frequently.)

scale1	REAL for slag2;
	DOUBLE PRECISION for dlag2.
	A scaling factor used to avoid over-/underflow in the
	eigenvalue equation which defines the first eigenvalue.
	If the eigenvalues are complex, then the eigenvalues are $(wr1 +/- wii)/scale1$ (which may lie outside the exponent range of the machine), $scale1=scale2$ , and $scale1$ will always be positive. If the eigenvalues are real, then the first (real) eigenvalue is $wr1/scale1$ , but this may overflow or underflow, and in fact, $scale1$ may be zero or less than the
	underflow threshhold if the exact eigenvalue is sufficiently large.
scale2	REAL for slag2;
	DOUBLE PRECISION for dlag2.
	A scaling factor used to avoid over-/underflow in the
	eigenvalue equation which defines the second
	eigenvalue. If the eigenvalues are complex, then scale2=scale1. If the eigenvalues are real, then the second (real) eigenvalue is wr2/scale2, but this may overflow or underflow, and in fact, scale2 may be zero or less than the underflow threshold if the exact eigenvalue is sufficiently large.
wrl	REAL for slag2;
	DOUBLE PRECISION for dlag2. If the eigenvalue is real, then wr1 is scale1 times the

eigenvalue closest to the (2,2) element of  $AB^{-1}$ . If the eigenvalue is complex, then *wr1=wr2* is *scale1* times the real part of the eigenvalues.

REAL for slag2;

DOUBLE PRECISION for dlag2.

If the eigenvalue is real, then *wr2* is *scale2* times the other eigenvalue. If the eigenvalue is complex, then *wr1=wr2* is *scale1* times the real part of the eigenvalues.

wi

wr2

REAL for slag2;

DOUBLE PRECISION for dlag2.

If the eigenvalue is real, then *wi* is zero. If the eigenvalue is complex, then *wi* is *scale1* times the imaginary part of the eigenvalues. *wi* will always be non-negative.

# ?lags2

Computes 2-by-2 orthogonal matrices U, V, and Q, and applies them to matrices A and B such that the rows of the transformed A and B are parallel.

### **Discussion**

This routine computes 2-by-2 orthogonal matrices U, V and Q, such that if upper = .TRUE, then

$$U' *A*Q = U' * \begin{bmatrix} A_1 & A_2 \\ 0 & A_3 \end{bmatrix} * Q = \begin{bmatrix} x & 0 \\ x & x \end{bmatrix}$$

and

$$V' *B*Q = V' * \begin{bmatrix} B_1 & B_2 \\ 0 & B_3 \end{bmatrix} *Q = \begin{bmatrix} x & 0 \\ x & x \end{bmatrix}$$

or if *upper* =.FALSE., then

$$U' *A*Q = U' * \begin{bmatrix} A_1 & 0 \\ A_2 & A_3 \end{bmatrix} * Q = \begin{bmatrix} x & x \\ 0 & x \end{bmatrix}$$

and

$$V' *B*Q = V' * \begin{bmatrix} B_1 & 0 \\ B_2 & B_3 \end{bmatrix} *Q = \begin{bmatrix} x & x \\ 0 & x \end{bmatrix}$$

The rows of the transformed A and B are parallel, where

$$U = \begin{bmatrix} csu & snu \\ -snu & csu \end{bmatrix}, V = \begin{bmatrix} csv & snv \\ -snv & csv \end{bmatrix}, Q = \begin{bmatrix} csq & snq \\ -snq & csq \end{bmatrix}$$

Here Z' denotes the transpose of Z.

### **Input Parameters**

upper	LOGICAL.
	If $upper = . TRUE .$ , the input matrices A and B are upper
	triangular;
	If <i>upper</i> = . FALSE., the input matrices A and B are
	lower triangular.
a1, a2, a3	REAL for slags2
	DOUBLE PRECISION for dlags2
	On entry, $a_1$ , $a_2$ and $a_3$ are elements of the input
	2-by-2 upper (lower) triangular matrix A.
b1, b2, b3	REAL for slags2
	DOUBLE PRECISION for dlags2
	On entry, <b>b1</b> , <b>b2</b> and <b>b3</b> are elements of the input
	2-by-2 upper (lower) triangular matrix <i>B</i> .

Csu, snu	REAL for slags2 DOUBLE PRECISION for dlags2 The desired orthogonal matrix U.
csv, snv	REAL for slags2 DOUBLE PRECISION for dlags2 The desired orthogonal matrix V.
csq, snq	REAL for slags2 DOUBLE PRECISION for dlags2 The desired orthogonal matrix $Q$ .

## ?lagtf

Computes an LU factorization of a matrix T- $\lambda I$ , where T is a general tridiagonal matrix, and  $\lambda$  a scalar, using partial pivoting with row interchanges.

call slagtf ( n, a, lambda, b, c, tol, d, in, info )
call dlagtf ( n, a, lambda, b, c, tol, d, in, info )

#### **Discussion**

This routine factorizes the matrix (T - lambda*I), where T is an n-by-n tridiagonal matrix and lambda is a scalar, as

T - lambda * I = P L U,

where P is a permutation matrix, L is a unit lower tridiagonal matrix with at most one non-zero sub-diagonal elements per column and U is an upper triangular matrix with at most two non-zero super-diagonal elements per column. The factorization is obtained by Gaussian elimination with partial pivoting and implicit row scaling. The parameter *lambda* is included in the routine so that <code>?lagtf</code> may be used, in conjunction with <code>?lagts</code>, to obtain eigenvectors of T by inverse iteration.

п	<b>INTEGER.</b> The order of the matrix $T (n \ge 0)$ .
a, b, c	REAL for slagtf DOUBLE PRECISION for dlagtf Arrays, dimension $a(n)$ , $b(n-1)$ , $c(n-1)$ : On entry, $a(*)$ must contain the diagonal elements of the matrix <i>T</i> . On entry, $b(*)$ must contain the $(n-1)$ super-diagonal elements of <i>T</i> . On entry, $c(*)$ must contain the $(n-1)$ sub-diagonal elements of <i>T</i> .
	elements of <i>I</i> .

#### tol

#### REAL for slagtf DOUBLE PRECISION for dlagtf

On entry, a relative tolerance used to indicate whether or not the matrix (T - lambda*I) is nearly singular. tol should normally be chose as approximately the largest relative error in the elements of *T*. For example, if the elements of *T* are correct to about 4 significant figures, then tol should be set to about  $5*10^{-4}$ . If tol is supplied as less than eps, where eps is the relative machine precision, then the value eps is used in place of tol.

#### **Output Parameters**

a	On exit, a is overwritten by the $n$ diagonal elements of the upper triangular matrix $U$ of the factorization of $T$ .
Ь	On exit, $b$ is overwritten by the $n$ -1 super-diagonal elements of the matrix $U$ of the factorization of $T$ .
С	On exit, $c$ is overwritten by the $n$ -1 sub-diagonal elements of the matrix $L$ of the factorization of $T$ .
d	<b>REAL</b> for slagtf <b>DOUBLE PRECISION</b> for dlagtf Array, dimension ( $n$ -2). On exit, $d$ is overwritten by the $n$ -2 second super-diagonal elements of the matrix $U$ of the factorization of $T$ .
in	INTEGER. Array, dimension $(n)$ . On exit, <i>in</i> contains details of the permutation matrix <i>P</i> . If an interchange occurred at the k-th step of the elimination, then <i>in</i> (k) = 1, otherwise <i>in</i> (k) = 0. The element <i>in</i> ( <i>n</i> ) returns the smallest positive integer <i>j</i> such that

 $abs(u(j,j)) \le norm((T - lambda*I)(j))*tol,$ where norm(A(j)) denotes the sum of the absolute values of the j-th row of the matrix A. If no such j exists then in(n) is returned as zero. If in(n) is returned as positive, then a diagonal element of U is small, indicating that (T - lambda * I) is singular or nearly singular.

info

#### INTEGER.

If info = 0, the execution is successful. If info = -k, the *k*th parameter had an illegal value.

## ?lagtm

Performs a matrix-matrix product of the form  $C = \alpha AB + \beta C$ , where A is a tridiagonal matrix, B and C are rectangular matrices, and  $\alpha$  and  $\beta$  are scalars, which may be 0, 1, or -1.

call slagtm(	trans, n	, nrhs,	alpha,	dl,	d,	du,	x,	ldx,	beta,	b,	ldb)
call dlagtm(	trans, n	, nrhs,	alpha,	dl,	d,	du,	х,	ldx,	beta,	b,	ldb)
call clagtm(	trans, n	, nrhs,	alpha,	dl,	d,	du,	х,	ldx,	beta,	b,	ldb)
call zlagtm(	trans, n	, nrhs,	alpha,	dl,	d,	du,	x,	ldx,	beta,	b,	ldb)

### **Discussion**

This routine performs a matrix-vector product of the form :

B := alpha * A * X + beta * B

where *A* is a tridiagonal matrix of order *n*, *B* and *X* are *n*-by-*nrhs* matrices, and *alpha* and *beta* are real scalars, each of which may be 0., 1., or -1.

trans	CHARACTER*1. Must be 'N' or 'T' or 'C'.
	Indicates the form of the equations:
	If $trans = 'N'$ , then $B := alpha * A * X + beta * B$
	(no transpose);
	If $trans = 'T'$ , then $B := alpha * A^T * X + beta * B$
	(transpose);
	If $trans = 'C'$ , then $B := alpha * A^H * X + beta * B$
	(conjugate transpose)
n	<b>INTEGER.</b> The order of the matrix $A \ (n \ge 0)$ .
nrhs	<b>INTEGER.</b> The number of right-hand sides, i.e., the number of columns in <i>X</i> and <i>B</i> ( $nrhs \ge 0$ ).

alpha, beta	REAL for slagtm/clagtm
	DOUBLE PRECISION for dlagtm/zlagtm
	The scalars $\alpha$ and $\beta$ . <u>alpha</u> must be 0., 1., or -1.;
	otherwise, it is assumed to be 0. <i>beta</i> must be 0., 1., or
	-1.; otherwise, it is assumed to be 1.
dl,d,du	REAL for slagtm
	DOUBLE PRECISION for dlagtm
	COMPLEX for clagtm
	COMPLEX*16 for zlagtm.
	Arrays: $dl(n - 1)$ , $d(n)$ , $du(n - 1)$ .
	The array $d1$ contains the $(n - 1)$ sub-diagonal elements
	of T.
	The array $d$ contains the $n$ diagonal elements of $T$ .
	The array $du$ contains the $(n - 1)$ super-diagonal
	elements of T.
x, b	REAL for slagtm
	DOUBLE PRECISION for dlagtm
	COMPLEX for clagtm
	COMPLEX*16 for zlagtm.
	Arrays:
	x(ldx, *) contains the <i>n</i> -by- <i>nrhs</i> matrix X. The
	second dimension of $x$ must be at least max(1, <i>nrhs</i> ).
	b(ldb,*) contains the <i>n</i> -by- <i>nrhs</i> matrix B. The
	second dimension of <b>b</b> must be at least $max(1, nrhs)$ .
1	
ldx	<b>INTEGER.</b> The leading dimension of the array $x$ ; $ldx \ge max(1, n)$ .
ldb	<b>INTEGER</b> . The leading dimension of the array <i>b</i> ;
	$ldb \geq max(1, n).$

b	Overwritten by the matrix expression
	B := alpha*A*X + beta*B

## ?lagts

Solves the system of equations  $(T-\lambda I)x = y$ or  $(T-\lambda I)^T x = y$ , where T is a general tridiagonal matrix and  $\lambda$  a scalar, using the LU factorization computed by <code>?lagtf</code>.

call slagts ( job, n, a, b, c, d, in, y, tol, info )
call dlagts ( job, n, a, b, c, d, in, y, tol, info )

### **Discussion**

This routine may be used to solve for *x* one of the systems of equations:

(T - lambda*I)*x = y or (T - lambda*I)'*x = y, where *T* is an *n*-by-*n* tridiagonal matrix, following the factorization of (T - lambda*I) as

T - lambda * I = P L U,

computed by the routine ?lagtf.

The choice of equation to be solved is controlled by the argument *job*, and in each case there is an option to perturb zero or very small diagonal elements of *U*, this option being intended for use in applications such as inverse iteration.

### **Input Parameters**

job

**INTEGER.** Specifies the job to be performed by **?lagts** as follows:

= 1: The equations (T - lambda*I)x = y are to be solved, but diagonal elements of *U* are not to be perturbed.

= -1: The equations (T - lambda*I)x = y are to be solved and, if overflow would otherwise occur, the diagonal elements of *U* are to be perturbed. See argument *tol* below.

	= 2: The equations $(T - lambda*I)' x = y$ are to be solved, but diagonal elements of U are not to be perturbed. = -2: The equations $(T - lambda*I)' x = y$ are to be
	solved and, if overflow would otherwise occur, the diagonal elements of <i>U</i> are to be perturbed. See argument <i>tol</i> below.
n	<b>INTEGER.</b> The order of the matrix $T (n \ge 0)$ .
a, b, c, d	REAL for slagts DOUBLE PRECISION for dlagts Arrays, dimension $a(n)$ , $b(n-1)$ , $c(n-1)$ , $d(n-2)$ : On entry, $a(*)$ must contain the diagonal elements of U as returned from ?lagtf. On entry, $b(*)$ must contain the first super-diagonal elements of $U$ as returned from ?lagtf. On entry, $c(*)$ must contain the sub-diagonal elements of $L$ as returned from ?lagtf. On entry, $d(*)$ must contain the second super-diagonal elements of $U$ as returned from ?lagtf.
in	INTEGER. Array, dimension ( <i>n</i> ). On entry, <i>in</i> (*) must contain details of the matrix <i>P</i> as returned from ?lagtf.
У	REAL for slagts DOUBLE PRECISION for dlagts Array, dimension ( <i>n</i> ). On entry, the right hand side vector <i>y</i> .
tol	REAL for slagtf DOUBLE PRECISION for dlagtf. On entry, with <i>job</i> < 0, <i>tol</i> should be the minimum perturbation to be made to very small diagonal elements of <i>U</i> . <i>tol</i> should normally be chosen as about <i>eps</i> *norm( <i>U</i> ), where <i>eps</i> is the relative machine

precision, but if *tol* is supplied as non-positive, then it is reset to eps*max(abs(u(i,j))). If job>0 then tol is not referenced.

### **Output Parameters**

Y	On exit, $y$ is overwritten by the solution vector $x$ .
tol	On exit, <i>tol</i> is changed as described in <i>Input</i> <i>Parameters</i> section above, only if <i>tol</i> is non-positive on entry. Otherwise <i>tol</i> is unchanged.
info	INTEGER. If $info = 0$ , the execution is successful. If $info = -i$ , the <i>i</i> th parameter had an illegal value. If $info = i > 0$ , overflow would occur when computing the <i>i</i> th element of the solution vector <i>x</i> . This can only occur when <i>job</i> is supplied as positive and either means that a diagonal element of <i>U</i> is very small, or that the elements of the right-hand side vector <i>y</i> are very large.

## ?lagv2

Computes the Generalized Schur factorization of a real 2-by-2 matrix pencil (A,B) where B is upper triangular.

#### **Discussion**

This routine computes the Generalized Schur factorization of a real 2-by-2 matrix pencil (*A*,*B*) where *B* is upper triangular. The routine computes orthogonal (rotation) matrices given by *cs1*, *sn1* and *csr*, *snr* such that:

1) if the pencil (A,B) has two real eigenvalues (include 0/0 or 1/0 types), then

$$\begin{bmatrix} a_{11} & a_{12} \\ 0 & a_{22} \end{bmatrix} = \begin{bmatrix} csl & snl \\ -snl & csl \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} csr & -snr \\ snr & csr \end{bmatrix}$$
$$\begin{bmatrix} b_{11} & b_{12} \\ 0 & b_{22} \end{bmatrix} = \begin{bmatrix} csl & snl \\ -snl & csl \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} \\ 0 & b_{22} \end{bmatrix} \begin{bmatrix} csr & -snr \\ snr & csr \end{bmatrix}$$

2) if the pencil (A, B) has a pair of complex conjugate eigenvalues, then

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} csl & snl \\ -snl & csl \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} csr & -snr \\ snr & csr \end{bmatrix}$$
$$\begin{bmatrix} b_{11} & 0 \\ 0 & b_{22} \end{bmatrix} = \begin{bmatrix} csl & snl \\ -snl & csl \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} \\ 0 & b_{22} \end{bmatrix} \begin{bmatrix} csr & -snr \\ snr & csr \end{bmatrix}$$
where  $b_{11} \ge b_{22} > 0$ .

### **Input Parameters**

a, b	REAL for slagv2 DOUBLE PRECISION for dlagv2 Arrays: a(lda,2) contains the 2-by-2 matrix A; b(ldb,2) contains the upper triangular 2-by-2 matrix B.
lda	<b>INTEGER.</b> The leading dimension of the array $a$ ; $1da \ge 2$ .
ldb	<b>INTEGER.</b> The leading dimension of the array $b$ ; <i>ldb</i> $\geq 2$ .

a	On exit, a is overwritten by the "A-part" of the generalized Schur form.
b	On exit, <i>b</i> is overwritten by the " <i>B</i> -part" of the generalized Schur form.
alphar,alphai,	
beta	REAL for slagv2 DOUBLE PRECISION for dlagv2. Arrays, dimension (2) each.
	(alphar(k) + i * alphai(k))/beta(k) are the eigenvalues of the pencil $(A,B)$ , k=1,2 and $i = $ sqrt(-1). Note that $beta(k)$ may be zero.
csl, snl	REAL for slagv2 DOUBLE PRECISION for dlagv2 The cosine and sine of the left rotation matrix, respectively.
csr, snr	REAL for slagv2 DOUBLE PRECISION for dlagv2 The cosine and sine of the right rotation matrix, respectively.

## ?lahqr

Computes the eigenvalues and Schur factorization of an upper Hessenberg matrix, using the double-shift/single-shift QR algorithm.

### **Discussion**

This routine is an auxiliary routine called by ?hseqr to update the eigenvalues and Schur decomposition already computed by ?hseqr, by dealing with the Hessenberg submatrix in rows and columns *ilo* to *ihi*.

wantt	LOGICAL. If <i>wantt</i> = .TRUE., the full Schur form <i>T</i> is required; If <i>wantt</i> = .FALSE., eigenvalues only are required.
wantz	LOGICAL. If wantz = .TRUE., the matrix of Schur vectors Z is required; If wantz = .FALSE., Schur vectors are not required.
n	<b>INTEGER</b> . The order of the matrix $H(n \ge 0)$ .
ilo, ihi	<b>INTEGER.</b> It is assumed that <i>H</i> is already upper quasi-triangular in rows and columns $ihi+1:n$ , and that $H(ilo,ilo-1) = 0$ (unless $ilo = 1$ ). The routine ?lahqr works primarily

	with the Hessenberg submatrix in rows and columns <i>ilo</i> to <i>ihi</i> , but applies transformations to all of <i>H</i> if <i>wantt</i> = .TRUE Constraints: $1 \leq ilo \leq max(1, ihi); ihi \leq n.$
h, z	<pre>REAL for slahqr DOUBLE PRECISION for dlahqr COMPLEX for clahqr COMPLEX*16 for zlahqr. Arrays: h(ldh,*) contains the upper Hessenberg matrix H. The second dimension of h must be at least max(1, n).</pre>
	<pre>z(ldz,*) If wantz = .TRUE., then, on entry, z must contain the current matrix Z of transformations accumulated by ?hseqr. If wantz = .FALSE., then z is not referenced. The second dimension of z must be at least max(1, n).</pre>
ldh	<b>INTEGER.</b> The first dimension of $h$ ; at least max $(1, n)$ .
ldz	<b>INTEGER</b> . The first dimension of $z$ ; at least max $(1, n)$ .
iloz, ihiz	<b>INTEGER.</b> Specify the rows of Z to which transformations must be applied if $wantz = .TRUE$ $1 \le i loz \le i lo; ihi \le ihiz \le n.$

h	On exit, if <i>wantt</i> = .TRUE., <i>H</i> is upper quasi-triangular (upper triangular for complex flavors) in rows and columns <i>ilo:ihi</i> , with any 2-by-2 diagonal blocks in standard form. If <i>wantt</i> = .FALSE., the contents of <i>H</i> are unspecified on exit.
wr, wi	REAL for slahqr DOUBLE PRECISION for dlahqr Arrays, DIMENSION at least max (1, <i>n</i> ) each. Used with real flavors only. The real and imaginary parts, respectively, of the

	computed eigenvalues <i>ilo</i> to <i>ihi</i> are stored in the corresponding elements of <i>wr</i> and <i>wi</i> . If two eigenvalues are computed as a complex conjugate pair, they are stored in consecutive elements of <i>wr</i> and <i>wi</i> , say the i-th and (i+1)th, with <i>wi</i> (i) > 0 and <i>wi</i> (i+1) < 0. If <i>wantt</i> = . TRUE ., the eigenvalues are stored in the same order as on the diagonal of the Schur form returned in <i>H</i> , with <i>wr</i> (i) = <i>H</i> (i,i), and, if <i>H</i> (i:i+1, i:i+1) is a 2-by-2 diagonal block, <i>wi</i> (i) = sqrt( <i>H</i> (i+1,i)* <i>H</i> (i,i+1)) and <i>wi</i> (i+1) = - <i>wi</i> (i).
W	COMPLEX for clahqr COMPLEX*16 for zlahqr. Array, DIMENSION at least max (1, <i>n</i> ). Used with complex flavors only. The computed eigenvalues <i>ilo</i> to <i>ihi</i> are stored in the corresponding elements of <i>w</i> . If <i>wantt</i> = . TRUE ., the eigenvalues are stored in the same order as on the diagonal of the Schur form returned in <i>H</i> , with <i>w</i> (i) = <i>H</i> (i,i).
Ζ	If $wantz = .$ TRUE., then, on exit z has been updated; transformations are applied only to the submatrix Z(iloz:ihiz, ilo:ihi).
info	<pre>INTEGER. If info = 0, the execution is successful. If info = i &gt; 0, ?lahqr failed to compute all the eigenvalues ilo to ihi in a total of 30*(ihi-ilo+1) iterations; elements i+1:ihi of wr and wi (for slahqr/dlahqr) or w (for clahqr/zlahqr) contain those eigenvalues which have been successfully computed.</pre>

## ?lahrd

Reduces the first nb columns of a general rectangular matrix A so that elements below the k-th subdiagonal are zero, and returns auxiliary matrices which are needed to apply the transformation to the unreduced part of A.

call	slahrd	(	n,	k,	nb,	a,	lda,	tau,	t,	ldt,	Y'	ldy	)
call	dlahrd	(	n,	k,	nb,	a,	lda,	tau,	t,	ldt,	Y'	ldy	)
call	clahrd	(	n,	k,	nb,	a,	lda,	tau,	t,	ldt,	Y'	ldy	)
call	zlahrd	(	n,	k,	nb,	a,	lda,	tau,	t,	ldt,	Y'	ldy	)

### **Discussion**

The routine reduces the first *nb* columns of a real/complex general *n*-by-(*n*-*k*+1) matrix *A* so that elements below the *k*-th subdiagonal are zero. The reduction is performed by an orthogonal/unitary similarity transformation Q' A Q. The routine returns the matrices *V* and *T* which determine *Q* as a block reflector *I* - *VTV'*, and also the matrix *Y* = *A VT*.

The matrix Q is represented as products of *nb* elementary reflectors:  $Q = H(1) H(2) \dots H(nb)$ 

Each H(i) has the form

 $H(\mathbf{i}) = I - tau * v * v'$ 

where *tau* is a real/complex scalar, and v is a real/complex vector.

This is an auxiliary routine called by ?gehrd.

n	<b>INTEGER.</b> The order of the matrix $A (n \ge 0)$ .
k	<b>INTEGER</b> . The offset for the reduction. Elements below the $k$ -th subdiagonal in the first $nb$ columns are reduced
	to zero.
nb	<b>INTEGER</b> . The number of columns to be reduced.

а	REAL for slahrd DOUBLE PRECISION for dlahrd COMPLEX for clahrd COMPLEX*16 for zlahrd.
	Array $a(lda, n-k+1)$ contains the n-by- $(n-k+1)$ general matrix A to be reduced.
lda	<b>INTEGER.</b> The first dimension of $a$ ; at least max $(1, n)$ .
ldt	<b>INTEGER.</b> The first dimension of the output array $t$ ; must be at least max $(1, nb)$ .
ldy	<b>INTEGER.</b> The first dimension of the output array $y$ ; must be at least max $(1, n)$ .
Output Parame	ters
a	On exit, the elements on and above the $k$ -th subdiagonal in the first $nb$ columns are overwritten with the corresponding elements of the reduced matrix; the elements below the $k$ -th subdiagonal, with the array tau, represent the matrix $Q$ as a product of elementary reflectors. The other columns of $a$ are unchanged. See <i>Application Notes</i> below.
tau	REAL for slahrd

DOUBLE PRECISION for dlahrd COMPLEX for clahrd COMPLEX*16 for zlahrd.

> Array, DIMENSION (*nb*). Contains scalar factors of the elementary reflectors.

t, y

REAL for slahrd DOUBLE PRECISION for dlahrd COMPLEX for clahrd COMPLEX*16 for zlahrd.

Arrays, dimension t(ldt, nb), y(ldy, nb). The array t contains upper triangular matrix T. The array y contains the *n*-by-*nb* matrix Y.

### **Application Notes**

For the elementary reflector H(i),

v(1:i+k-1) = 0, v(i+k) = 1; v(i+k+1:n) is stored on exit in a(i+k+1:n, i)and *tau* is stored in *tau*(i).

The elements of the vectors v together form the (n-k+1)-by-nb matrix V which is needed, with T and Y, to apply the transformation to the unreduced part of the matrix, using an update of the form:

$$A := (I - V T V') * (A - Y V')$$

The contents of A on exit are illustrated by the following example with n = 7, k = 3 and nb = 2:

$$\begin{bmatrix} a & h & a & a & a \\ a & h & a & a & a \\ a & h & a & a & a \\ h & h & a & a & a \\ v_1 & h & a & a & a \\ v_1 & v_2 & a & a & a \\ v_1 & v_2 & a & a & a \end{bmatrix}$$

where *a* denotes an element of the original matrix *A*, *h* denotes a modified element of the upper Hessenberg matrix *H*, and  $v_i$  denotes an element of the vector defining *H*(i).

## ?laic1

Applies one step of incremental condition estimation.

call slaic1 ( job, j, x, sest, w, gamma, sestpr, s, c )
call dlaic1 ( job, j, x, sest, w, gamma, sestpr, s, c )
call claic1 ( job, j, x, sest, w, gamma, sestpr, s, c )
call zlaic1 ( job, j, x, sest, w, gamma, sestpr, s, c )

### **Discussion**

The routine **?laic1** applies one step of incremental condition estimation in its simplest version.

Let x,  $||x||_2 = 1$  (where  $||a||_2$  denotes the 2-norm of a), be an approximate singular vector of an j-by-j lower triangular matrix L, such that

 $||L^*x||_2 = sest$ 

Then ?laic1 computes *sestpr*, *s*, *c* such that the vector

$$xhat = \begin{bmatrix} s * x \\ c \end{bmatrix}$$

is an approximate singular vector of

$$Lhat = \begin{bmatrix} L & 0 \\ w' & gamma \end{bmatrix}$$

in the sense that

 $||Lhat *xhat||_2 = sestpr.$ 

Depending on *job*, an estimate for the largest or smallest singular value is computed.

Note that [sc]' and  $sestpr^2$  is an eigenpair of the system (for slaicl/claic)

diag(sest*sest, 0) + [alpha gamma] * 
$$\begin{bmatrix} alpha \\ gamma \end{bmatrix}$$
  
where  $alpha = x' *w$ ;  
or of the system (for claic1/zlaic)  
diag(sest*sest, 0) + [alpha gamma] *  $\begin{bmatrix} \operatorname{conjg}(alpha) \\ \operatorname{conjg}(gamma) \end{bmatrix}$   
where  $alpha = \operatorname{conig}(x)' *w$ 

where alpha = conjg(x)' * w.

job	<pre>INTEGER. If job =1, an estimate for the largest singular value is computed; If job =2, an estimate for the smallest singular value is computed;</pre>
j	INTEGER. Length of $x$ and $w$ .
x, w	REAL for slaic1 DOUBLE PRECISION for dlaic1 COMPLEX for claic1 COMPLEX*16 for zlaic1. Arrays, dimension ( <i>j</i> ) each. Contain vectors <i>x</i> and <i>w</i> , respectively.
sest	REAL for slaic1/claic1; DOUBLE PRECISION for dlaic1/zlaic1. Estimated singular value of <i>j</i> -by- <i>j</i> matrix <i>L</i> .
gamma	REAL for slaic1 DOUBLE PRECISION for dlaic1 COMPLEX for claic1 COMPLEX*16 for zlaic1. The diagonal element <i>gamma</i> .

sestpr	REAL for slaic1/claic1; DOUBLE PRECISION for dlaic1/zlaic1. Estimated singular value of $(j+1)$ -by- $(j+1)$ matrix <i>Lhat</i> .
s, C	REAL for slaic1 DOUBLE PRECISION for dlaic1 COMPLEX for claic1 COMPLEX*16 for zlaic1. Sine and cosine needed in forming <i>xhat</i> .

## ?laln2

Solves a 1-by-1 or 2-by-2 linear system of equations of the specified form.

```
call slaln2( ltrans, na, nw, smin, ca, a, lda, d1, d2,
            b, ldb, wr, wi, x, ldx, scale, xnorm, info )
call dlaln2( ltrans, na, nw, smin, ca, a, lda, d1, d2,
            b, ldb, wr, wi, x, ldx, scale, xnorm, info )
```

#### **Discussion**

The routine solves a system of the form

(ca A - w D) X = s B or (ca A' - w D) X = s Bwith possible scaling (s) and perturbation of A (A' means A-transpose.)

A is an *na*-by-*na* real matrix, *ca* is a real scalar, *D* is an *na*-by-*na* real diagonal matrix, *w* is a real or complex value, and *X* and *B* are *na*-by-1 matrices: real if *w* is real, complex if *w* is complex. The parameter *na* may be 1 or 2.

If *w* is complex, *X* and *B* are represented as *na*-by-2 matrices, the first column of each being the real part and the second being the imaginary part.

The routine computes the scaling factor  $s (\leq 1)$  so chosen that X can be computed without overflow. X is further scaled if necessary to assure that norm(*ca* A - w D)*norm(X) is less than overflow.

If both singular values of (ca A - w D) are less than smin, smin * I (where I stands for identity) will be used instead of (ca A - w D). If only one singular value is less than smin, one element of (ca A - w D) will be perturbed enough to make the smallest singular value roughly smin. If both singular values are at least smin, (ca A - w D) will not be perturbed. In any case, the perturbation will be at most some small multiple of

 $\max(smin, ulp * norm(ca A - w D)).$ 

The singular values are computed by infinity-norm approximations, and thus will only be correct to a factor of 2 or so.



**NOTE.** All input quantities are assumed to be smaller than overflow by a reasonable factor (see bignum).

trans	LOGICAL.
	If trans = .TRUE., A- transpose will be used. If trans = .FALSE., A will be used (not transposed.)
na	<b>INTEGER</b> . The size of the matrix <i>A</i> . May only be 1 or 2.
<i>1</i> 2W	<b>INTEGER.</b> This parameter must be 1 if <i>w</i> is real, and 2 if <i>w</i> is complex. May only be 1 or 2.
smin	REAL for slaln2 DOUBLE PRECISION for dlaln2. The desired lower bound on the singular values of <i>A</i> . This should be a safe distance away from underflow or overflow, for example, between ( <i>underflow/machine_precision</i> ) and ( <i>machine_precision</i> * overflow). (See bignum and ulp).
Ca	REAL for slaln2 DOUBLE PRECISION for dlaln2. The coefficient by which <i>A</i> is multiplied.
a	REAL for slaln2 DOUBLE PRECISION for dlaln2. Array, DIMENSION ( <i>lda,na</i> ). The <i>na</i> -by- <i>na</i> matrix A.
lda	<b>INTEGER.</b> The leading dimension of <b>a</b> . Must be at least <i>na</i> .
d1, d2	<b>REAL for slaln2</b> <b>DOUBLE PRECISION for dlaln2.</b> The (1,1) and (2,2) elements in the diagonal matrix $D$ , respectively. $d2$ is not used if $nw = 1$ .

b	REAL for slaln2
	DOUBLE PRECISION for dlaln2.
	Array, DIMENSION ( <i>ldb,nw</i> ). The <i>na</i> -by- <i>nw</i> matrix <i>B</i> (right-hand side). If $nw = 2$ ( <i>w</i> is complex), column 1 contains the real part of <i>B</i> and column 2 contains the imaginary part.
ldb	INTEGER. The leading dimension of <i>b</i> . Must be at least
	na.
wr, wi	REAL for slaln2
	DOUBLE PRECISION for dlaln2.
	The real and imaginary part of the scalar w, respectively. wi is not used if $nw = 1$ .
ldx	<b>INTEGER.</b> The leading dimension of the output array $x$ . Must be at least $na$ .

x	<b>REAL</b> for slaln2 <b>DOUBLE PRECISION</b> for dlaln2. Array, <b>DIMENSION</b> ( <i>ldx,nw</i> ). The <i>na</i> -by- <i>nw</i> matrix X (unknowns), as computed by the routine. If $nw = 2$ ( <i>w</i> is complex), on exit, column 1 will contain the real part of X and column 2 will contain the imaginary part.
scale	<b>REAL</b> for slaln2 <b>DOUBLE PRECISION</b> for dlaln2. The scale factor that <i>B</i> must be multiplied by to insure that overflow does not occur when computing <i>X</i> . Thus $(ca A - w D) X$ will be <i>scale</i> * <i>B</i> , not <i>B</i> (ignoring perturbations of <i>A</i> .) It will be at most 1.
xnorm	REAL for slaln2 DOUBLE PRECISION for dlaln2. The infinity-norm of X, when X is regarded as an <i>na</i> -by- <i>nw</i> real matrix.
info	<b>INTEGER</b> . An error flag. It will be zero if no error occurs, a negative number if an argument is in error, or a positive

number if (ca A - w D) had to be perturbed. The possible values are: If *info* = 0: no error occurred, and (ca A - w D) did not have to be perturbed. If *info* = 1: (ca A - w D) had to be perturbed to make its smallest (or only) singular value greater than *smin*.



**NOTE.** *In the interests of speed, this routine does not check the inputs for errors.* 

## ?lals0

Applies back multiplying factors in solving the least squares problem using divide and conquer SVD approach. Used by ?gelsd.

- call slals0( icompq, nl, nr, sqre, nrhs, b, ldb, bx, ldbx, perm, givptr, givcol, ldgcol, givnum, ldgnum, poles, difl, difr, z, k, c, s, work, info )
- call dlals0( icompq, nl, nr, sqre, nrhs, b, ldb, bx, ldbx, perm, givptr, givcol, ldgcol, givnum, ldgnum, poles, difl, difr, z, k, c, s, work, info )
- call clals0 ( icompq, nl, nr, sqre, nrhs, b, ldb, bx, ldbx, perm, givptr, givcol, ldgcol, givnum, ldgnum, poles, difl, difr, z, k, c, s, rwork, info )
- call zlals0 ( icompq, nl, nr, sqre, nrhs, b, ldb, bx, ldbx, perm, givptr, givcol, ldgcol, givnum, ldgnum, poles, difl, difr, z, k, c, s, rwork, info )

### Discussion

The routine applies back the multiplying factors of either the left or right singular vector matrix of a diagonal matrix appended by a row to the right hand side matrix *B* in solving the least squares problem using the divide-and-conquer SVD approach.

For the left singular vector matrix, three types of orthogonal matrices are involved:

(1L) Givens rotations: the number of such rotations is *givptr*; the pairs of columns/rows they were applied to are stored in *givcol*; and the *c*- and *s*-values of these rotations are stored in *givnum*.

(2L) Permutation. The (nl+1)-st row of *B* is to be moved to the first row, and for j=2:n, *perm*(j)-th row of *B* is to be moved to the j-th row.

(3L) The left singular vector matrix of the remaining matrix.

For the right singular vector matrix, four types of orthogonal matrices are involved:

(1R) The right singular vector matrix of the remaining matrix.

(2R) If *sqre* = 1, one extra Givens rotation to generate the right null space.

(3R) The inverse transformation of (2L).

(4R) The inverse transformation of (1L).

icompq	<pre>INTEGER. Specifies whether singular vectors are to be computed in factored form: If icompq = 0: Left singular vector matrix. If icompq = 1: Right singular vector matrix.</pre>
nl	<b>INTEGER</b> . The row dimension of the upper block. $nl \ge 1$ .
nr	<b>INTEGER</b> . The row dimension of the lower block. $nr \ge 1$ .
sqre	INTEGER. If sqre = 0: the lower block is an <i>nr</i> -by- <i>nr</i> square matrix. If sqre = 1: the lower block is an <i>nr</i> -by-( <i>nr</i> +1)

	rectangular matrix. The bidiagonal matrix has row dimension $n = nl + nr + 1$ , and column dimension $m = n + sqre$ .
nrhs	<b>INTEGER.</b> The number of columns of <i>b</i> and <i>bx</i> . Must be at least 1.
b	REAL for slals0 DOUBLE PRECISION for dlals0 COMPLEX for clals0 COMPLEX*16 for zlals0. Array, DIMENSION ( <i>ldb</i> , <i>nrhs</i> ). Contains the right hand sides of the least squares problem in rows 1 through <i>m</i> .
ldb	<b>INTEGER.</b> The leading dimension of <b>b</b> . Must be at least $\max(1, \max(m, n))$ .
bx	REAL for slals0 DOUBLE PRECISION for dlals0 COMPLEX for clals0 COMPLEX*16 for zlals0. Workspace array, DIMENSION ( <i>ldbx</i> , <i>nrhs</i> ).
ldbx	INTEGER. The leading dimension of <i>bx</i> .
perm	<b>INTEGER.</b> Array, <b>DIMENSION</b> ( <i>n</i> ). The permutations (from deflation and sorting) applied to the two blocks.
givptr	<b>INTEGER.</b> The number of Givens rotations which took place in this subproblem.
givcol	<b>INTEGER.</b> Array, <b>DIMENSION</b> ( <i>ldgcol</i> , 2). Each pair of numbers indicates a pair of rows/columns involved in a Givens rotation.
ldgcol	<b>INTEGER.</b> The leading dimension of <i>givcol</i> , must be at least $n$ .

givnum	REAL for slals0 /clals0 DOUBLE PRECISION for dlals0/zlals0 Array, DIMENSION ( <i>ldgnum</i> , 2 ). Each number indicates the c or s value used in the corresponding Givens rotation.
ldgnum	<b>INTEGER</b> . The leading dimension of arrays <i>difr</i> , <i>poles</i> and <i>givnum</i> , must be at least <i>k</i> .
poles	REAL for slals0 /clals0 DOUBLE PRECISION for dlals0/zlals0 Array, DIMENSION ( <i>ldgnum</i> , 2 ). On entry, <i>poles</i> (1: <i>k</i> , 1) contains the new singular values obtained from solving the secular equation, and <i>poles</i> (1: <i>k</i> , 2) is an array containing the poles in the secular equation.
difl	REAL for slals0 /clals0 DOUBLE PRECISION for dlals0/zlals0 Array, DIMENSION ( k ). On entry, difl(i) is the distance between <i>i</i> -th updated (undeflated) singular value and the <i>i</i> -th (undeflated) old singular value.
difr	REAL for slals0 /clals0 DOUBLE PRECISION for dlals0/zlals0 Array, DIMENSION ( <i>ldgnum</i> , 2 ). On entry, <i>difr(i</i> , 1) contains the distances between <i>i</i> -th updated (undeflated) singular value and the <i>i</i> +1-th (undeflated) old singular value. And <i>difr(i</i> , 2) is the normalizing factor for the <i>i</i> -th right singular vector.
Ζ	REAL for slals0 /clals0 DOUBLE PRECISION for dlals0/zlals0 Array, DIMENSION (k). Contains the components of the deflation-adjusted updating row vector.
k	<b>INTEGER.</b> Contains the dimension of the non-deflated matrix. This is the order of the related secular equation. $1 \leq n \leq n$ .

С	REAL for slals0 /clals0
	DOUBLE PRECISION for dlals0/zlals0
	Contains garbage if $sqre = 0$ and the <i>c</i> value of a Givens rotation related to the right null space if $sqre = 1$ .
S	REAL for slals0 /clals0
	DOUBLE PRECISION for dlals0/zlals0
	Contains garbage if <i>sqre</i> =0 and the <i>s</i> value of a Givens
	rotation related to the right null space if $sqre = 1$ .
work	REAL for slals0
	DOUBLE PRECISION for dlals0
	Workspace array, <b>DIMENSION</b> ( <i>k</i> ). Used with real
	flavors only.
rwork	REAL for clals0
	DOUBLE PRECISION for zlals0
	Workspace array, DIMENSION ( $k*(1+nrhs) + 2*nrhs$ ).
	Used with complex flavors only.

b	On exit, contains the solution $X$ in rows 1 through $n$ .
info	INTEGER. If $info = 0$ : successful exit. If $info = -i < 0$ , the <i>i</i> -th argument had an illegal value.

## ?lalsa

Computes the SVD of the coefficient matrix in compact form. Used by ?gelsd.

<pre>call slalsa ( icompq, smlsiz, n, nrhs, b, ldb, bx, ldbx,</pre>
<pre>call dlalsa ( icompq, smlsiz, n, nrhs, b, ldb, bx, ldbx,</pre>
<pre>call clalsa ( icompq, smlsiz, n, nrhs, b, ldb, bx, ldbx,</pre>
<pre>call zlalsa ( icompq, smlsiz, n, nrhs, b, ldb, bx, ldbx, u, ldu, vt, k, difl, difr, z, poles, givptr, givcol, ldgcol, perm, givnum, c, s, rwork, iwork, info )</pre>

### Discussion

The routine is an itermediate step in solving the least squares problem by computing the SVD of the coefficient matrix in compact form. The singular vectors are computed as products of simple orthorgonal matrices.

If *icompq* = 0, **?lalsa** applies the inverse of the left singular vector matrix of an upper bidiagonal matrix to the right hand side; and if

icompq = 1, the routine applies the right singular vector matrix to the right hand side. The singular vector matrices were generated in the compact form by ?lalsa.

icompq	<b>INTEGER.</b> Specifies whether the left or the right singular vector matrix is involved. If <i>icompq</i> = 0: left singular vector matrix is used If <i>icompq</i> = 1: right singular vector matrix is used.
smlsiz	<b>INTEGER.</b> The maximum size of the subproblems at the bottom of the computation tree.
п	<b>INTEGER.</b> The row and column dimensions of the upper bidiagonal matrix.
nrhs	<b>INTEGER.</b> The number of columns of <i>b</i> and <i>bx</i> . Must be at least 1.
b	REAL for slalsa DOUBLE PRECISION for dlalsa COMPLEX for clalsa COMPLEX*16 for zlalsa Array, DIMENSION ( <i>ldb</i> , <i>nrhs</i> ). Contains the right hand sides of the least squares problem in rows 1 through <i>m</i> .
ldb	<b>INTEGER.</b> The leading dimension of $b$ in the calling subprogram. Must be at least max $(1, \max(m, n))$ .
ldbx	<b>INTEGER</b> . The leading dimension of the output array <i>bx</i> .
u	REAL for slalsa/clalsa DOUBLE PRECISION for dlalsa/zlalsa Array, DIMENSION ( <i>ldu</i> , <i>smlsiz</i> ). On entry, <i>u</i> contains the left singular vector matrices of all subproblems at the bottom level.
ldu	<b>INTEGER</b> , $ldu \ge n$ . The leading dimension of arrays $u$ , $vt$ , $difl$ , $difr$ , $poles$ , $givnum$ , and $z$ .
vt	REAL for slalsa/clalsa DOUBLE PRECISION for dlalsa/zlalsa Array, DIMENSION ( <i>ldu</i> , <i>smlsiz</i> +1). On entry, contains the right singular vector matrices of all subproblems at the bottom level.
k	INTEGER array, DIMENSION ( n ).

difl	REAL for slalsa/clalsa DOUBLE PRECISION for dlalsa/zlalsa Array, DIMENSION ( <i>ldu</i> , <i>nlvl</i> ), where <i>nlvl</i> = int(log ₂ ( <i>n/(smlsiz</i> +1))) + 1.
difr	REAL for slalsa/clalsa DOUBLE PRECISION for dlalsa/zlalsa Array, DIMENSION ( <i>ldu</i> , 2* <i>nlv1</i> ). On entry, <i>dif1</i> (*, <i>i</i> ) and <i>difr</i> (*, 2 <i>i</i> -1) record distances between singular values on the <i>i</i> -th level and singular values on the ( <i>i</i> -1)-th level, and <i>difr</i> (*, 2 <i>i</i> ) record the normalizing factors of the right singular vectors matrices of subproblems on <i>i</i> -th level.
Ζ	REAL for slalsa/clalsa DOUBLE PRECISION for dlalsa/zlalsa Array, DIMENSION ( <i>ldu</i> , <i>nlv1</i> ). On entry, <i>z</i> (1, <i>i</i> ) contains the components of the deflation- adjusted updating the row vector for subproblems on the <i>i</i> -th level.
poles	REAL for slalsa/clalsa DOUBLE PRECISION for dlalsa/zlalsa Array, DIMENSION ( <i>ldu</i> , 2* <i>nlv1</i> ). On entry, <i>poles</i> (*, 2 <i>i</i> -1: 2 <i>i</i> ) contains the new and old singular values involved in the secular equations on the <i>i</i> -th level.
givptr	<pre>INTEGER. Array, DIMENSION ( n ). On entry, givptr( i ) records the number of Givens rotations performed on the <i>i</i>-th problem on the computation tree.</pre>
givcol	INTEGER. Array, DIMENSION ( <i>ldgcol</i> , 2* <i>nlvl</i> ). On entry, for each <i>i</i> , <i>givcol</i> (*, 2 <i>i</i> -1: 2 <i>i</i> ) records the locations of Givens rotations performed on the <i>i</i> -th level on the computation tree.

ldgcol	<b>INTEGER</b> , $ldgcol \ge n$ . The leading dimension of arrays <i>givcol</i> and <i>perm</i> .
perm	<pre>INTEGER. Array, DIMENSION ( ldgcol, nlvl ). On entry, perm(*, i) records permutations done on the i-th level of the computation tree.</pre>
givnum	REAL for slalsa/clalsa DOUBLE PRECISION for dlalsa/zlalsa Array, DIMENSION ( <i>ldu</i> , 2* <i>nlv1</i> ). On entry, <i>givnum</i> (*, 2 <i>i</i> -1 : 2 <i>i</i> ) records the <i>c</i> and <i>s</i> values of Givens rotations performed on the <i>i</i> -th level on the computation tree.
С	<b>REAL</b> for slalsa/clalsa DOUBLE PRECISION for dlalsa/zlalsa Array, DIMENSION ( $n$ ). On entry, if the <i>i</i> -th subproblem is not square, $c(i)$ contains the $c$ value of a Givens rotation related to the right null space of the <i>i</i> -th subproblem.
S	REAL for slalsa/clalsa DOUBLE PRECISION for dlalsa/zlalsa Array, DIMENSION ( $n$ ). On entry, if the <i>i</i> -th subproblem is not square, $s(i)$ contains the <i>s</i> -value of a Givens rotation related to the right null space of the <i>i</i> -th subproblem.
work	REAL for slalsa DOUBLE PRECISION for dlalsa Workspace array, DIMENSION at least (n). Used with real flavors only.
rwork	REAL for clalsa DOUBLE PRECISION for zlalsa Workspace array, DIMENSION at least max( n, ( <i>smlsz</i> +1)* <i>nrhs</i> *3). Used with complex flavors only.
iwork	<b>INTEGER</b> . Workspace array, <b>DIMENSION</b> at least (3 <i>n</i> ).

b	On exit, contains the solution <i>X</i> in rows 1 through <i>n</i> .
bx	REAL for slalsa DOUBLE PRECISION for dlalsa COMPLEX for clalsa COMPLEX*16 for zlalsa Array, DIMENSION ( <i>ldbx</i> , <i>nrhs</i> ). On exit, the result of applying the left or right singular vector matrix to <i>b</i> .
info	INTEGER. If $info = 0$ : successful exit If $info = -i < 0$ , the <i>i</i> -th argument had an illegal value.

## ?lalsd

Uses the singular value decomposition of A to solve the least squares problem.

call slalsd (	uplo, smlsiz, n, nrhs, d, e, b, ldb, rcond, rank, work, iwork, info )
call dlalsd (	uplo, smlsiz, n, nrhs, d, e, b, ldb, rcond, rank, work, iwork, info )
call clalsd (	uplo, smlsiz, n, nrhs, d, e, b, ldb, rcond, rank, work, rwork, iwork, info )
call zlalsd (	uplo, smlsiz, n, nrhs, d, e, b, ldb, rcond, rank, work, rwork, iwork, info )

### **Discussion**

The routine uses the singular value decomposition of A to solve the least squares problem of finding X to minimize the Euclidean norm of each column of AX-B, where A is *n*-by-*n* upper bidiagonal, and X and B are *n*-by-*nrhs*. The solution X overwrites B.

The singular values of *A* smaller than *rcond* times the largest singular value are treated as zero in solving the least squares problem; in this case a minimum norm solution is returned. The actual singular values are returned in *d* in ascending order.

This code makes very mild assumptions about floating point arithmetic. It will work on machines with a guard digit in add/subtract, or on those binary machines without guard digits which subtract like the Cray XMP, Cray YMP, Cray C 90, or Cray 2.

It could conceivably fail on hexadecimal or decimal machines without guard digits, but we know of none.

uplo	CHARACTER*1. If $uplo = 'U'$ , $d$ and $e$ define an upper bidiagonal matrix. If $uplo = 'L'$ , $d$ and $e$ define a lower bidiagonal matrix.
smlsiz	<b>INTEGER.</b> The maximum size of the subproblems at the bottom of the computation tree.
п	<b>INTEGER.</b> The dimension of the bidiagonal matrix. $n \ge 0$ .
nrhs	<b>INTEGER.</b> The number of columns of <i>B</i> . Must be at least 1.
d	REAL for slalsd/clalsd DOUBLE PRECISION for dlalsd/zlalsd Array, DIMENSION ( <i>n</i> ). On entry, <i>d</i> contains the main diagonal of the bidiagonal matrix.
е	REAL for slalsd/clalsd DOUBLE PRECISION for dlalsd/zlalsd Array, DIMENSION ( <i>n</i> -1). Contains the super-diagonal entries of the bidiagonal matrix. On exit, <i>e</i> is destroyed.
b	REAL for slalsd DOUBLE PRECISION for dlalsd COMPLEX for clalsd COMPLEX*16 for zlalsd

	Array, <b>DIMENSION</b> ( <i>1db,nrhs</i> ). On input, <i>b</i> contains the right hand sides of the least squares problem. On output, <i>b</i> contains the solution <i>X</i> .
ldb	<b>INTEGER</b> . The leading dimension of $b$ in the calling subprogram. Must be at least max $(1,n)$ .
rcond	<b>REAL</b> for slalsd/clalsd <b>DOUBLE PRECISION</b> for dlalsd/zlalsd The singular values of <i>A</i> less than or equal to <i>rcond</i> times the largest singular value are treated as zero in solving the least squares problem. If <i>rcond</i> is negative, machine precision is used instead. For example, if diag( <i>S</i> )* <i>X</i> = <i>B</i> were the least squares problem, where diag( <i>S</i> ) is a diagonal matrix of singular values, the solution would be $X(i) = B(i) / S(i)$ if $S(i)$ is greater than <i>rcond</i> *max( <i>S</i> ), and $X(i) = 0$ if $S(i)$ is less than or equal to <i>rcond</i> *max( <i>S</i> ).
rank	<b>INTEGER</b> . The number of singular values of <i>A</i> greater than <i>rcond</i> times the largest singular value.
work	REAL for slalsd DOUBLE PRECISION for dlalsd COMPLEX for clalsd COMPLEX*16 for zlalsd Workspace array. DIMENSION for real flavors at least $(9n+2n*smlsiz+8n*nlvl+n*nrhs+(smlsiz+1)^2)$ , where $nlvl = max(0, int(log_2(n/(smlsiz+1))) + 1)$ . DIMENSION for complex flavors at least $(n*nrhs)$ .
rwork	REAL for clalsd DOUBLE PRECISION for zlalsd Workspace array, used with complex flavors only. DIMENSION at least $(9n + 2n*smlsiz + 8n*nlv1 + 3*mlsiz*nrhs + (smlsiz+1)^2)$ , where $nlv1 = max(0, int(log_2(min(m,n)/(smlsiz+1))) + 1)$ .

*iwork* INTEGER. Workspace array, DIMENSION at least (3n*nlvl + 11n).

### **Output Parameters**

d	On exit, if $info = 0$ , <i>d</i> contains singular values of the bidiagonal matrix.
b	On exit, $b$ contains the solution $X$ .
info	INTEGER. If $info = 0$ : successful exit. If $info = -i < 0$ , the <i>i</i> -th argument had an illegal value. If $info > 0$ : The algorithm failed to compute a singular value while working on the submatrix lying in rows and columns $info/(n+1)$ through mod( $info,n+1$ ).

# ?lamch

Determines machine parameters for floating-point arithmetic.

val = slamch ( cmach )
val = dlamch ( cmach )

### **Discussion**

The function **?lamch** determines single precision and double precision machine parameters.

### **Input Parameters**

cmach CHARACTER*1. Specifies the value to be returned by
?lamch:
= 'E' or 'e', val = eps
= 'S' or 's, val = sfmin
= 'B' or 'b', val = base
= 'P' or 'p', val = eps*base

= 'N' or 'n', val = t = 'R' or 'r', val = rnd = 'M' or 'm', val = emin = 'U' or 'u', val = rmin = '*L*' or '*1*', *val* = *emax* = '0' or 'o', val = rmax where *eps* = relative machine precision; *sfmin* = safe minimum, such that 1/*sfmin* does not overflow: *base* = base of the machine; prec = eps*base; = number of (base) digits in the mantissa; t rnd = 1.0 when rounding occurs in addition, 0.0 otherwise; *emin* = minimum exponent before (gradual) underflow; rmin = underflow_threshold - base**(emin-1); *emax* = largest exponent before overflow; rmax = overflow threshold - (base**emax)*(1-eps).

### **Output Parameters**

val

REAL for slamch DOUBLE PRECISION for dlamch Value returned by the function.

### ?lamc1

Called from ?lamc2. Determines machine parameters given by beta, t, rnd, ieee1.

call slamc1 ( beta, t, rnd, ieee1 )
call dlamc1 ( beta, t, rnd, ieee1 )

### **Discussion**

The routine ?lamc1 determines machine parameters given by *beta*, *t*, *rnd*, *ieee1*.

### **Output Parameters**

beta	<b>INTEGER</b> . The base of the machine.
t	<b>INTEGER.</b> The number of ( <i>beta</i> ) digits in the mantissa.
rnd	LOGICAL. Specifies whether proper rounding ( <i>rnd</i> = .TRUE.) or chopping ( <i>rnd</i> = .FALSE.) occurs in addition. This may not be a reliable guide to the way in which the machine performs its arithmetic.
ieeel	LOGICAL. Specifies whether rounding appears to be done in the <i>ieee</i> 'round to nearest' style.

# ?lamc2

Used by ?lamch. Determines machine parameters specified in its arguments list.

call slamc2 ( beta, t, rnd, eps, emin, rmin, emax, rmax )
call dlamc2 ( beta, t, rnd, eps, emin, rmin, emax, rmax )

### **Discussion**

The routine **?lamc2** determines machine parameters specified in its arguments list.

### **Output Parameters**

beta	<b>INTEGER</b> . The base of the machine.
t	<b>INTEGER</b> . The number of ( <i>beta</i> ) digits in the mantissa.

rnd	LOGICAL. Specifies whether proper rounding ( <i>rnd</i> = .TRUE.) or chopping ( <i>rnd</i> = .FALSE.) occurs in addition. This may not be a reliable guide to the way in which the machine performs its arithmetic.
eps	REAL for slamc2 DOUBLE PRECISION for dlamc2 The smallest positive number such that fl(1.0 - eps) < 1.0, where fl denotes the computed value.
emin	<b>INTEGER.</b> The minimum exponent before (gradual) underflow occurs.
rmin	REAL for slamc2 DOUBLE PRECISION for dlamc2 The smallest normalized number for the machine, given by base ^{emin-1} , where base is the floating point value of beta.
emax	<b>INTEGER</b> . The maximum exponent before overflow occurs.
rmax	REAL for slamc2 DOUBLE PRECISION for dlamc2 The largest positive number for the machine, given by base ^{emax (1 - eps)} , where base is the floating point value of beta.

# ?lamc3

Called from ?lamc1-?lamc5. Intended to force a and b to be stored prior to doing the addition of a and b.

```
val = slamc3 (a, b)
val = dlamc3 (a, b)
```

### Discussion

The routine is intended to force a and b to be stored prior to doing the addition of a and b, for use in situations where optimizers might hold one of these in a register.

### **Input Parameters**

a,b REAL for slamc3 DOUBLE PRECISION for dlamc3 The values a and b.

### **Output Parameters**

val	REAL for slamc3
	DOUBLE PRECISION for dlamc3
	The result of adding values <i>a</i> and <i>b</i> .

### ?lamc4

*This is a service routine for* **?lamc2**.

call slamc4 (emin, start, base)
call dlamc4 (emin, start, base)

### **Discussion**

This is a service routine for **?lamc2**.

start	REAL for slamc4
	DOUBLE PRECISION for dlamc4
	The starting point for determining <i>emin</i> .
base	<b>INTEGER.</b> The base of the machine.

emin

**INTEGER.** The minimum exponent before (gradual) underflow, computed by setting *a* = *start* and dividing by *base* until the previous *a* can not be recovered.

### ?lamc5

Called from ?lamc2. Attempts to compute the largest machine floating-point number, without overflow.

call slamc5 ( beta, p, emin, ieee, emax, rmax )
call dlamc5 ( beta, p, emin, ieee, emax, rmax )

### **Discussion**

The routine ?lamc5 attempts to compute *rmax*, the largest machine floating-point number, without overflow. It assumes that *emax* + abs(*emin*) sum approximately to a power of 2. It will fail on machines where this assumption does not hold, for example, the Cyber 205 (*emin* = -28625, *emax* = 28718). It will also fail if the value supplied for *emin* is too large (that is, too close to zero), probably with overflow.

beta	<b>INTEGER</b> . The base of floating-point arithmetic.
p	<b>INTEGER</b> . The number of base <i>beta</i> digits in the mantissa of a floating-point value.
emin	<b>INTEGER.</b> The minimum exponent before (gradual) underflow.
ieee	<b>LOGICAL</b> . A logical flag specifying whether or not the arithmetic system is thought to comply with the IEEE standard.

emax	<b>INTEGER</b> . The largest exponent before overflow.
rmax	REAL for slamc5
	DOUBLE PRECISION for dlamc5
	The largest machine floating-point number.

# ?lamrg

Creates a permutation list to merge the entries of two independently sorted sets into a single set sorted in acsending order.

call slamrg ( n1, n2, a, strd1, strd2, index )
call dlamrg ( n1, n2, a, strd1, strd2, index )

### **Discussion**

The routine creates a permutation list which will merge the elements of *a* (which is composed of two independently sorted sets) into a single set which is sorted in ascending order.

n1, n2	INTEGER.
	These arguments contain the respective lengths of the
	two sorted lists to be merged.
а	REAL for slamrg
	DOUBLE PRECISION for dlamrg.
	Array, DIMENSION $(n1+n2)$ .
	The first n1 elements of a contain a list of numbers
	which are sorted in either ascending or descending
	order. Likewise for the final n2 elements.

strd1, strd2 INTEGER. These are the strides to be taken through the array a. Allowable strides are 1 and -1. They indicate whether a subset of a is sorted in ascending (strdx = 1) or descending (strdx = -1) order.

### **Output Parameters**

index

INTEGER. Array, DIMENSION (n1+n2). On exit, this array will contain a permutation such that if b(i) = a(index(i)) for i=1, n1+n2, then b will be sorted in ascending order.

### ?langb

Returns the value of the 1-norm, Frobenius norm, infinity-norm, or the largest absolute value of any element of general band matrix.

val = slangb ( norm, n, kl, ku, ab, ldab, work )
val = dlangb ( norm, n, kl, ku, ab, ldab, work )
val = clangb ( norm, n, kl, ku, ab, ldab, work )
val = zlangb ( norm, n, kl, ku, ab, ldab, work )

#### **Discussion**

The function returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n-by-n band matrix A, with kl sub-diagonals and ku super-diagonals.

The value *val* returned by the function is:

val = max(abs(A_{ij})), if norm = 'M' or 'm' = norm1(A), if norm = '1' or '0' or 'o' = norm1(A), if norm = '1' or 'i' = normF(A), if norm = 'F', 'f', 'E' or 'e'

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

norm	CHARACTER*1. Specifies the value to be returned by the routine as described above.
п	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ . When $n = 0$ , <b>?langb</b> is set to zero.
kl	<b>INTEGER.</b> The number of sub-diagonals of the matrix <i>A</i> . $kl \ge 0$ .
ku	<b>INTEGER.</b> The number of super-diagonals of the matrix <i>A</i> . $ku \ge 0$ .
ab	REAL for slangb DOUBLE PRECISION for dlangb COMPLEX for clangb COMPLEX*16 for zlangb Array, DIMENSION ( <i>ldab,n</i> ). The band matrix <i>A</i> , stored in rows 1 to $kl+ku+1$ . The <i>j</i> -th column of <i>A</i> is stored in the <i>j</i> -th column of the array <i>ab</i> as follows: ab(ku+1+i-j,j) = a(i,j) for max(1, <i>j</i> -ku) $\leq i \leq \min(n,j+k1)$ .
ldab	<b>INTEGER.</b> The leading dimension of the array <u>ab</u> . $1dab \ge kl+ku+1$ .
work	REAL for slangb/clangb DOUBLE PRECISION for dlangb/zlangb Workspace array, DIMENSION ( <i>lwork</i> ), where $lwork \ge n$ when $norm = 'I'$ ; otherwise, <i>work</i> is not referenced.

val

REAL for slangb/clangb DOUBLE PRECISION for dlangb/zlangb Value returned by the function.

# ?lange

Returns the value of the 1-norm, Frobenius norm, infinity-norm, or the largest absolute value of any element of a general rectangular matrix.

val = slange ( norm, m, n, a, lda, work )
val = dlange ( norm, m, n, a, lda, work )
val = clange ( norm, m, n, a, lda, work )
val = zlange ( norm, m, n, a, lda, work )

### **Discussion**

The function **?lange** returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real/complex matrix *A*.

The value *val* returned by the function is:

<b>val</b> = $max(abs(A_{ij}))$	), if <i>norm</i> = 'M' or 'm'
= $norm1(A)$ ,	if <i>norm</i> = '1' or ' <b>0</b> ' or 'o'
= normI(A),	if <i>norm</i> = 'I' or 'i'
$= \operatorname{normF}(A)$ ,	if <i>norm</i> = 'F', 'f', 'E' or 'e'

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

### **Input Parameters**

norm	CHARACTER*1. Specifies the value to be returned in <b>?lange</b> as described above.
m	<b>INTEGER.</b> The number of rows of the matrix A. $m \ge 0$ . When $m = 0$ , <b>?lange</b> is set to zero.
п	<b>INTEGER.</b> The number of columns of the matrix A. $n \ge 0$ . When $n = 0$ , <b>?lange</b> is set to zero.
a	REAL for slange DOUBLE PRECISION for dlange COMPLEX for clange COMPLEX*16 for zlange Array, DIMENSION ( <i>lda</i> , <i>n</i> ). The <i>m</i> -by- <i>n</i> matrix <i>A</i> .
lda	<b>INTEGER.</b> The leading dimension of the array $a$ . <i>lda</i> $\geq \max(m, 1)$ .
work	<pre>REAL for slange and clange. DOUBLE PRECISION for dlange and zlange. Workspace array, DIMENSION (lwork), where lwork ≥ m when norm = 'I'; otherwise, work is not referenced.</pre>

### **Output Parameters**

val	REAL for slange/clange
	DOUBLE PRECISION for dlange/zlange
	Value returned by the function.

# ?langt

Returns the value of the 1-norm, Frobenius norm, infinity-norm, or the largest absolute value of any element of a general tridiagonal matrix.

val = slangt ( norm, n, dl, d, du )

```
val = dlangt ( norm, n, dl, d, du )
val = clangt ( norm, n, dl, d, du )
val = zlangt ( norm, n, dl, d, du )
```

#### **Discussion**

The routine returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real/complex tridiagonal matrix *A*.

The value *val* returned by the function is:

<b>val</b> = $max(abs(A_{ij}))$ , if $norm = 'M'$ or 'm'		
= $norm1(A)$ ,	if <i>norm</i> = '1' or ' <b>0</b> ' or 'o'	
= $normI(A)$ ,	if <i>norm</i> = '1' or 'i'	
= $\operatorname{norm} F(A)$ ,	if <i>norm</i> = 'F', 'f', 'E' or 'e'	

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

norm	CHARACTER*1. Specifies the value to be returned in <b>?langt</b> as described above.
n	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ . When $n = 0$ , <b>?langt</b> is set to zero.
dl, d, du	REAL for slangt DOUBLE PRECISION for dlangt COMPLEX for clangt COMPLEX*16 for zlangt Arrays: dl (n-1), d (n), du (n-1). The array dl contains the (n-1) sub-diagonal elements of A. The array d contains the diagonal elements of A. The array du contains the (n-1) super-diagonal elements of A.

val REAL for slangt/clangt DOUBLE PRECISION for dlangt/zlangt Value returned by the function.

### ?lanhs

Returns the value of the 1-norm, Frobenius norm, infinity-norm, or the largest absolute value of any element of an upper Hessenberg matrix.

val = slanhs ( norm, n, a, lda, work )
val = dlanhs ( norm, n, a, lda, work )
val = clanhs ( norm, n, a, lda, work )
val = zlanhs ( norm, n, a, lda, work )

#### **Discussion**

The function **?lanhs** returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a Hessenberg matrix *A*.

The value *val* returned by the function is:

```
val = max(abs(A<sub>ij</sub>)), if norm = 'M' or 'm'
= norm1(A), if norm = '1' or 'O' or 'o'
= norm1(A), if norm = '1' or 'i'
= normF(A), if norm = 'F', 'f', 'E' or 'e'
```

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

### **Input Parameters**

· · · · ·	
norm	CHARACTER*1. Specifies the value to be returned in <b>?lanhs</b> as described above.
п	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ . When $n = 0$ , <b>?lanhs</b> is set to zero.
a	REAL for slanhs DOUBLE PRECISION for dlanhs COMPLEX for clanhs COMPLEX*16 for zlanhs Array, DIMENSION ( <i>lda</i> , <i>n</i> ). The <i>n</i> -by- <i>n</i> upper Hessenberg matrix <i>A</i> ; the part of <i>A</i> below the first sub-diagonal is not referenced.
lda	<b>INTEGER.</b> The leading dimension of the array $a$ . $lda \ge max(n,1)$ .
work	REAL for slanhs and clanhs. DOUBLE PRECISION for dlange and zlange. Workspace array, DIMENSION ( <i>lwork</i> ), where <i>lwork</i> $\geq$ <i>n</i> when <i>norm</i> = 'I'; otherwise, <i>work</i> is not referenced.

### **Output Parameters**

	Value returned by the function.
	DOUBLE PRECISION for dlanhs/zlanhs
val	REAL for slanhs/clanhs

# ?lansb

Returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a symmetric band matrix.

val = slansb ( norm, uplo, n, k, ab, ldab, work )
val = dlansb ( norm, uplo, n, k, ab, ldab, work )

val = clansb ( norm, uplo, n, k, ab, ldab, work )
val = zlansb ( norm, uplo, n, k, ab, ldab, work )

#### **Discussion**

The function **?lansb** returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n-by-n real/complex symmetric band matrix A, with k super-diagonals.

The value *val* returned by the function is:

<b>val</b> = $\max(abs(A_{ij}))$	), if <i>norm</i> = 'M' or 'm'
= $norml(A)$ ,	if <i>norm</i> = '1' or ' <b>O</b> ' or 'o'
= $normI(A)$ ,	if <i>norm</i> = 'I' or 'i'
= $normF(A)$ ,	if <i>norm</i> = 'F', 'f', 'E' or 'e'

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

norm	CHARACTER*1. Specifies the value to be returned in <b>?lansb</b> as described above.
uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the band matrix $A$ is supplied. If $uplo = 'U'$ : upper triangular part is supplied; If $uplo = 'L'$ : lower triangular part is supplied.
п	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ . When $n = 0$ , <b>?lansb</b> is set to zero.
k	<b>INTEGER.</b> The number of super-diagonals or sub-diagonals of the band matrix A. $k \ge 0$ .
ab	REAL for slansb DOUBLE PRECISION for dlansb COMPLEX for clansb COMPLEX*16 for zlansb Array, DIMENSION ( <i>ldab,n</i> ). The upper or lower triangle of the symmetric band matrix <i>A</i> , stored in the

	first $k+1$ rows of $ab$ . The <i>j</i> -th column of $A$ is stored in the <i>j</i> -th column of the array $ab$ as follows: if $uplo = 'U'$ , $ab(k+1+i-j,j) = a(i,j)$ for $max(1,j-k) \le i \le j$ ; if $uplo = 'L'$ , $ab(1+i-j,j) = a(i,j)$ for $j \le min(n,j+k)$ .
ldab	<b>INTEGER</b> . The leading dimension of the array <i>ab</i> . $1dab \ge k+1$ .
work	<b>REAL</b> for slansb and clansb. DOUBLE PRECISION for dlansb and zlansb. Workspace array, DIMENSION ( <i>lwork</i> ), where $lwork \ge n$ when $norm = 'I'$ or '1' or 'O'; otherwise, <i>work</i> is not referenced.

val

REAL for slansb/clansb DOUBLE PRECISION for dlansb/zlansb Value returned by the function.

# ?lanhb

Returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a Hermitian band matrix.

val = clanhb ( norm, uplo, n, k, ab, ldab, work )
val = zlanhb ( norm, uplo, n, k, ab, ldab, work )

### **Discussion**

The routine returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n-by-n Hermitian band matrix A, with k super-diagonals.

The value *val* returned by the function is:

**val** =  $max(abs(A_{ij}))$ , if *norm* = 'M' or 'm'

- = norm1(*A*), if *norm* = '1' or '0' or 'o'
- = normI(*A*), if *norm* = 'I' or 'i'
- = normF(A), if norm = 'F', 'f', 'E' or 'e'

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

norm	CHARACTER*1. Specifies the value to be returned in ?lanhb as described above.
uplo	<b>CHARACTER*1.</b> Specifies whether the upper or lower triangular part of the band matrix A is supplied. If $uplo = 'U'$ : upper triangular part is supplied; If $uplo = 'L'$ : lower triangular part is supplied.
n	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ . When $n = 0$ , <b>?lanhb</b> is set to zero.
k	<b>INTEGER.</b> The number of super-diagonals or sub-diagonals of the band matrix A. $k \ge 0$ .
ab	COMPLEX for clanhb. COMPLEX*16 for zlanhb. Array, DIMENSION ( <i>ldab</i> , <i>n</i> ). The upper or lower triangle of the Hermitian band matrix <i>A</i> , stored in the first <i>k</i> +1 rows of <i>ab</i> . The <i>j</i> -th column of <i>A</i> is stored in the <i>j</i> -th column of the array <i>ab</i> as follows: if $uplo = 'U'$ , $ab(k+1+i-j,j) = a(i,j)$ for $max(1,j-k) \le i \le j$ ; if $uplo = 'L'$ , $ab(1+i-j,j) = a(i,j)$ for $j \le snin(n,j+k)$ . Note that the imaginary parts of the diagonal elements
	need not be set and are assumed to be zero.
ldab	<b>INTEGER.</b> The leading dimension of the array <i>ab</i> . $ldab \ge k+1$ .

work

REAL for clanhb.
DOUBLE PRECISION for zlanhb.
Workspace array, DIMENSION (lwork), where
lwork ≥ n when norm = 'I' or '1' or 'O'; otherwise, work
is not referenced.

### **Output Parameters**

val

REAL for slanhb/clanhb DOUBLE PRECISION for dlanhb/zlanhb Value returned by the function.

### ?lansp

Returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a symmetric matrix supplied in packed form.

val = slansp ( norm, uplo, n, ap, work )
val = dlansp ( norm, uplo, n, ap, work )
val = clansp ( norm, uplo, n, ap, work )
val = zlansp ( norm, uplo, n, ap, work )

### **Discussion**

The function **?lansp** returns the value of the l-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real/complex symmetric matrix *A*, supplied in packed form.

The value *val* returned by the function is:

```
val = max(abs(A<sub>ij</sub>)), if norm = 'M' or 'm'
= norm1(A), if norm = '1' or 'O' or 'o'
= norm1(A), if norm = '1' or 'i'
```

= normF(A), if norm = 'F', 'f', 'E' or 'e'

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

### **Input Parameters**

norm	CHARACTER*1. Specifies the value to be returned in <b>?lansp</b> as described above.
uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the symmetric matrix $A$ is supplied. If $uplo = 'U'$ : Upper triangular part of $A$ is supplied If $uplo = 'L'$ : Lower triangular part of $A$ is supplied.
п	<b>INTEGER.</b> The order of the matrix <i>A</i> . $n \ge 0$ . When $n = 0$ , <b>?lansp</b> is set to zero.
ap	REAL for slansp DOUBLE PRECISION for dlansp COMPLEX for clansp COMPLEX*16 for zlansp Array, DIMENSION $(n(n+1)/2)$ . The upper or lower triangle of the symmetric matrix $A$ , packed columnwise in a linear array. The <i>j</i> -th column of $A$ is stored in the array <i>ap</i> as follows: if <i>uplo</i> = 'U', <i>ap</i> ( <i>i</i> + ( <i>j</i> -1) <i>j</i> /2) = $A(i,j)$ for $1 \le i \le j$ ; if <i>uplo</i> = 'L', <i>ap</i> ( <i>i</i> + ( <i>j</i> -1)(2 <i>n</i> - <i>j</i> )/2) = $A(i,j)$ for $j \le \le$ .
work	REAL for slansp and clansp. DOUBLE PRECISION for dlansp and zlansp. Workspace array, DIMENSION ( <i>lwork</i> ), where $lwork \ge n$ when $norm = 'I'$ or '1' or 'O'; otherwise, <i>work</i> is not referenced.

### **Output Parameters**

valREAL for slansp/clanspDOUBLEPRECISION for dlansp/zlanspValue returned by the function.

# ?lanhp

Returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex Hermitian matrix supplied in packed form.

```
val = clanhp ( norm, uplo, n, ap, work )
val = zlanhp ( norm, uplo, n, ap, work )
```

### **Discussion**

The function **?lanhp** returns the value of the l-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex Hermitian matrix *A*, supplied in packed form.

The value *val* returned by the function is:

<b>val</b> = $\max(abs(A_{ij}))$	), if <i>norm</i> = 'M' or 'm'
= $norm1(A)$ ,	if <i>norm</i> = '1' or ' <b>0</b> ' or 'o'
= $normI(A)$ ,	if <i>norm</i> = 'I' or 'i'
= $\operatorname{norm} F(A)$ ,	if <i>norm</i> = 'F', 'f', 'E' or 'e'

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

norm	CHARACTER*1. Specifies the value to be returned in ?lanhp as described above.
uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the Hermitian matrix $A$ is supplied. If $uplo = 'U'$ : Upper triangular part of $A$ is supplied If $uplo = 'L'$ : Lower triangular part of $A$ is supplied.

n	<b>INTEGER.</b> The order of the matrix <i>A</i> . $n \ge 0$ . When $n = 0$ , <b>?lanhp</b> is set to zero.
ap	COMPLEX for clanhp. COMPLEX*16 for zlanhp. Array, DIMENSION $(n(n+1)/2)$ . The upper or lower triangle of the Hermitian matrix $A$ , packed columnwise in a linear array. The <i>j</i> -th column of $A$ is stored in the array <i>ap</i> as follows: if <i>uplo</i> = 'U', <i>ap</i> ( <i>i</i> + ( <i>j</i> -1) <i>j</i> /2) = $A(i,j)$ for $1 \le i \le j$ ; if <i>uplo</i> = 'L', <i>ap</i> ( <i>i</i> + ( <i>j</i> -1)(2 <i>n</i> - <i>j</i> )/2) = $A(i,j)$ for $j \le \le$ .
work	<pre>REAL for clanhp. DOUBLE PRECISION for zlanhp. Workspace array, DIMENSION (lwork), where lwork ≥ n when norm = 'I' or '1' or 'O'; otherwise, work is not referenced.</pre>

valREAL for clanhp.DOUBLEPRECISION for zlanhp.Value returned by the function.

# ?lanst/?lanht

Returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real symmetric or complex Hermitian tridiagonal matrix.

val = slanst ( norm, n, d, e )
val = dlanst ( norm, n, d, e )
val = clanht ( norm, n, d, e )
val = zlanht ( norm, n, d, e )

### **Discussion**

The functions **?lanst/?lanht** return the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real symmetric or a complex Hermitian tridiagonal matrix *A*.

The value *val* returned by the function is:

val = max(abs(A_{ij})), if norm = 'M' or 'm' = norm1(A), if norm = '1' or 'O' or 'o' = norm1(A), if norm = '1' or 'i' = normF(A), if norm = 'F', 'f', 'E' or 'e'

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

### **Input Parameters**

norm	CHARACTER*1. Specifies the value to be returned in ?lanst/?lanht as described above.
п	<b>INTEGER.</b> The order of the matrix <i>A</i> . $n \ge 0$ . When $n = 0$ , <b>?lanst/?lanht</b> is set to zero.
d	REAL for slanst/clanht DOUBLE PRECISION for dlanst/zlanht Array, DIMENSION (n). The diagonal elements of A.
e	REAL for slanst DOUBLE PRECISION for dlanst COMPLEX for clanht COMPLEX*16 for zlanht Array, DIMENSION ( <i>n</i> -1). The ( <i>n</i> -1) sub-diagonal or super-diagonal elements of A.

### **Output Parameters**

val

REAL for slanst/clanht DOUBLE PRECISION for dlanst/zlanht Value returned by the function.

### ?lansy

Returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real/complex symmetric matrix.

val = slansy ( norm, uplo, n, a, lda, work )
val = dlansy ( norm, uplo, n, a, lda, work )
val = clansy ( norm, uplo, n, a, lda, work )
val = zlansy ( norm, uplo, n, a, lda, work )

### **Discussion**

The function **?lansy** returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a real/complex symmetric matrix *A*.

The value *val* returned by the function is:

<b>val</b> = $max(abs(A_{ij}))$ , if <i>norm</i> = 'M' or 'm'			
= $norml(A)$ ,	if <i>norm</i> = '1' or ' <b>0</b> ' or 'o'		
= $normI(A)$ ,	if <i>norm</i> = 'I' or 'i'		
= norm $F(A)$ ,	if <i>norm</i> = 'F', 'f', 'E' or 'e'		

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

### **Input Parameters**

norm

CHARACTER*1. Specifies the value to be returned in ?lansy as described above.

uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the symmetric matrix <i>A</i> is to be referenced. = 'U': Upper triangular part of <i>A</i> is referenced. = 'L': Lower triangular part of <i>A</i> is referenced
n	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ . When $n = 0$ , <b>?lansy</b> is set to zero.
a	REAL for slansy DOUBLE PRECISION for dlansy COMPLEX for clansy COMPLEX*16 for zlansy Array, DIMENSION ( <i>lda,n</i> ). The symmetric matrix A. If uplo = 'U', the leading <i>n</i> -by- <i>n</i> upper triangular part of <i>a</i> contains the upper triangular part of the matrix A, and the strictly lower triangular part of <i>a</i> is not referenced. If $uplo = 'L'$ , the leading <i>n</i> -by- <i>n</i> lower triangular part of <i>a</i> contains the lower triangular part of the matrix A, and the strictly upper triangular part of the matrix A, and the strictly upper triangular part of <i>a</i> is not referenced.
lda	<b>INTEGER.</b> The leading dimension of the array <i>a</i> . $1 da \ge max(n,1)$ .
work	REAL for slansy and clansy. DOUBLE PRECISION for dlansy and zlansy. Workspace array, DIMENSION ( <i>lwork</i> ), where $lwork \ge n$ when $norm = 'I'$ or '1' or 'O'; otherwise, <i>work</i> is not referenced.

val	REAL for slansy/clansy
	DOUBLE PRECISION for dlansy/zlansy
	Value returned by the function.

### ?lanhe

Returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex Hermitian matrix.

val = clanhe ( norm, uplo, n, a, lda, work )
val = zlanhe ( norm, uplo, n, a, lda, work )

### **Discussion**

The function **?lanke** returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a complex Hermitian matrix *A*.

The value *val* returned by the function is:

val =  $max(abs(A_{ii}))$ , if norm = M' or m'

- = norm1(*A*), if *norm* = '1' or '0' or 'o'
- = normI(*A*), if *norm* = 'I' or 'i'
- = normF(A), if norm = 'F', 'f', 'E' or 'e'

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

norm	CHARACTER*1. Specifies the value to be returned in <b>?lanhe</b> as described above.
uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the Hermitian matrix <i>A</i> is to be referenced. = 'U': Upper triangular part of <i>A</i> is referenced. = 'L': Lower triangular part of <i>A</i> is referenced

n	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ . When $n = 0$ , <b>?lanhe</b> is set to zero.
a	COMPLEX for clanhe. COMPLEX*16 for zlanhe. Array, DIMENSION ( <i>lda,n</i> ). The Hermitian matrix <i>A</i> . If $uplo = 'U'$ , the leading <i>n</i> -by- <i>n</i> upper triangular part of <i>a</i> contains the upper triangular part of the matrix <i>A</i> , and the strictly lower triangular part of <i>a</i> is not referenced. If $uplo = 'L'$ , the leading <i>n</i> -by- <i>n</i> lower triangular part of <i>a</i> contains the lower triangular part of the matrix <i>A</i> , and the strictly upper triangular part of the matrix <i>A</i> , and the strictly upper triangular part of <i>a</i> is not referenced.
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $lda \ge max(n,1)$ .
work	REAL for clanhe. DOUBLE PRECISION for zlanhe. Workspace array, DIMENSION ( <i>lwork</i> ), where $lwork \ge n$ when $norm = 'I'$ or '1' or '0'; otherwise, <i>work</i> is not referenced.

	-
va	1

REAL for clanhe. DOUBLE PRECISION for zlanhe. Value returned by the function.

# ?lantb

Returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a triangular band matrix.

val = slantb ( norm, uplo, diag, n, k, ab, ldab, work )
val = dlantb ( norm, uplo, diag, n, k, ab, ldab, work )

val = clantb ( norm, uplo, diag, n, k, ab, ldab, work )
val = zlantb ( norm, uplo, diag, n, k, ab, ldab, work )

#### **Discussion**

The function ?lantb returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of an n-by-n triangular band matrix A, with (k + 1) diagonals.

The value *val* returned by the function is:

<b>val</b> = $max(abs(A_{ij}))$	), if <i>norm</i> = 'M' or 'm'
= $norml(A)$ ,	if <i>norm</i> = '1' or ' <b>0</b> ' or 'o'
= $normI(A)$ ,	if <i>norm</i> = 'I' or 'i'
= $normF(A)$ ,	if <i>norm</i> = 'F', 'f', 'E' or 'e'

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

norm	CHARACTER*1. Specifies the value to be returned in <b>?lantb</b> as described above.
uplo	CHARACTER*1. Specifies whether the matrix <i>A</i> is upper or lower triangular. = 'U': Upper triangular = 'L': Lower triangular.
diag	CHARACTER*1. Specifies whether or not the matrix A is unit triangular. = 'N': Non-unit triangular = 'U': Unit triangular.
п	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ . When $n = 0$ , <b>?lantb</b> is set to zero.
k	<b>INTEGER.</b> The number of super-diagonals of the matrix A if $uplo = 'U'$ , or the number of sub-diagonals of the matrix A if $uplo = 'L'$ . $k \ge 0$ .

ab	REAL for slantb
	DOUBLE PRECISION for dlantb
	COMPLEX for clantb
	COMPLEX*16 for zlantb
	Array, <b>DIMENSION</b> ( <i>ldab</i> , <i>n</i> ). The upper or lower
	triangular band matrix A, stored in the first $k+1$ rows of
	<i>ab</i> . The <i>j</i> -th column of <i>A</i> is stored in the <i>j</i> -th column of
	the array ab as follows:
	if $uplo = U'$ , $ab(k+1+i-j,j) = a(i,j)$ for
	$\max(1, j-k) \le i \le j;$
	if $uplo = L'$ , $ab(1+i-j,j) = a(i,j)$ for
	$j \leq i \leq \min(n, j+k).$
	Note that when $diag = 'U'$ , the elements of the array <i>ab</i> corresponding to the diagonal elements of the matrix <i>A</i> are not referenced, but are assumed to be one.
ldab	<b>INTEGER.</b> The leading dimension of the array <u>ab</u> . $1dab \ge k+1$ .
work	REAL for slantb and clantb.
	DOUBLE PRECISION for dlantb and zlantb.
	Workspace array, <b>DIMENSION</b> ( <i>lwork</i> ), where
	$lwork \ge n$ when $norm = 'I'$ ; otherwise, $work$ is not
	referenced.
Output Deven	to up

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REAL for slantb/clantb. DOUBLE PRECISION for dlantb/zlantb. Value returned by the function.

### ?lantp

Returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a triangular matrix supplied in packed form.

val = slantp ( norm, uplo, diag, n, ap, work )
val = dlantp ( norm, uplo, diag, n, ap, work )
val = clantp ( norm, uplo, diag, n, ap, work )
val = zlantp ( norm, uplo, diag, n, ap, work )

### **Discussion**

The function **?lantp** returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a triangular matrix *A*, supplied in packed form.

The value *val* returned by the function is:

val = max(abs(A_{ij})), if norm = 'M' or 'm' = norm1(A), if norm = '1' or 'O' or 'o' = norm1(A), if norm = 'I' or 'i' = normF(A), if norm = 'F', 'f', 'E' or 'e'

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

### **Input Parameters**

norm

CHARACTER*1. Specifies the value to be returned in ?lantp as described above.

uplo	CHARACTER*1. Specifies whether the matrix A is upper or lower triangular. = 'u': Upper triangular = 'L': Lower triangular.
diag	CHARACTER*1. Specifies whether or not the matrix A is unit triangular. = 'N': Non-unit triangular = 'U': Unit triangular.
п	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ . When $n = 0$ , <b>?lantp</b> is set to zero.
ap	REAL for slantp DOUBLE PRECISION for dlantp COMPLEX for clantp COMPLEX*16 for zlantp Array, DIMENSION $(n(n+1)/2)$ . The upper or lower triangular matrix A, packed columnwise in a linear array. The j-th column of A is stored in the array ap as follows: if $uplo = 'U'$ , $AP(i + (j-1)j/2) = a(i,j)$ for $1 \le i \le j$ ; if $uplo = 'L'$ , $ap(i + (j-1)(2n-j)/2) = a(i,j)$ for $j \le i \le n$ . Note that when $diag = 'U'$ , the elements of the array ap corresponding to the diagonal elements of the matrix A are not referenced, but are assumed to be one.
work	REAL for slantp and clantp. DOUBLE PRECISION for dlantp and zlantp. Workspace array, DIMENSION ( <i>lwork</i> ), where $lwork \ge n$ when $norm = 'I'$ ; otherwise, <i>work</i> is not referenced.
Output Parameters	
wo 1	PEAL for glantn/glantn

val

REAL for slantp/clantp. DOUBLE PRECISION for dlantp/zlantp. Value returned by the function.

### ?lantr

Returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a trapezoidal or triangular matrix.

val = slantr ( norm, uplo, diag, m, n, a, lda, work )
val = dlantr ( norm, uplo, diag, m, n, a, lda, work )
val = clantr ( norm, uplo, diag, m, n, a, lda, work )
val = zlantr ( norm, uplo, diag, m, n, a, lda, work )

### **Discussion**

The function **?lantr** returns the value of the 1-norm, or the Frobenius norm, or the infinity norm, or the element of largest absolute value of a trapezoidal or triangular matrix *A*.

The value *val* returned by the function is:

<b>val</b> = $\max(abs(A_{ij}))$	), if <u>norm</u> = 'M' or 'm'
= $norml(A)$ ,	if <i>norm</i> = '1' or ' <b>0</b> ' or 'o'
= $normI(A)$ ,	if <i>norm</i> = 'I' or 'i'
= $\operatorname{norm} F(A)$ ,	if <i>norm</i> = 'F', 'f', 'E' or 'e'

where norm1 denotes the 1-norm of a matrix (maximum column sum), norm1 denotes the infinity norm of a matrix (maximum row sum) and normF denotes the Frobenius norm of a matrix (square root of sum of squares). Note that  $\max(abs(A_{ij}))$  is not a matrix norm.

### **Input Parameters**

norm

CHARACTER*1. Specifies the value to be returned in ?lantr as described above.

uplo	CHARACTER*1. Specifies whether the matrix <i>A</i> is upper or lower trapezoidal. = 'U': Upper trapezoidal = 'L': Lower trapezoidal. Note that <i>A</i> is triangular instead of trapezoidal if <i>m</i> = <i>n</i> .
diag	CHARACTER*1. Specifies whether or not the matrix <i>A</i> has unit diagonal. = 'N': Non-unit diagonal = 'U': Unit diagonal.
m	<b>INTEGER.</b> The number of rows of the matrix A. $m \ge 0$ , and if $uplo = 'U', m \le n$ . When $m = 0$ , ?lantr is set to zero.
n	<b>INTEGER.</b> The number of columns of the matrix A. $n \ge 0$ , and if $uplo = L', n \le m$ . When $n = 0$ , ?lantr is set to zero.
a	REAL for slantr DOUBLE PRECISION for dlantr COMPLEX for clantr COMPLEX*16 for zlantr Array, DIMENSION ( <i>lda</i> , <i>n</i> ).
	The trapezoidal matrix $A$ ( $A$ is triangular if $m = n$ ). If $uplo = 'U'$ , the leading $m$ -by- $n$ upper trapezoidal part of the array $a$ contains the upper trapezoidal matrix, and the strictly lower triangular part of $a$ is not referenced. If $uplo = 'L'$ , the leading $m$ -by- $n$ lower trapezoidal part of the array $a$ contains the lower trapezoidal matrix, and the strictly upper triangular part of $a$ is not referenced. Note that when $diag = 'U'$ , the diagonal elements of $a$ are not referenced and are assumed to be one.
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $lda \ge max(m,1)$ .

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REAL for slantr/clantrp. DOUBLE PRECISION for dlantr/zlantr. Workspace array, DIMENSION (*lwork*), where *lwork* ≥ m when norm = 'I'; otherwise, work is not referenced.

### **Output Parameters**

val

work

REAL for slantr/clantrp. DOUBLE PRECISION for dlantr/zlantr. Value returned by the function.

### ?lanv2

Computes the Schur factorization of a real 2-by-2 nonsymmetric matrix in standard form.

call slanv2 ( a, b, c, d, rt1r, rt1i, rt2r, rt2i, cs, sn ) call dlanv2 ( a, b, c, d, rt1r, rt1i, rt2r, rt2i, cs, sn )

### **Discussion**

The routine computes the Schur factorization of a real 2-by-2 nonsymmetric matrix in standard form:

 $\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} cs & -sn \\ sn & cs \end{bmatrix} \begin{bmatrix} aa & bb \\ cc & dd \end{bmatrix} \begin{bmatrix} cs & sn \\ -sn & cs \end{bmatrix}$ 

where either

- 1. cc = 0 so that *aa* and *dd* are real eigenvalues of the matrix, or
- 2. aa = dd and bb*cc < 0, so that  $aa \pm \text{sqrt}(bb*cc)$  are complex conjugate eigenvalues.

The routine was adjusted to reduce the risk of cancellation errors, when computing real eigenvalues, and to ensure, if possible, that  $abs(rtlr) \ge abs(rt2r)$ .

### **Input Parameters**

a, b, c, d	REAL for slanv2
	DOUBLE PRECISION for dlanv2.
	On entry, elements of the input matrix.

### **Output Parameters**

a, b, c, d	On exit, overwritten by the elements of the standardized Schur form.
rt1r, rt1i, rt2r, rt2i,	<b>REAL</b> for slanv2 <b>DOUBLE PRECISION</b> for dlanv2. The real and imaginary parts of the eigenvalues. If the eigenvalues are a complex conjugate pair, $rt1i > 0$ .
cs, sn	REAL for slanv2 DOUBLE PRECISION for dlanv2. Parameters of the rotation matrix.

# ?lapll

Measures the linear dependence of two vectors.

```
call slapl1 ( n, x, incx, y, incy, ssmin )
call dlapl1 ( n, x, incx, y, incy, ssmin )
call clapl1 ( n, x, incx, y, incy, ssmin )
call zlapl1 ( n, x, incx, y, incy, ssmin )
```

### **Discussion**

Given two column vectors x and y of length n, let

A = (x y) be the *n*-by-2 matrix.

The routine **?lapl1** first computes the *QR* factorization of *A* as A = QR and then computes the SVD of the 2-by-2 upper triangular matrix *R*. The smaller singular value of *R* is returned in *ssmin*, which is used as the measurement of the linear dependency of the vectors *x* and *y*.

### **Input Parameters**

n	<b>INTEGER.</b> The length of the vectors $x$ and $y$ .
x	REAL for slapl1 DOUBLE PRECISION for dlapl1 COMPLEX for clapl1 COMPLEX*16 for zlapl1 Array, DIMENSION (1+(n-1)incx). On entry, x contains the <i>n</i> -vector x.
У	REAL for slapl1 DOUBLE PRECISION for dlapl1 COMPLEX for clapl1 COMPLEX*16 for zlapl1 Array, DIMENSION (1+(n-1)incy). On entry, y contains the <i>n</i> -vector y.
incx	<b>INTEGER.</b> The increment between successive elements of <i>x</i> ; $incx > 0$ .
incy	<b>INTEGER</b> . The increment between successive elements of <i>y</i> ; <i>incy</i> > 0.

### **Output Parameters**

x	On exit, $\mathbf{x}$ is overwritten.
Y	On exit, $y$ is overwritten.
ssmin	<b>REAL</b> for slapll/clapl1 DOUBLE PRECISION for dlapl1/zlapl1 The smallest singular value of the <i>n</i> -by-2 matrix $A = (x \ y)$ .

# ?lapmt

Performs a forward or backward permutation of the columns of a matrix.

```
call slapmt ( forwrd, m, n, x, ldx, k )
call dlapmt ( forwrd, m, n, x, ldx, k )
call clapmt ( forwrd, m, n, x, ldx, k )
call zlapmt ( forwrd, m, n, x, ldx, k )
```

### **Discussion**

The routine ?lapmt rearranges the columns of the *m*-by-*n* matrix X as specified by the permutation k(1),k(2),...,k(n) of the integers 1,...,n.

If *forwrd* = .TRUE., forward permutation: X(*,k(j)) is moved to X(*,j) for j=1,2,...,n.

If *forwrd* = .FALSE., backward permutation:

X(*, j) is moved to X(*, k(j)) for j = 1, 2, ..., n.

forwrd	LOGICAL. If <i>forwrd</i> = .TRUE., forward permutation If <i>forwrd</i> = .FALSE., backward permutation
m	<b>INTEGER.</b> The number of rows of the matrix <i>X</i> . $m \ge 0$ .
п	<b>INTEGER.</b> The number of columns of the matrix <i>X</i> . $n \ge 0$ .
x	REAL for slapmt DOUBLE PRECISION for dlapmt COMPLEX for clapmt COMPLEX*16 for zlapmt Array, DIMENSION ( <i>ldx,n</i> ). On entry, the <i>m</i> -by- <i>n</i> matrix <i>X</i> .

ldx	<b>INTEGER.</b> The leading dimension of the array $x$ , $ldx \ge max(1,m)$ .	
k	<b>INTEGER.</b> Array, <b>DIMENSION</b> ( <i>n</i> ). On entry, <i>k</i> contains the permutation vector.	
Output Parameters		
x	On exit, $\mathbf{x}$ contains the permuted matrix X.	

# ?lapy2

*Returns* sqrt( $x^2 + y^2$ ).

val = slapy2 ( x, y )
val = dlapy2 ( x, y )

## **Discussion**

The function ?lapy2 returns  $sqrt(x^2+y^2)$ , avoiding unnecessary overflow or harmful underflow.

## **Input Parameters**

x, yREAL for slapy2DOUBLEPRECISION for dlapy2Specify the input values x and y.

## **Output Parameters**

val	REAL for slapy2
	DOUBLE PRECISION for dlapy2.
	Value returned by the function.

## **?lapy3** *Returns* sqrt( $x^2+y^2+z^2$ ).

val = slapy3 ( x, y, z ) val = dlapy3 ( x, y, z )

#### **Discussion**

The function ?lapy3 returns  $sqrt(x^2+y^2+z^2)$ , avoiding unnecessary overflow or harmful underflow.

## **Input Parameters**

x, y, z	REAL for slapy3
	DOUBLE PRECISION for dlapy3
	Specify the input values <i>x</i> , <i>y</i> and <i>z</i> .

#### **Output Parameters**

DOUBLE PRECISION for dlapy3.
Value returned by the function.

# ?laqgb

Scales a general band matrix, using row and column scaling factors computed by ?gbequ.

## Discussion

The routine equilibrates a general m-by-n band matrix A with kl subdiagonals and ku superdiagonals using the row and column scaling factors in the vectors r and c.

m	<b>INTEGER.</b> The number of rows of the matrix <i>A</i> . $m \ge 0$ .
п	<b>INTEGER.</b> The number of columns of the matrix <i>A</i> . $n \ge 0$ .
kl	<b>INTEGER.</b> The number of subdiagonals within the band of <i>A</i> . $kl \ge 0$ .
ku	<b>INTEGER.</b> The number of superdiagonals within the band of A. $ku \ge 0$ .
ab	REAL for slaqgb DOUBLE PRECISION for dlaqgb COMPLEX for claqgb COMPLEX*16 for zlaqgb Array, DIMENSION ( <i>ldab</i> , <i>n</i> ). On entry, the matrix <i>A</i> in band storage, in rows 1 to $k1+ku+1$ . The <i>j</i> -th column of A is stored in the <i>j</i> -th column of the array <i>ab</i> as follows: ab(ku+1+i-j,j) = A(i,j) for $max(1,j-ku) \leq i \leq min(m,j+k1)$ .
ldab	<b>INTEGER.</b> The leading dimension of the array <i>ab</i> . $1da \ge kl+ku+1$ .
amax	REAL for slaqgb/claqgb DOUBLE PRECISION for dlaqgb/zlaqgb Absolute value of largest matrix entry.

ab	On exit, the equilibrated matrix, in the same storage format as <i>A</i> . See <i>equed</i> for the form of the equilibrated matrix.
r, c	REAL for slaqgb/claqgb DOUBLE PRECISION for dlaqgb/zlaqgb Arrays $r(m)$ , $c(n)$ . Contain the row and column scale factors for $A$ , respectively.
rowcnd	REAL for slaqgb/claqgb DOUBLE PRECISION for dlaqgb/zlaqgb Ratio of the smallest $r(i)$ to the largest $r(i)$ .
colcnd	REAL for slaqgb/claqgb DOUBLE PRECISION for dlaqgb/zlaqgb Ratio of the smallest $c(i)$ to the largest $c(i)$ .
equed	CHARACTER*1. Specifies the form of equilibration that was done. If equed = 'N': No equilibration If equed = 'R': Row equilibration, that is, A has been premultiplied by diag( $r$ ). If equed = 'C': Column equilibration, that is, A has been postmultiplied by diag( $c$ ). If equed = 'B': Both row and column equilibration, that is, A has been replaced by diag( $r$ )*A*diag( $c$ ).

### **Application Notes**

The routine uses internal parameters thresh, large, and small, which have the following meaning. thresh is a threshold value used to decide if row or column scaling should be done based on the ratio of the row or column scaling factors. If rowcnd < thresh, row scaling is done, and if colcnd < thresh, column scaling is done. large and small are threshold values used to decide if row scaling should be done based on the absolute size of the largest matrix element. If amax > large or amax < small, row scaling is done.

## ?laqge

Scales a general rectangular matrix, using row and column scaling factors computed by ?geequ.

call slaqge ( m, n, a, lda, r, c, rowcnd, colcnd, amax, equed ) call dlaqge ( m, n, a, lda, r, c, rowcnd, colcnd, amax, equed ) call claqge ( m, n, a, lda, r, c, rowcnd, colcnd, amax, equed ) call zlaqge ( m, n, a, lda, r, c, rowcnd, colcnd, amax, equed )

## **Discussion**

The routine equilibrates a general m-by-n matrix A using the row and scaling factors in the vectors r and c.

m	<b>INTEGER.</b> The number of rows of the matrix <i>A</i> . $m \ge 0$ .
п	<b>INTEGER.</b> The number of columns of the matrix <i>A</i> . $n \ge 0$ .
a	REAL for slagge DOUBLE PRECISION for dlagge COMPLEX for clagge COMPLEX*16 for zlagge Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the <i>m</i> -by- <i>n</i> matrix <i>A</i> .
lda	<b>INTEGER.</b> The leading dimension of the array <i>A</i> . $Ida \ge \max(m, 1)$ .
r	REAL for slangge/clagge DOUBLE PRECISION for dlagge/zlagge Array, DIMENSION (m). The row scale factors for A.

С	REAL for slangge/clagge DOUBLE PRECISION for dlagge/zlagge Array, DIMENSION (n). The column scale factors for A.
rowcnd	REAL for slangge/clagge DOUBLE PRECISION for dlagge/zlagge Ratio of the smallest $r(i)$ to the largest $r(i)$ .
colcnd	REAL for slangge/clagge DOUBLE PRECISION for dlagge/zlagge Ratio of the smallest $c(i)$ to the largest $c(i)$ .
amax	REAL for slangge/clagge DOUBLE PRECISION for dlagge/zlagge Absolute value of largest matrix entry.

a	On exit, the equilibrated matrix. See <i>equed</i> for the form of the equilibrated matrix.
equed	CHARACTER*1. Specifies the form of equilibration that was done. If equed = 'N': No equilibration If equed = 'R': Row equilibration, that is, A has been premultiplied by diag( $r$ ). If equed = 'C': Column equilibration, that is, A has been postmultiplied by diag( $c$ ). If equed = 'B': Both row and column equilibration, that is, A has been replaced by diag( $r$ )*A*diag( $c$ ).

### **Application Notes**

The routine uses internal parameters *thresh*, *large*, and *small*, which have the following meaning. *thresh* is a threshold value used to decide if row or column scaling should be done based on the ratio of the row or column scaling factors. If *rowcnd < thresh*, row scaling is done, and if *colcnd < thresh*, column scaling is done. *large* and *small* are threshold values used to decide if row scaling should be done based on the absolute size of the largest matrix element. If *amax > large* or *amax < small*, row scaling is done.

# ?laqp2

Computes a QR factorization with column pivoting of the matrix block.

call slaqp2 ( m, n, offset, a, lda, jpvt, tau, vn1, vn2, work )
call dlaqp2 ( m, n, offset, a, lda, jpvt, tau, vn1, vn2, work )
call claqp2 ( m, n, offset, a, lda, jpvt, tau, vn1, vn2, work )
call zlaqp2 ( m, n, offset, a, lda, jpvt, tau, vn1, vn2, work )

## **Discussion**

The routine computes a QR factorization with column pivoting of the block A(offset+1:m,1:n). The block A(1:offset,1:n) is accordingly pivoted, but not factorized.

m	<b>INTEGER.</b> The number of rows of the matrix <i>A</i> . $m \ge 0$ .
n	<b>INTEGER.</b> The number of columns of the matrix <i>A</i> . $n \ge 0$ .
offset	<b>INTEGER</b> . The number of rows of the matrix A that must be pivoted but no factorized. offset $\geq 0$ .
a	REAL for slaqp2 DOUBLE PRECISION for dlaqp2 COMPLEX for claqp2 COMPLEX*16 for zlaqp2 Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the <i>m</i> -by- <i>n</i> matrix <i>A</i> .
lda	<b>INTEGER</b> . The leading dimension of the array A. $1 da \ge max(1,m)$ .

jpvt	<b>INTEGER</b> . Array, <b>DIMENSION</b> ( <i>n</i> ). On entry, if $jpvt(i) \neq 0$ , the <i>i</i> -th column of <i>A</i> is permuted to the front of $A * P$ (a leading column); if $jpvt(i) = 0$ , the <i>i</i> -th column of <i>A</i> is a free column.	
vn1, vn2	REAL for slaqp2/claqp2 DOUBLE PRECISION for dlaqp2/zlaqp2 Arrays, DIMENSION ( <i>n</i> ) each. Contain the vectors with the partial and exact column norms, respectively.	
work	REAL for slaqp2 DOUBLE PRECISION for dlaqp2 COMPLEX for claqp2 COMPLEX*16 for zlaqp2 Workspace array, DIMENSION (n).	
Output Parameters		
a	On exit, the upper triangle of block $A(offset+1:m,1:n)$ is the triangular factor obtained; the elements in block $A(offset+1:m,1:n)$ below the diagonal, together with the array <i>tau</i> , represent the orthogonal matrix <i>Q</i> as a product of elementary reflectors. Block $A(1:offset,1:n)$ has been accordingly pivoted, but not factorized.	
jpvt	On exit, if $jpvt(i) = k$ , then the <i>i</i> -th column of $A*P$ was the <i>k</i> -th column of <i>A</i> .	
tau	REAL for slaqp2 DOUBLE PRECISION for dlaqp2 COMPLEX for claqp2 COMPLEX*16 for zlaqp2 Array, DIMENSION (min( <i>m</i> , <i>n</i> )). The scalar factors of the elementary reflectors.	
vn1, vn2	Contain the vectors with the partial and exact column norms, respectively.	

## ?laqps

Computes a step of QR factorization with column pivoting of a real m-by-n matrix A by using BLAS level 3.

### **Discussion**

This routine computes a step of QR factorization with column pivoting of a real *m*-by-*n* matrix *A* by using BLAS level 3. The routine tries to factorize *nb* columns from *A* starting from the row *offset*+1, and updates all of the matrix with BLAS level 3 routine ?gemm.

In some cases, due to catastrophic cancellations, **?lagps** cannot factorize *nb* columns. Hence, the actual number of factorized columns is returned in *kb*.

Block A(1:offset,1:n) is accordingly pivoted, but not factorized.

m	<b>INTEGER.</b> The number of rows of the matrix <i>A</i> . $m \ge 0$ .
n	<b>INTEGER.</b> The number of columns of the matrix <i>A</i> . $n \ge 0$ .
offset	<b>INTEGER</b> . The number of rows of <i>A</i> that have been factorized in previous steps.
nb	<b>INTEGER</b> . The number of columns to factorize.

a	REAL for slaqps DOUBLE PRECISION for dlaqps COMPLEX for claqps COMPLEX*16 for zlaqps Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the <i>m</i> -by- <i>n</i> matrix <i>A</i> .
lda	<b>INTEGER</b> . The leading dimension of the array <b>a</b> . $1da \ge \max(1,m)$ .
jpvt	INTEGER. Array, DIMENSION ( <i>n</i> ). If $jpvt(i) = k$ then column <i>k</i> of the full matrix <i>A</i> has been permuted into position <i>i</i> in <i>AP</i> .
vn1, vn2	REAL for slaqps/claqps DOUBLE PRECISION for dlaqps/zlaqps Arrays, DIMENSION ( <i>n</i> ) each. Contain the vectors with the partial and exact column norms, respectively.
auxv	REAL for slaqps DOUBLE PRECISION for dlaqps COMPLEX for claqps COMPLEX*16 for zlaqps Array, DIMENSION ( <i>nb</i> ). Auxiliary vector.
f	REAL for slaqps DOUBLE PRECISION for dlaqps COMPLEX for claqps COMPLEX*16 for zlaqps Array, DIMENSION ( $ldf,nb$ ). Matrix $F' = L*Y'*A$ .
ldf	<b>INTEGER</b> . The leading dimension of the array $f$ . $ldf \ge \max(1,n)$ .

kb	<b>INTEGER</b> . The number of columns actually factorized.
a	On exit, block $A(offset+1:m,1:kb)$ is the triangular factor obtained and block $A(1:offset,1:n)$ has been
	accordingly pivoted, but no factorized. The rest of the
	matrix, block A(offset+1:m,kb+1:n) has been updated.

jpvt	<b>INTEGER</b> array, <b>DIMENSION</b> $(n)$ . If $jpvt(i) = k$ then column $k$ of the full matrix $A$ has been permuted into position $i$ in $AP$ .
tau	REAL for slaqps DOUBLE PRECISION for dlaqps COMPLEX for claqps COMPLEX*16 for zlaqps Array, DIMENSION ( <i>kb</i> ). The scalar factors of the elementary reflectors.
vn1, vn2	The vectors with the partial and exact column norms, respectively.
auxv	Auxiliary vector.
f	Matrix $F' = L * Y' * A$ .

# ?laqsb

Scales a symmetric/Hermitian band matrix, using scaling factors computed by ?pbequ.

call slaqsb ( uplo, n, kd, ab, ldab, s, scond, amax, equed )
call dlaqsb ( uplo, n, kd, ab, ldab, s, scond, amax, equed )
call claqsb ( uplo, n, kd, ab, ldab, s, scond, amax, equed )
call zlaqsb ( uplo, n, kd, ab, ldab, s, scond, amax, equed )

## **Discussion**

The routine equilibrates a symmetric band matrix A using the scaling factors in the vector s.

## **Input Parameters**

input i aramot	
uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the symmetric matrix A is stored. If $uplo = 'U'$ : upper triangular. If $uplo = 'L'$ : lower triangular.
n	<b>INTEGER.</b> The order of the matrix <i>A</i> . $n \ge 0$ .
kd	<b>INTEGER.</b> The number of super-diagonals of the matrix A if $uplo = 'U'$ , or the number of sub-diagonals if $uplo = 'L'$ . $kd \ge 0$ .
ab	REAL for slaqsb DOUBLE PRECISION for dlaqsb COMPLEX for claqsb COMPLEX*16 for zlaqsb Array, DIMENSION ( <i>ldab,n</i> ). On entry, the upper or lower triangle of the symmetric band matrix A, stored in the first kd+1 rows of the array. The <i>j</i> -th column of A is stored in the <i>j</i> -th column of the array <i>ab</i> as follows: if $uplo = 'U'$ , $ab(kd+1+i-j,j) = A(i,j)$ for $max(1,j-kd) \le i \le j$ ; if $uplo = 'L'$ , $ab(1+i-j,j) = A(i,j)$ for $j \le i \le min(n,j+kd)$ .
ldab	<b>INTEGER.</b> The leading dimension of the array <i>ab</i> . $ldab \ge kd+1$ .
scond	REAL for slaqsb/claqsb DOUBLE PRECISION for dlaqsb/zlaqsb Ratio of the smallest $s(i)$ to the largest $s(i)$ .
amax	REAL for slaqsb/claqsb DOUBLE PRECISION for dlaqsb/zlaqsb Absolute value of largest matrix entry.

## **Output Parameters**

ab

On exit, if info = 0, the triangular factor U or L from the Cholesky factorization A = U'U or A = LL' of the band matrix A, in the same storage format as A.

S	REAL for slaqsb/claqsb
	DOUBLE PRECISION for dlaqsb/zlaqsb
	Array, <b>DIMENSION</b> ( <i>n</i> ). The scale factors for <i>A</i> .
equed	CHARACTER*1.
	Specifies whether or not equilibration was done.
	If $equed = 'N'$ : No equilibration.
	If equed = 'Y': Equilibration was done, that is, A has
	been replaced by $diag(s) * A * diag(s)$ .

## **Application Notes**

s

The routine uses internal parameters thresh, large, and small, which have the following meaning. thresh is a threshold value used to decide if scaling should be based on the ratio of the scaling factors. If scond < thresh, scaling is done. large and small are threshold values used to decide if scaling should be done based on the absolute size of the largest matrix element. If *amax* > *large* or *amax* < *small*, scaling is done.

## ?laqsp

Scales a symmetric/Hermitian matrix in packed storage, using scaling factors computed by ?ppequ.

> call slagsp (uplo, n, ap, s, scond, amax, equed) call dlagsp (uplo, n, ap, s, scond, amax, equed) call claqsp (uplo, n, ap, s, scond, amax, equed) call zlagsp (uplo, n, ap, s, scond, amax, equed)

### Discussion

The routine **?lagsp** equilibrates a symmetric matrix A using the scaling factors in the vector *s*.

## **Internal Parameters**

uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the symmetric matrix A is stored. If $uplo = 'U'$ : upper triangular. If $uplo = 'L'$ : lower triangular.
п	<b>INTEGER</b> . The order of the matrix <i>A</i> . $n \ge 0$ .
ap	REAL for slaqsp DOUBLE PRECISION for dlaqsp COMPLEX for claqsp COMPLEX*16 for zlaqsp Array, DIMENSION ( $n(n+1)/2$ ). On entry, the upper or lower triangle of the symmetric matrix $A$ , packed columnwise in a linear array. The <i>j</i> -th column of A is stored in the array <i>ap</i> as follows: if $uplo = 'U'$ , $ap(i + (j-1)j/2) = A(i,j)$ for $1 \le i \le j$ ; if $uplo = 'L'$ , $ap(i + (j-1)(2n-j)/2) = A(i,j)$ for $j \le \le$ .
S	REAL for slaqsp/claqsp DOUBLE PRECISION for dlaqsp/zlaqsp Array, DIMENSION (n). The scale factors for A.
scond	REAL for slaqsp/claqsp DOUBLE PRECISION for dlaqsp/zlaqsp Ratio of the smallest $s(i)$ to the largest $s(i)$ .
amax	REAL for slaqsp/claqsp DOUBLE PRECISION for dlaqsp/zlaqsp Absolute value of largest matrix entry.

## **Output Parameters**

ар	On exit, the equilibrated matrix: $diag(s)*A*diag(s)$ , in the same storage format as <i>A</i> .
equed	CHARACTER*1. Specifies whether or not equilibration was done. If $equed = 'N'$ : No equilibration. If $equed = 'Y'$ : Equilibration was done, that is, A has been replaced by diag(s)*A*diag(s).

### **Application Notes**

The routine uses internal parameters thresh, large, and small, which have the following meaning. thresh is a threshold value used to decide if scaling should be based on the ratio of the scaling factors. If scond < thresh, scaling is done. large and small are threshold values used to decide if scaling should be done based on the absolute size of the largest matrix element. If amax > large or amax < small, scaling is done.

## ?laqsy

Scales a symmetric/Hermitian matrix, using scaling factors computed by ?poequ.

call	slaqsy	(	uplo,	n,	a,	lda,	s,	scond,	amax,	equed	)
call	dlaqsy	(	uplo,	n,	a,	lda,	s,	scond,	amax,	equed	)
call	claqsy	(	uplo,	n,	a,	lda,	s,	scond,	amax,	equed	)
call	zlaqsy	(	uplo,	n,	a,	lda,	s,	scond,	amax,	equed	)

### **Discussion**

The routine equilibrates a symmetric matrix A using the scaling factors in the vector s.

uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the symmetric matrix $A$ is stored. If $uplo = 'U'$ : upper triangular. If $uplo = 'L'$ : lower triangular.
п	<b>INTEGER</b> . The order of the matrix <i>A</i> . $n \ge 0$ .
a	REAL for slaqsy DOUBLE PRECISION for dlaqsy COMPLEX for claqsy

	COMPLEX*16 for zlaqsy Array, DIMENSION ( <i>lda,n</i> ). On entry, the symmetric matrix A. If $uplo = 'U'$ , the leading <i>n</i> -by- <i>n</i> upper triangular part of <i>a</i> contains the upper triangular part of the matrix A, and the strictly lower triangular part of <i>a</i> is not referenced. If $uplo = 'L'$ , the leading <i>n</i> -by- <i>n</i> lower triangular part of <i>a</i> contains the lower triangular part of the matrix A, and the strictly upper triangular part of <i>a</i> is not referenced.
lda	<b>INTEGER.</b> The leading dimension of the array <i>a</i> . $1da \ge \max(n,1)$ .
S	REAL for slaqsy/claqsy DOUBLE PRECISION for dlaqsy/zlaqsy Array, DIMENSION (n). The scale factors for A.
scond	REAL for slaqsy/claqsy DOUBLE PRECISION for dlaqsy/zlaqsy Ratio of the smallest $s(i)$ to the largest $s(i)$ .
amax	REAL for slaqsy/claqsy DOUBLE PRECISION for dlaqsy/zlaqsy Absolute value of largest matrix entry.

equedCHARACTER*1.Specifies whether or not equilibration was done.If equed = 'N': No equilibration.If equed = 'Y': Equilibration was done, i.e., A has replaced by diag(s)*A*diag(s).	as been

## **Application Notes**

The routine uses internal parameters *thresh*, *large*, and *small*, which have the following meaning. *thresh* is a threshold value used to decide if scaling should be based on the ratio of the scaling factors. If *scond* <

thresh, scaling is done. large and small are threshold values used to decide if scaling should be done based on the absolute size of the largest matrix element. If amax > large or amax < small, scaling is done.

## ?laqtr

Solves a real quasi-triangular system of equations, or a complex quasi-triangular system of special form, in real arithmetic.

### **Discussion**

The routine <code>?laqtr</code> solves the real quasi-triangular system op(T) * p = scale * c, if *lreal* = .TRUE. or the complex quasi-triangular systems op(T + iB)*(p+iq) = scale*(c+id), if *lreal* = .FALSE. in real arithmetic, where T is upper quasi-triangular.

If lreal = .FALSE., then the first diagonal block of T must be 1-by-1, B is the specially structured matrix

$$B = \begin{bmatrix} b_1 & b_2 & \dots & b_n \\ & w & & \\ & & w & \\ & & & \ddots & \\ & & & & w \end{bmatrix}$$

op(A) = A or A', A' denotes the conjugate transpose of matrix A. On input,

$$\mathbf{x} = \begin{bmatrix} c \\ d \end{bmatrix}$$
, on output  $\mathbf{x} = \begin{bmatrix} p \\ q \end{bmatrix}$ 

This routine is designed for the condition number estimation in routine ?trsna.

ltran	LOGICAL. On entry, <i>ltran</i> specifies the option of conjugate transpose: = .FALSE., $op(T + iB) = T + iB$ , = .TRUE., $op(T + iB) = (T + iB)'$ .
lreal	LOGICAL. On entry, <i>lreal</i> specifies the input matrix structure: = .FALSE., the input is complex = .TRUE., the input is real.
n	<b>INTEGER.</b> On entry, <i>n</i> specifies the order of $T + iB$ . $n \ge 0$ .
t	<b>REAL</b> for slaqtr <b>DOUBLE PRECISION</b> for dlaqtr Array, dimension $(ldt,n)$ . On entry, <i>t</i> contains a matrix in Schur canonical form. If $lreal = .FALSE.$ , then the first diagonal block of <i>t</i> must be 1-by-1.
ldt	<b>INTEGER.</b> The leading dimension of the matrix <i>T</i> . $1dt \ge \max(1,n)$ .
b	<b>REAL</b> for slaqtr <b>DOUBLE PRECISION</b> for dlaqtr Array, dimension $(n)$ . On entry, $b$ contains the elements to form the matrix $B$ as described above. If lreal = .TRUE., b is not referenced.
W	REAL for slaqtr DOUBLE PRECISION for dlaqtr On entry, w is the diagonal element of the matrix B. If <i>lreal</i> = .TRUE., w is not referenced.

x	REAL for slaqtr DOUBLE PRECISION for dlaqtr Array, dimension $(2n)$ . On entry, x contains the right hand side of the system.
work	REAL for slaqtr DOUBLE PRECISION for dlaqtr Workspace array, dimension ( <i>n</i> ).
Output Parame	ters
scale	REAL for slaqtr DOUBLE PRECISION for dlaqtr On exit, <i>scale</i> is the scale factor.
x	On exit, $\mathbf{x}$ is overwritten by the solution.
info	<pre>INTEGER. If info = 0: successful exit. If info = 1: the some diagonal 1-by-1 block has been perturbed by a small number smin to keep nonsingularity. If info = 2: the some diagonal 2-by-2 block has been perturbed by a small number in ?laln2 to keep nonsingularity.</pre>



**NOTE.** *In the interests of speed, this routine does not check the inputs for errors.* 

## ?lar1v

Computes the (scaled)  $\mathbf{r}$ -th column of the inverse of the submatrix in rows b1 through bn of the tridiagonal matrix  $LDL^{T} - \mathbf{q}$ .

## **Discussion**

The routine ?larlv computes the (scaled) r-th column of the inverse of the submatrix in rows *b1* through *bn* of the tridiagonal matrix  $LDL^{T}$  -  $\mathbf{O}^{*}I$ .

The following steps accomplish this computation :

- 1. Stationary *qd* transform,  $LDL^T \mathbf{G} \cdot I = L(+) D(+) L(+)^T$
- 2. Progressive *qd* transform,  $LDL^T \sigma I = U(-) D(-) U(-)^T$ ,
- 3. Computation of the diagonal elements of the inverse of  $LDL^{T}$   $\sigma I$  by combining the above transforms, and choosing r as the index where the diagonal of the inverse is (one of the) largest in magnitude.
- 4. Computation of the (scaled) *r*-th column of the inverse using the twisted factorization obtained by combining the top part of the stationary and the bottom part of the progressive transform.

п	<b>INTEGER.</b> The order of the matrix $LDL^{T}$ .
b1	<b>INTEGER.</b> First index of the submatrix of $LDL^{T}$ .

bn	<b>INTEGER.</b> Last index of the submatrix of $LDL^{T}$ .
sigma	<b>REAL for slarlv/clarlv</b> <b>DOUBLE PRECISION for dlarlv/zlarlv</b> The shift. Initially, when $r = 0$ , <i>sigma</i> should be a good approximation to an eigenvalue of $LDL^{T}$ .
1	REAL for slarlv/clarlv DOUBLE PRECISION for dlarlv/zlarlv Array, DIMENSION ( <i>n</i> -1). The ( <i>n</i> -1) subdiagonal elements of the unit bidiagonal matrix <i>L</i> , in elements 1 to <i>n</i> -1.
d	REAL for slarlv/clarlv DOUBLE PRECISION for dlarlv/zlarlv Array, DIMENSION ( <i>n</i> ). The <i>n</i> diagonal elements of the diagonal matrix <i>D</i> .
ld	REAL for slarlv/clarlv DOUBLE PRECISION for dlarlv/zlarlv Array, DIMENSION ( $n$ -1). The $n$ -1 elements $L_i^*D_i$ .
11d	REAL for slarlv/clarlv DOUBLE PRECISION for dlarlv/zlarlv Array, DIMENSION ( <i>n</i> -1). The <i>n</i> -1 elements $L_i^*L_i^*D_i$ .
gersch	REAL for slarlv/clarlv DOUBLE PRECISION for dlarlv/zlarlv Array, DIMENSION (2n). The <i>n</i> Gerschgorin intervals. These are used to restrict the initial search for <i>r</i> , when <i>r</i> is input as 0.
r	INTEGER. Initially $r$ should be input to be 0 and is then output as the index where the diagonal element of the inverse is largest in magnitude. In later iterations, this same value of $r$ should be input.
work	REAL for slarlv/clarlv DOUBLE PRECISION for dlarlv/zlarlv Workspace array, DIMENSION (4 <i>n</i> ).

Ζ	REAL for slarlv DOUBLE PRECISION for dlarlv COMPLEX for clarlv COMPLEX*16 for zlarlv Array, DIMENSION ( <i>n</i> ). The (scaled) <i>r</i> -th column of the
	inverse. $z(r)$ is returned to be 1.
ztz	REAL for slarlv/clarlv DOUBLE PRECISION for dlarlv/zlarlv The square of the norm of z.
mingma	<b>REAL</b> for slarlv/clarlv <b>DOUBLE PRECISION</b> for dlarlv/zlarlv The reciprocal of the largest (in magnitude) diagonal element of the inverse of $LDL^T$ - $\sigma$ * <i>I</i> .
r	On output, $\mathbf{r}$ is the index where the diagonal element of the inverse is largest in magnitude.
isuppz	INTEGER. Array, DIMENSION (2). The support of the vector in $z$ , that is, the vector $z$ is nonzero only in elements isuppz(1) through $isuppz(2)$ .

## ?lar2v

Applies a vector of plane rotations with real cosines and real/complex sines from both sides to a sequence of 2-by-2 symmetric/Hermitian matrices.

call slar2v ( n, x, y, z, incx, c, s, incc )
call dlar2v ( n, x, y, z, incx, c, s, incc )
call clar2v ( n, x, y, z, incx, c, s, incc )
call zlar2v ( n, x, y, z, incx, c, s, incc )

## Discussion

The routine  $2 \ln 2v$  applies a vector of real/complex plane rotations with real cosines from both sides to a sequence of 2-by-2 real symmetric or complex Hermitian matrices, defined by the elements of the vectors x, y and z. For i = 1, 2, ..., n

$$\begin{bmatrix} x_i & z_i \\ \operatorname{conjg}(z_i) & y_i \end{bmatrix} : = \begin{bmatrix} c(i) & \operatorname{conjg}(s(i)) \\ -s(i) & c(i) \end{bmatrix} \begin{bmatrix} x_i & z_i \\ \operatorname{conjg}(z_i) & y_i \end{bmatrix} \begin{bmatrix} c(i) & -\operatorname{conjg}(s(i)) \\ s(i) & c(i) \end{bmatrix}$$

п	<b>INTEGER</b> . The number of plane rotations to be applied.
x, y, z	REAL for slar2v DOUBLE PRECISION for dlar2v COMPLEX for clar2v COMPLEX*16 for zlar2v Arrays, DIMENSION $(1+(n-1)*incx)$ each. Contain the vectors $x$ , $y$ and $z$ , respectively. For all flavors of ?lar2v, elements of $x$ and $y$ are assumed to be real.
incx	<b>INTEGER.</b> The increment between elements of $x$ , $y$ , and $z$ . <i>incx</i> > 0.
С	REAL for slar2v/clar2v DOUBLE PRECISION for dlar2v/zlar2v Array, DIMENSION (1+(n-1)*incc). The cosines of the plane rotations.
S	REAL for slar2v DOUBLE PRECISION for dlar2v COMPLEX for clar2v COMPLEX*16 for zlar2v Array, DIMENSION (1+(n-1)*incc). The sines of the plane rotations.
incc	<b>INTEGER.</b> The increment between elements of $c$ and $s$ . inc $c > 0$ .

x, y, z Vectors x, y and z, containing the results of transform.

## ?larf

Applies an elementary reflector to a general rectangular matrix.

call slarf ( side, m, n, v, incv, tau, c, ldc, work )
call dlarf ( side, m, n, v, incv, tau, c, ldc, work )
call clarf ( side, m, n, v, incv, tau, c, ldc, work )
call zlarf ( side, m, n, v, incv, tau, c, ldc, work )

#### **Discussion**

The routine applies a real/complex elementary reflector H to a real/complex m-by-n matrix C, from either the left or the right. H is represented in the form

H = I - tau * v * v',

where tau is a real/complex scalar and v is a real/complex vector.

If tau = 0, then *H* is taken to be the unit matrix. For clarf/zlarf, to apply *H*' (the conjugate transpose of *H*), supply conjg(tau) instead of tau.

side	CHARACTER*1.
	If <b>side</b> = 'L': form $H * C$
	If <b>side</b> = 'R': form $C * H$ .
m	<b>INTEGER</b> . The number of rows of the matrix $C$ .
n	INTEGER. The number of columns of the matrix $C$ .
v	REAL for slarf
	DOUBLE PRECISION for dlarf
	COMPLEX for clarf

	COMPLEX*16 for zlarf Array, DIMENSION (1 + (m-1)*abs(incv)) if side = 'L' or (1 + (n-1)*abs(incv)) if side = 'R'. The vector $v$ in the representation of $H$ . $v$ is not used if tau = 0.
incv	<b>INTEGER.</b> The increment between elements of $v$ . incv $\neq 0$ .
tau	REAL for slarf DOUBLE PRECISION for dlarf COMPLEX for clarf COMPLEX*16 for zlarf The value <i>tau</i> in the representation of <i>H</i> .
c	REAL for slarf DOUBLE PRECISION for dlarf COMPLEX for clarf COMPLEX*16 for zlarf Array, DIMENSION ( <i>ldc</i> , <i>n</i> ). On entry, the <i>m</i> -by- <i>n</i> matrix <i>C</i> .
ldc	<b>INTEGER.</b> The leading dimension of the array $c$ . $ldc \ge max(1,m)$ .
work	REAL for slarf DOUBLE PRECISION for dlarf COMPLEX for clarf COMPLEX*16 for zlarf Workspace array, DIMENSION (n) if side = 'L' or (m) if side = 'R'.

c On exit, c is overwritten by the matrix H*C if side = 'L', or C*H if side = 'R'.

## ?larfb

Applies a block reflector or its transpose/conjugate-transpose to a general rectangular matrix.

call slarfb (			storev, m, n, k, v, work, ldwork )
call dlarfb (			storev, m, n, k, v, work, ldwork )
call clarfb (	side, trans,	direct,	storev, m, n, k, v,
	ldv, t, ldt,	c, ldc,	work, ldwork )

## **Discussion**

The routine ?larfb applies a complex block reflector H or its transpose H' to a complex *m*-by-*n* matrix C from either left or right.

side	CHARACTER*1. If <i>side</i> = 'L': apply <i>H</i> or <i>H'</i> from the left If <i>side</i> = 'R': apply <i>H</i> or <i>H'</i> from the right
trans	CHARACTER*1. If <i>trans</i> = 'N': apply <i>H</i> (No transpose) If <i>trans</i> = 'C': apply <i>H</i> ' (Conjugate transpose)
direct	CHARACTER*1. Indicates how <i>H</i> is formed from a product of elementary reflectors If <i>direct</i> = 'F': $H = H(1) H(2) \dots H(k)$ (forward) If <i>direct</i> = 'B': $H = H(k) \dots H(2) H(1)$ (backward)
storev	CHARACTER*1. Indicates how the vectors which define the elementary reflectors are stored: If <i>storev</i> = 'C': Column-wise If <i>storev</i> = 'R': Row-wise

т	<b>INTEGER.</b> The number of rows of the matrix $C$ .
n	<b>INTEGER</b> . The number of columns of the matrix C.
k	<b>INTEGER.</b> The order of the matrix $T$ (equal to the number of elementary reflectors whose product defines the block reflector).
V	REAL for slarfb DOUBLE PRECISION for dlarfb COMPLEX for clarfb COMPLEX*16 for zlarfb Array, DIMENSION (ldv, k) if storev = 'C' (ldv, m) if storev = 'R' and side = 'L' (ldv, n) if storev = 'R' and side = 'R' The matrix V.
ldv	INTEGER. The leading dimension of the array v. If <i>storev</i> = 'C' and <i>side</i> = 'L', $1dv \ge max(1,m)$ ; if <i>storev</i> = 'C' and <i>side</i> = 'R', $1dv \ge max(1,n)$ ; if <i>storev</i> = 'R', $1dv \ge k$ .
t	REAL for slarfb DOUBLE PRECISION for dlarfb COMPLEX for clarfb COMPLEX*16 for zlarfb Array, DIMENSION ( <i>ldt</i> , <i>k</i> ). Contains the triangular <i>k</i> -by- <i>k</i> matrix <i>T</i> in the representation of the block reflector.
ldt	<b>INTEGER.</b> The leading dimension of the array $t$ . ldt $\geq k$ .
С	REAL for slarfb DOUBLE PRECISION for dlarfb COMPLEX for clarfb COMPLEX*16 for zlarfb Array, DIMENSION ( <i>ldc</i> , <i>n</i> ). On entry, the <i>m</i> -by- <i>n</i> matrix <i>C</i> .

ldc	<b>INTEGER</b> . The leading dimension of the array $c$ . $ldc \ge max(1,m)$ .
work	REAL for slarfb DOUBLE PRECISION for dlarfb COMPLEX for clarfb COMPLEX*16 for zlarfb Workspace array, DIMENSION ( <i>ldwork</i> , <i>k</i> ).
ldwork	<b>INTEGER.</b> The leading dimension of the array work. If $side = 'L'$ , $ldwork \ge max(1, n)$ ; if $side = 'R'$ , $ldwork \ge max(1, m)$ .

On exit, c is overwritten by  $H^*C$  or H' *C or  $C^*H$  or  $C^*H'$ .

# ?larfg

Generates an elementary reflector (Householder matrix).

С

call slarfg ( n, alpha, x, incx, tau )
call dlarfg ( n, alpha, x, incx, tau )
call clarfg ( n, alpha, x, incx, tau )
call zlarfg ( n, alpha, x, incx, tau )

### **Discussion**

$$H' * \begin{bmatrix} alpha \\ x \end{bmatrix} = \begin{bmatrix} beta \\ 0 \end{bmatrix}, \quad H' * H = I,$$

where *alpha* and *beta* are scalars (with *beta* real for all flavors), and x is an (*n*-1)-element real/complex vector. *H* is represented in the form

$$H = I - tau^* \begin{bmatrix} 1 \\ v \end{bmatrix} * \begin{bmatrix} 1 & v' \end{bmatrix}$$

where tau is a real/complex scalar and v is a real/complex (n-1)-element vector. Note that for clarfg/zlarfg, H is not Hermitian.

If the elements of x are all zero (and, for complex flavors, *alpha* is real), then tau = 0 and H is taken to be the unit matrix.

Otherwise,  $1 \leq tau \leq 2$  (for real flavors), or  $1 \leq \operatorname{Re}(tau) \leq 2$  and  $\operatorname{abs}(tau-1) \leq 1$  (for complex flavors).

## **Input Parameters**

n	<b>INTEGER</b> . The order of the elementary reflector.
alpha	REAL for slarfg DOUBLE PRECISION for dlarfg COMPLEX for clarfg COMPLEX*16 for zlarfg On entry, the value <i>alpha</i> .
x	REAL for slarfg DOUBLE PRECISION for dlarfg COMPLEX for clarfg COMPLEX*16 for zlarfg Array, DIMENSION (1+(n-2)*abs( <i>incx</i> )). On entry, the vector <i>x</i> .
incx	INTEGER. The increment between elements of $x$ . $incx > 0$ .

### **Output Parameters**

alpha	On exit, it is overwritten with the value <i>beta</i> .
x	On exit, it is overwritten with the vector <i>v</i> .

tau

REAL for slarfg DOUBLE PRECISION for dlarfg COMPLEX for clarfg COMPLEX*16 for zlarfg The value *tau*.

## ?larft

Forms the triangular factor T of a block reflector  $H = I \cdot VTV^{H}$ .

```
call slarft ( direct, storev, n, k, v, ldv, tau, t, ldt )
call dlarft ( direct, storev, n, k, v, ldv, tau, t, ldt )
call clarft ( direct, storev, n, k, v, ldv, tau, t, ldt )
call zlarft ( direct, storev, n, k, v, ldv, tau, t, ldt )
```

#### **Discussion**

The routine <code>?larft</code> forms the triangular factor T of a real/complex block reflector H of order n, which is defined as a product of k elementary reflectors.

If direct = F',  $H = H(1) H(2) \dots H(k)$  and T is upper triangular;

If direct = B',  $H = H(k) \dots H(2) H(1)$  and T is lower triangular.

If *storev* = 'C', the vector which defines the elementary reflector H(i) is stored in the *i*-th column of the array *v*, and H = I - V * T * V'.

If *storev* = 'R', the vector which defines the elementary reflector H(i) is stored in the *i*-th row of the array *v*, and H = I - V' * T * V.

## **Input Parameters**

direct

CHARACTER*1. Specifies the order in which the elementary reflectors are multiplied to form the block reflector:

= '**F**':  $H = H(1) H(2) \dots H(k)$  (forward) = '**B**':  $H = H(k) \dots H(2) H(1)$  (backward)

storev	CHARACTER*1. Specifies how the vectors which define the elementary reflectors are stored (see also <i>Application Notes</i> below): = 'C': column-wise = 'R': row-wise.
п	<b>INTEGER</b> . The order of the block reflector <i>H</i> . $n \ge 0$ .
k	<b>INTEGER.</b> The order of the triangular factor <i>T</i> (equal to the number of elementary reflectors). $k \ge 1$ .
V	REAL for slarft DOUBLE PRECISION for dlarft COMPLEX for clarft COMPLEX*16 for zlarft Array, DIMENSION (ldv, k) if storev = 'C' or (ldv, n) if storev = 'R'. The matrix V.
ldv	<b>INTEGER.</b> The leading dimension of the array v. If $storev = 'C'$ , $ldv \ge max(1,n)$ ; if $storev = 'R'$ , $ldv \ge k$ .
tau	REAL for slarft DOUBLE PRECISION for dlarft COMPLEX for clarft COMPLEX*16 for zlarft Array, DIMENSION (k). tau(i) must contain the scalar factor of the elementary reflector $H(i)$ .
ldt	<b>INTEGER</b> . The leading dimension of the output array $t$ . $ldt \ge k$ .

t	REAL for slarft
	DOUBLE PRECISION for dlarft
	COMPLEX for clarft
	COMPLEX*16 for zlarft
	Array, DIMENSION ( <i>ldt</i> , <i>k</i> ). The <i>k</i> -by- <i>k</i> triangular factor

*T* of the block reflector. If *direct* = 'F', *T* is upper triangular; if *direct* = 'B', *T* is lower triangular. The rest of the array is not used.

v

The matrix V.

## **Application Notes**

The shape of the matrix V and the storage of the vectors which define the H(i) is best illustrated by the following example with n = 5 and k = 3. The elements equal to 1 are not stored; the corresponding array elements are modified but restored on exit. The rest of the array is not used.

direct = 'F' and storev = 'C': direct = 'F' and storev = 'R':

$\begin{bmatrix} 1 \end{bmatrix}$	
$v_1$ 1	$\begin{bmatrix} 1 & v_1 & v_1 & v_1 \\ v_1 & v_1 & v_1 \end{bmatrix}$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$1 v_2 v_2 v_2$
$v_1 \ v_2 \ v_3$	$1 v_3 v_3$
$v_1 v_2 v_3$	

direct = 'B' and storev = 'C': direct = 'B' and storev = 'R':

$$\begin{bmatrix} v_1 & v_2 & v_3 \\ v_1 & v_2 & v_3 \\ 1 & v_2 & v_3 \\ 1 & v_3 \\ 1 \end{bmatrix}$$
$$\begin{bmatrix} v_1 & v_1 & 1 \\ v_2 & v_2 & v_2 & 1 \\ v_3 & v_3 & v_3 & v_3 & 1 \end{bmatrix}$$

## ?larfx

Applies an elementary reflector to a general rectangular matrix, with loop unrolling when the reflector has order  $\leq 10$ .

call slarfx ( side, m, n, v, tau, c, ldc, work )
call dlarfx ( side, m, n, v, tau, c, ldc, work )
call clarfx ( side, m, n, v, tau, c, ldc, work )
call zlarfx ( side, m, n, v, tau, c, ldc, work )

#### **Discussion**

The routine ?larfx applies a real/complex elementary reflector H to a real/complex *m*-by-*n* matrix C, from either the left or the right. H is represented in the form H = I - tau * v * v', where tau is a real/complex scalar and v is a real/complex vector.

If tau = 0, then *H* is taken to be the unit matrix

side	CHARACTER*1. If side = 'L': form $H*C$ If side = 'R': form $C*H$ .
m	<b>INTEGER.</b> The number of rows of the matrix $C$ .
n	<b>INTEGER.</b> The number of columns of the matrix $C$ .
V	REAL for slarfx DOUBLE PRECISION for dlarfx COMPLEX for clarfx COMPLEX*16 for zlarfx Array, DIMENSION (m) if side = 'L' or (n) if side = 'R'. The vector v in the representation of H.

tau	REAL for slarfx DOUBLE PRECISION for dlarfx COMPLEX for clarfx COMPLEX*16 for zlarfx The value <i>tau</i> in the representation of <i>H</i> .
С	REAL for slarfx DOUBLE PRECISION for dlarfx COMPLEX for clarfx COMPLEX*16 for zlarfx Array, DIMENSION ( <i>ldc</i> , <i>n</i> ). On entry, the <i>m</i> -by- <i>n</i> matrix C.
ldc	<b>INTEGER</b> . The leading dimension of the array $c$ . $lda \ge (1,m)$ .
work	REAL for slarfx DOUBLE PRECISION for dlarfx COMPLEX for clarfx COMPLEX*16 for zlarfx Workspace array, DIMENSION (n) if side = 'L' or (m) if side = 'R'. work is not referenced if H has order < 11.

С

On exit, C is overwritten by the matrix  $H^*C$  if *side* = 'L', or  $C^*H$  if *side* = 'R'.

# ?largv

Generates a vector of plane rotations with real cosines and real/complex sines.

call slargv ( n, x, incx, y, incy, c, incc )

call dlargv ( n, x, incx, y, incy, c, incc )
call clargv ( n, x, incx, y, incy, c, incc )
call zlargv ( n, x, incx, y, incy, c, incc )

#### **Discussion**

The routine generates a vector of real/complex plane rotations with real cosines, determined by elements of the real/complex vectors x and y.

For slargv/dlargv:

$$\begin{bmatrix} \mathbf{c}(i) & s(i) \\ -s(i) & \mathbf{c}(i) \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix} = \begin{bmatrix} a_i \\ 0 \end{bmatrix} , \text{ for } i = 1, 2, \dots, n$$

For clargv/zlargv:

$$\begin{bmatrix} \mathbf{c}(i) & s(i) \\ -\operatorname{conjg}(s(i)) & \mathbf{c}(i) \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix} = \begin{bmatrix} r_i \\ 0 \end{bmatrix}, \text{ for } i = 1, 2, \dots, n$$

where  $c(i)^2 + abs(s(i))^2 = 1$  and the following conventions are used (these are the same as in clartg/zlartg but differ from the BLAS Level 1 routine crotg/zrotg):

If  $y_i = 0$ , then c(i) = 1 and s(i) = 0; If  $x_i = 0$ , then c(i) = 0 and s(i) is chosen so that  $r_i$  is real.

n	<b>INTEGER.</b> The number of plane rotations to be generated.
х, у	REAL for slargv DOUBLE PRECISION for dlargv COMPLEX for clargv COMPLEX*16 for zlargv Arrays, DIMENSION $(1+(n-1)*incx)$ and $(1+(n-1)*incy)$ , respectively. On entry, the vectors <i>x</i> and <i>y</i> .
incx	<b>INTEGER.</b> The increment between elements of $x$ . <i>incx</i> > 0.

incy	<b>INTEGER</b> . The increment between elements of <i>y</i> . <i>incy</i> $> 0$ .
incc	<b>INTEGER.</b> The increment between elements of the output array $c$ . <i>incc</i> > 0.
Output Parameters	
x	On exit, $\mathbf{x}(i)$ is overwritten by $a_i$ (for real flavors), or by $r_i$ (for complex flavors), for $i = 1,, n$ .
Y	On exit, the sines $s(i)$ of the plane rotations.
С	<b>REAL</b> for slargv/clargv DOUBLE PRECISION for dlargv/zlargv Array, DIMENSION $(1+(n-1)*incc)$ . The cosines of the plane rotations.

## ?larnv

Returns a vector of random numbers from a uniform or normal distribution.

```
call slarnv ( idist, iseed, n, x )
call dlarnv ( idist, iseed, n, x )
call clarnv ( idist, iseed, n, x )
call zlarnv ( idist, iseed, n, x )
```

### **Discussion**

The routine **?larnv** returns a vector of *n* random real/complex numbers from a uniform or normal distribution.

This routine calls the auxiliary routine **?laruv** to generate random real numbers from a uniform (0,1) distribution, in batches of up to 128 using vectorisable code. The Box-Muller method is used to transform numbers from a uniform to a normal distribution.

## **Input Parameters**

idist	<pre>INTEGER. Specifies the distribution of the random numbers: for slarnv and dlanrv: = 1: uniform (0,1) = 2: uniform (-1,1) = 3: normal (0,1). for clarnv and zlanrv: = 1: real and imaginary parts each uniform (0,1) = 2: real and imaginary parts each uniform (-1,1) = 3: real and imaginary parts each normal (0,1) = 4: uniformly distributed on the disc abs(z) &lt; 1 = 5: uniformly distributed on the circle abs(z) = 1</pre>
iseed	INTEGER. Array, DIMENSION (4). On entry, the seed of the random number generator; the array elements must be between 0 and 4095, and <i>iseed</i> (4) must be odd.
n	<b>INTEGER</b> . The number of random numbers to be generated.
Output Parame	eters
x	REAL for slarnv DOUBLE PRECISION for dlarnv COMPLEX for clarnv COMPLEX*16 for zlarnv Array, DIMENSION (n). The generated random numbers.

*iseed* On exit, the seed is updated.

# ?larrb

*Provides limited bisection to locate eigenvalues for more accuracy.* 

#### Discussion

Given the relatively robust representation(RRR)  $LDL^T$ , the routine does "limited" bisection to locate the eigenvalues of  $LDL^T$ , w(ifirst) through w(ilast), to more accuracy. Intervals [*left*, *right*] are maintained by storing their mid-points and semi-widths in the arrays w and werr respectively.

n	<b>INTEGER</b> . The order of the matrix.
d	REAL for slarrb DOUBLE PRECISION for dlarrb Array, DIMENSION ( <i>n</i> ). The <i>n</i> diagonal elements of the diagonal matrix <i>D</i> .
1	REAL for slarrb DOUBLE PRECISION for dlarrb Array, DIMENSION ( <i>n</i> -1). The <i>n</i> -1 subdiagonal elements of the unit bidiagonal matrix <i>L</i> .
ld	REAL for slarrb DOUBLE PRECISION for dlarrb Array, DIMENSION ( $n$ -1). The $n$ -1 elements $L_i * D_i$ .
11d	REAL for slarrb DOUBLE PRECISION for dlarrb Array, DIMENSION ( $n$ -1). The $n$ -1 elements $L_i * L_i * D_i$ .
ifirst	<b>INTEGER.</b> The index of the first eigenvalue in the cluster.

ilast	<b>INTEGER.</b> The index of the last eigenvalue in the cluster.
sigma	<b>REAL</b> for slarrb DOUBLE PRECISION for dlarrb The shift used to form $LDL^T$ (see ?larrf).
reltol	REAL for slarrb DOUBLE PRECISION for dlarrb The relative tolerance.
W	<b>REAL</b> for slarrb <b>DOUBLE PRECISION</b> for dlarrb Array, <b>DIMENSION</b> ( <i>n</i> ). On input, $w(ifirst)$ through w(ilast) are estimates of the corresponding eigenvalues of $LDL^{T}$ .
wgap	<b>REAL</b> for slarrb <b>DOUBLE PRECISION</b> for dlarrb Array, <b>DIMENSION</b> ( <i>n</i> ). The gaps between the eigenvalues of $LDL^T$ .
werr	REAL for slarrb DOUBLE PRECISION for dlarrb Array, DIMENSION (n). On input, werr(ifirst) through werr(ilast) are the errors in the estimates w(ifirst) through w(ilast).
work	REAL for slarrb DOUBLE PRECISION for dlarrb Workspace array. Note that this parameter is never used in the routine.
iwork	INTEGER. Workspace array, DIMENSION (2 <i>n</i> ).
Output Parame	ters
W	On output these estimates of the eigenvalues are "refined".
wgap	Very small gaps are changed on output.
werr	On output, "refined" errors in the estimates $w(ifirst)$

r On output, "refined" errors in the estimates w(ifirst)through w(ilast). info

INTEGER.

Error flag. Note that this parameter is never set in the routine.

## ?larre

Given the tridiagonal matrix T, sets small off-diagonal elements to zero and for each unreduced block  $T_i$ , finds base representations and eigenvalues.

```
call slarre ( n, d, e, tol, nsplit, isplit, m, w, woff,
               gersch, work, info )
call dlarre ( n, d, e, tol, nsplit, isplit, m, w, woff,
               gersch, work, info )
```

#### Discussion

Given the tridiagonal matrix T, the routine sets "small" off-diagonal elements to zero, and for each unreduced block  $T_i$ , it finds

- the numbers  $\sigma_i$
- the base  $T_i \sigma_i I = L_i D_i L_i^T$  representations and eigenvalues of each  $L_i D_i L_i^T$ . •

The representations and eigenvalues found are then used by ?stegr to compute the eigenvectors of a symmetric tridiagonal matrix. Currently, the base representations are limited to being positive or negative definite, and the eigenvalues of the definite matrices are found by the dqds algorithm (subroutine ?lasq2). As an added benefit, ?larre also outputs the n Gerschgorin intervals for each  $L_i D_i L_i^T$ .

#### **Input Parameters**

n

**INTEGER**. The order of the matrix.

d	REAL for slarre DOUBLE PRECISION for dlarre Array, DIMENSION ( <i>n</i> ). On entry, the <i>n</i> diagonal elements of the tridiagonal matrix <i>T</i> .
e	<b>REAL</b> for slarre DOUBLE PRECISION for dlarre Array, DIMENSION ( <i>n</i> ). On entry, the ( <i>n</i> -1) subdiagonal elements of the tridiagonal matrix $T$ ; $e(n)$ need not be set.
tol	<b>REAL</b> for slarre <b>DOUBLE PRECISION</b> for dlarre The threshold for splitting. If on input $ e(i)  < tol$ , then the matrix <i>T</i> is split into smaller blocks.
nsplit	<b>INTEGER.</b> The number of blocks <i>T</i> splits into. $1 \leq n \leq n$ .
work	REAL for slarre DOUBLE PRECISION for dlarre Workspace array, DIMENSION (4* <i>n</i> ).
Output Parame	ters
d	On exit, the <i>n</i> diagonal elements of the diagonal matrices $D_i$ .

*e* On exit, the subdiagonal elements of the unit bidiagonal matrices  $L_i$ .

## isplit INTEGER.

т

Array, DIMENSION (2n). The splitting points, at which T breaks up into submatrices. The first submatrix consists of rows/columns 1 to *isplit*(1), the second of rows/columns *isplit*(1)+1 through *isplit*(2), etc., and the *nsplit*-th consists of rows/columns *isplit*(*nsplit*-1)+1 through *isplit*(*nsplit*)=n. INTEGER. The total number of eigenvalues (of all the  $L_i D_i L_i^T$ ) found.

W	<b>REAL</b> for slarre <b>DOUBLE PRECISION</b> for dlarre Array, <b>DIMENSION</b> ( <i>n</i> ). The first <i>m</i> elements contain the eigenvalues. The eigenvalues of each of the blocks, $L_i D_i L_i^T$ , are sorted in ascending order.
woff	REAL for slarre DOUBLE PRECISION for dlarre Array, DIMENSION ( $n$ ). The <i>nsplit</i> base points $\sigma_i$ .
gersch	<b>REAL</b> for slarre <b>DOUBLE PRECISION</b> for dlarre Array, <b>DIMENSION</b> (2 <i>n</i> ). The <i>n</i> Gerschgorin intervals.
info	<b>INTEGER.</b> Output error code from <b>?lasq2</b> .

## ?larrf

Finds a new relatively robust representation such that at least one of the eigenvalues is relatively isolated.

### **Discussion**

Given the initial representation  $LDL^T$  and its cluster of close eigenvalues (in a relative measure), w(ifirst), w(ifirst+1), ... w(ilast), the routine ?larrf finds a new relatively robust representation

 $LDL^{T} - \mathbf{G}_{i} I = L(+)D(+)L(+)^{T}$ 

such that at least one of the eigenvalues of  $L(+)D(+)L(+)^T$  is relatively isolated.

п	INTEGER. The order of the matrix.
d	REAL for slarrf DOUBLE PRECISION for dlarrf Array, DIMENSION ( <i>n</i> ). The <i>n</i> diagonal elements of the diagonal matrix <i>D</i> .
1	REAL for slarrf DOUBLE PRECISION for dlarrf Array, DIMENSION ( <i>n</i> -1). The ( <i>n</i> -1) subdiagonal elements of the unit bidiagonal matrix <i>L</i> .
1d	REAL for slarrf DOUBLE PRECISION for dlarrf Array, DIMENSION ( $n$ -1). The $n$ -1 elements $L_i * D_i$ .
11d	REAL for slarrf DOUBLE PRECISION for dlarrf Array, DIMENSION ( $n$ -1). The $n$ -1 elements $L_i * L_i * D_i$ .
ifirst	<b>INTEGER</b> . The index of the first eigenvalue in the cluster.
ilast	<b>INTEGER</b> . The index of the last eigenvalue in the cluster.
W	<b>REAL</b> for slarrf <b>DOUBLE</b> PRECISION for dlarrf Array, DIMENSION ( <i>n</i> ). On input, the eigenvalues of $LDL^{T}$ in ascending order. <i>w</i> ( <i>ifirst</i> ) through <i>w</i> ( <i>ilast</i> ) form the cluster of relatively close eigenvalues.
sigma	<b>REAL</b> for slarrf <b>DOUBLE PRECISION</b> for dlarrf The shift used to form $L(+)D(+)L(+)^T$ .
work	REAL for slarrf DOUBLE PRECISION for dlarrf Workspace array.

W	On output, $w(ifirst)$ through $w(ilast)$ are estimates of the corresponding eigenvalues of $L(+)D(+)L(+)^{T}$ .
dplus	<b>REAL for slarrf</b> <b>DOUBLE PRECISION for dlarrf</b> Array, <b>DIMENSION</b> ( <i>n</i> ). The <i>n</i> diagonal elements of the diagonal matrix $D(+)$ .
lplus	REAL for slarrf DOUBLE PRECISION for dlarrf Array, DIMENSION ( $n$ ). The first ( $n$ -1) elements of <i>lplus</i> contain the subdiagonal elements of the unit bidiagonal matrix $L(+)$ . <i>lplus</i> ( $n$ ) is set to <i>sigma</i> .

## ?larrv

Computes the eigenvectors of the tridiagonal matrix  $T = L D L^T$  given L, D and the eigenvalues of  $L D L^T$ .

### **Discussion**

The routine **?larrv** computes the eigenvectors of the tridiagonal matrix  $T = L D L^T$  given L, D and the eigenvalues of  $L D L^T$ . The input eigenvalues should have high relative accuracy with respect to the entries of L and D. The desired accuracy of the output can be specified by the input parameter **tol**.

n	<b>INTEGER</b> . The order of the matrix. $n \ge 0$ .
d	<b>REAL for slarrv/clarrv</b> <b>DOUBLE PRECISION for dlarrv/zlarrv</b> Array, <b>DIMENSION</b> ( <i>n</i> ). On entry, the <i>n</i> diagonal elements of the diagonal matrix <i>D</i> .
1	REAL for slarrv/clarrv DOUBLE PRECISION for dlarrv/zlarrv Array, DIMENSION ( <i>n</i> -1). On entry, the ( <i>n</i> -1) subdiagonal elements of the unit bidiagonal matrix <i>L</i> are contained in elements 1 to <i>n</i> -1 of 1. 1( <i>n</i> ) need not be set.
isplit	<b>INTEGER.</b> Array, <b>DIMENSION</b> ( <i>n</i> ). The splitting points, at which <i>T</i> breaks up into submatrices. The first submatrix consists of rows/columns 1 to <i>isplit</i> (1), the second of rows/columns <i>isplit</i> (1)+1 through <i>isplit</i> (2), etc.
tol	<ul> <li>REAL for slarrv/clarrv</li> <li>DOUBLE PRECISION for dlarrv/zlarrv</li> <li>The absolute error tolerance for the eigenvalues/eigenvectors.</li> <li>Errors in the input eigenvalues must be bounded by tol.</li> <li>The eigenvectors output have residual norms bounded by tol, and the dot products between different eigenvectors are bounded by tol. tol must be at least n*eps* T , where eps is the machine precision and  T  is the 1-norm of the tridiagonal matrix.</li> </ul>
m	<b>INTEGER.</b> The total number of eigenvalues found. $0 \le m \le n$ . If range = 'A', $m = n$ , and if range = 'I', $m = iu - il + 1$ .
W	REAL for slarrv/clarrv DOUBLE PRECISION for dlarrv/zlarrv Array, DIMENSION ( <i>n</i> ). The first <i>m</i> elements of <i>w</i> contain the eigenvalues for which eigenvectors are to be computed. The eigenvalues should be grouped by

within the block (The output array w from ?larre is expected here). Errors in w must be bounded by tol. INTEGER. iblock Array, **DIMENSION** (*n*). The submatrix indices associated with the corresponding eigenvalues in w; iblock(i)=1 if eigenvalue w(i) belongs to the first submatrix from the top, =2 if w(i) belongs to the second submatrix, etc. **INTEGER**. The leading dimension of the output array *z*. ldz  $ldz \ge 1$ , and if jobz = V',  $ldz \ge max(1,n)$ . REAL for slarry/clarry work DOUBLE PRECISION for dlarry/zlarry Workspace array, **DIMENSION** (13*n*). iwork INTEGER. Workspace array, **DIMENSION** (6*n*).

split-off block and ordered from smallest to largest

#### **Output Parameters**

d	On exit, <i>d</i> may be overwritten.
1	On exit, 1 is overwritten.
Ζ	REAL for slarrv DOUBLE PRECISION for dlarrv
	COMPLEX for clarry
	COMPLEX*16 for zlarrv
	Array, DIMENSION $(1dz, max(1,m))$ .
	If $jobz = 'V'$ , then if $info = 0$ , the first <i>m</i> columns
	of $z$ contain the orthonormal eigenvectors of the matrix
	T corresponding to the selected eigenvalues, with the
	$\mathbf{i}$ -th column of $\mathbf{z}$ holding the eigenvector associated

with w(i). If jobz = 'N', then z is not referenced.



**NOTE.** The user must ensure that at least max(1,m) columns are supplied in the array z; if range = 'V', the exact value of m is not known in advance and an upper bound must be used.

isuppz	<b>INTEGER</b> . Array, <b>DIMENSION</b> $(2*\max(1,m))$ . The support of the eigenvectors in $z$ , i.e., the indices indicating the nonzero elements in $z$ . The <i>i</i> -th eigenvector is nonzero only in elements <i>isuppz</i> (2 <i>i</i> -1) through <i>isuppz</i> (2 <i>i</i> ).
info	<pre>INTEGER. If info = 0: successful exit If info = -i &lt; 0: the i-th argument had an illegal value info &gt; 0: if info = 1, there is an internal error in ?larrb; if info = 2, there is an internal error in ?stein.</pre>

# ?lartg

Generates a plane rotation with real cosine and real/complex sine.

```
call slartg ( f, g, cs, sn, r )
call dlartg ( f, g, cs, sn, r )
call clartg ( f, g, cs, sn, r )
call zlartg ( f, g, cs, sn, r )
```

### Discussion

The routine generates a plane rotation so that

$$\begin{bmatrix} cs & sn \\ -conjg(sn) & cs \end{bmatrix} \cdot \begin{bmatrix} f \\ g \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}$$
  
where  $cs^{2} + |sn|^{2} = 1$ 

This is a slower, more accurate version of the BLAS Level 1 routine **?rotg**, except for the following differences.

For slartg/dlartg:

*f* and *g* are unchanged on return;

If g=0, then cs=1 and sn=0;

If f=0 and  $g \neq 0$ , then cs=0 and sn=1 without doing any floating point operations (saves work in ?bdsqr when there are zeros on the diagonal);

If *f* exceeds *g* in magnitude, *cs* will be positive.

For clartg/zlartg:

*f* and *g* are unchanged on return;

If g=0, then cs=1 and sn=0;

If f=0, then cs=0 and sn is chosen so that r is real.

### **Input Parameters**

f, g REAL for slartg
DOUBLE PRECISION for dlartg
COMPLEX for clartg
COMPLEX*16 for zlartg
The first and second component of vector to be rotated.

### **Output Parameters**

CS

REAL for slartg/clartg DOUBLE PRECISION for dlartg/zlartg The cosine of the rotation. REAL for slartg DOUBLE PRECISION for dlartg COMPLEX for clartg COMPLEX*16 for zlartg The sine of the rotation.

REAL for slartg DOUBLE PRECISION for dlartg COMPLEX for clartg COMPLEX*16 for zlartg The nonzero component of the rotated vector.

## ?lartv

Applies a vector of plane rotations with real cosines and real/complex sines to the elements of a pair of vectors.

sn

r

call	slartv	(	n,	x,	incx,	Y'	incy,	С,	s,	incc	)
call	dlartv	(	n,	x,	incx,	Y,	incy,	с,	s,	incc	)
call	clartv	(	n,	x,	incx,	Y,	incy,	с,	s,	incc	)
call	zlartv	(	n,	x,	incx,	Y'	incy,	с,	s,	incc	)

### **Discussion**

The routine applies a vector of real/complex plane rotations with real cosines to elements of the real/complex vectors x and y. For i = 1, 2, ..., n

$$\begin{bmatrix} x_i \\ y_i \end{bmatrix} : = \begin{bmatrix} c(i) & s(i) \\ -\text{conjg}(s(i)) & c(i) \end{bmatrix} \begin{bmatrix} x_i \\ y_i \end{bmatrix}$$

### **Input Parameters**

n

**INTEGER.** The number of plane rotations to be applied.

х, у	REAL for slartv DOUBLE PRECISION for dlartv COMPLEX for clartv COMPLEX*16 for zlartv Arrays, DIMENSION (1+(n-1)*incx) and (1+(n-1)*incy), respectively. The input vectors x and y.
incx	<b>INTEGER.</b> The increment between elements of $x$ . <i>incx</i> > 0.
incy	<b>INTEGER.</b> The increment between elements of $y$ . incy > 0.
С	REAL for slartv/clartv DOUBLE PRECISION for dlartv/zlartv Array, DIMENSION $(1+(n-1)*incc)$ . The cosines of the plane rotations.
8	REAL for slartv DOUBLE PRECISION for dlartv COMPLEX for clartv COMPLEX*16 for zlartv Array, DIMENSION (1+(n-1)*incc). The sines of the plane rotations.
incc	<b>INTEGER</b> . The increment between elements of $c$ and $s$ . incc > 0.

*x*, *y* The rotated vectors *x* and *y*.

## ?laruv

Returns a vector of n random real numbers from a uniform distribution.

```
call slaruv ( iseed, n, x )
call dlaruv ( iseed, n, x )
```

### **Discussion**

The routine ?laruv returns a vector of *n* random real numbers from a uniform (0,1) distribution ( $n \leq 28$ ).

This is an auxiliary routine called by ?larnv.

### **Input Parameters**

iseed	<b>INTEGER.</b> Array, <b>DIMENSION</b> (4). On entry, the seed of the random number generator; the array elements must be between 0 and 4095, and <i>iseed</i> (4) must be odd.
п	<b>INTEGER.</b> The number of random numbers to be generated. $n \leq 128$ .
Output Parame	ters
x	REAL for slaruv DOUBLE PRECISION for dlaruv Array, DIMENSION ( <i>n</i> ). The generated random numbers.
seed	On exit, the seed is updated.

## ?larz

Applies an elementary reflector (as returned by **?tzrzf**) to a general matrix.

> call slarz ( side, m, n, l, v, incv, tau, c, ldc, work ) call dlarz ( side, m, n, l, v, incv, tau, c, ldc, work ) call clarz ( side, m, n, l, v, incv, tau, c, ldc, work ) call zlarz ( side, m, n, l, v, incv, tau, c, ldc, work )

### Discussion

The routine ?larz applies a real/complex elementary reflector H to a real/complex *m*-by-*n* matrix C, from either the left or the right.

H is represented in the form

H = I - tau * v * v',

where tau is a real/complex scalar and v is a real/complex vector.

If tau = 0, then *H* is taken to be the unit matrix.

For complex flavors, to apply H' (the conjugate transpose of H), supply conjg(tau) instead of tau.

*H* is a product of *k* elementary reflectors as returned by **?tzrzf**.

side	CHARACTER*1. If side = 'L': form $H*C$ If side = 'R': form $C*H$
m	<b>INTEGER</b> . The number of rows of the matrix <i>C</i> .
n	<b>INTEGER</b> . The number of columns of the matrix <i>C</i> .
1	<b>INTEGER.</b> The number of entries of the vector $v$ containing the meaningful part of the Householder vectors. If <i>side</i> = 'L', $m \ge 1 \ge 0$ , if <i>side</i> = 'R', $n \ge 1 \ge 0$ .
v	REAL for slarz DOUBLE PRECISION for dlarz COMPLEX for clarz COMPLEX*16 for zlarz Array, DIMENSION $(1+(1-1)*abs(incv))$ . The vector $v$ in the representation of $H$ as returned by ?tzrzf. v is not used if $tau = 0$ .
incv	<b>INTEGER</b> . The increment between elements of $v$ . <i>incv</i> $\neq 0$ .
tau	REAL for slarz DOUBLE PRECISION for dlarz COMPLEX for clarz COMPLEX*16 for zlarz The value <i>tau</i> in the representation of <i>H</i> .

С	REAL for slarz
	DOUBLE PRECISION for dlarz
	COMPLEX for clarz
	COMPLEX*16 for zlarz
	Array, DIMENSION (1dc,n).
	On entry, the <i>m</i> -by- <i>n</i> matrix <i>C</i> .
ldc	<b>INTEGER.</b> The leading dimension of the array <i>c</i> .
	$ldc \geq \max(1,m).$
work	REAL for slarz
	DOUBLE PRECISION for dlarz
	COMPLEX for clarz
	COMPLEX*16 for zlarz
	Workspace array, DIMENSION
	(n) if $side = L'$ or
	(m) if $side = 'R'$ .
Output Parama	1
I WITCHT DOROMO	

С

On exit, *c* is overwritten by the matrix  $H^*C$  if *side* = 'L', or  $C^*H$  if *side* = 'R'.

## ?larzb

Applies a block reflector or its transpose/conjugate-transpose to a general matrix.

```
call slarzb ( side, trans, direct, storev, m, n, k, l,
                v, ldv, t, ldt, c, ldc, work, ldwork )
call dlarzb ( side, trans, direct, storev, m, n, k, l,
               v, ldv, t, ldt, c, ldc, work, ldwork )
call clarzb ( side, trans, direct, storev, m, n, k, l,
               v, ldv, t, ldt, c, ldc, work, ldwork )
call zlarzb ( side, trans, direct, storev, m, n, k, l,
               v, ldv, t, ldt, c, ldc, work, ldwork )
```

### Discussion

The routine applies a real/complex block reflector H or its transpose  $H^T$  (or  $H^H$  for complex flavors) to a real/complex distributed *m*-by-*n* matrix C from the left or the right.

Currently, only *storev* = 'R' and *direct* = 'B' are supported.

side	CHARACTER*1. If $side = 'L'$ : apply <i>H</i> or <i>H</i> ' from the left If $side = 'R'$ : apply <i>H</i> or <i>H</i> ' from the right
trans	CHARACTER*1. If <i>trans</i> = 'N': apply <i>H</i> (No transpose) If <i>trans</i> ='C': apply <i>H</i> ' (Transpose/conjugate transpose)
direct	CHARACTER*1. Indicates how <i>H</i> is formed from a product of elementary reflectors = 'F': $H = H(1) H(2) \dots H(k)$ (forward, not supported yet) = 'B': $H = H(k) \dots H(2) H(1)$ (backward)
storev	CHARACTER*1. Indicates how the vectors which define the elementary reflectors are stored: = 'C': Column-wise (not supported yet) = 'R': Row-wise.
m	<b>INTEGER</b> . The number of rows of the matrix <i>C</i> .
n	INTEGER. The number of columns of the matrix $C$ .
k	<b>INTEGER.</b> The order of the matrix $T$ (equal to the number of elementary reflectors whose product defines the block reflector).
1	<b>INTEGER.</b> The number of columns of the matrix V containing the meaningful part of the Householder reflectors. If <i>side</i> = 'L', $m \ge 1 \ge 0$ , if <i>side</i> = 'R', $n \ge 1 \ge 0$ .
V	REAL for slarzb DOUBLE PRECISION for dlarzb COMPLEX for clarzb

	COMPLEX*16 for zlarzb Array, DIMENSION ( <i>ldv</i> , nv). If storev = 'C', nv = k; if storev = 'R', nv = 1.
ldv	<b>INTEGER.</b> The leading dimension of the array $v$ . If <i>storev</i> = 'C', <i>ldv</i> $\geq$ <i>l</i> ; if <i>storev</i> = 'R', <i>ldv</i> $\geq$ <i>k</i> .
t	REAL for slarzb DOUBLE PRECISION for dlarzb COMPLEX for clarzb COMPLEX*16 for zlarzb Array, DIMENSION ( <i>ldt,k</i> ). The triangular <i>k</i> -by- <i>k</i> matrix <i>T</i> in the representation of the block reflector.
ldt	<b>INTEGER.</b> The leading dimension of the array $t$ . <i>ldt</i> $\geq k$ .
С	REAL for slarzb DOUBLE PRECISION for dlarzb COMPLEX for clarzb COMPLEX*16 for zlarzb Array, DIMENSION ( <i>ldc</i> , <i>n</i> ). On entry, the <i>m</i> -by- <i>n</i> matrix <i>C</i> .
ldc	<b>INTEGER.</b> The leading dimension of the array $c$ . $ldc \ge max(1,m)$ .
work	REAL for slarzb DOUBLE PRECISION for dlarzb COMPLEX for clarzb COMPLEX*16 for zlarzb Workspace array, DIMENSION ( <i>ldwork</i> , <i>k</i> ).
ldwork	<b>INTEGER.</b> The leading dimension of the array work. If $side = L'$ , $ldwork \ge max(1, n)$ ; if $side = R'$ , $ldwork \ge max(1, m)$ .

С	On exit, $c$ is overwritten by $H^*C$ or $H'^*C$ or $C^*H$ or
	<i>C</i> * <i>H</i> ′.

# ?larzt

Forms the triangular factor T of a block reflector  $H = I \cdot VTV^{H}$ .

```
call slarzt ( direct, storev, n, k, v, ldv, tau, t, ldt )
call dlarzt ( direct, storev, n, k, v, ldv, tau, t, ldt )
call clarzt ( direct, storev, n, k, v, ldv, tau, t, ldt )
call zlarzt ( direct, storev, n, k, v, ldv, tau, t, ldt )
```

### **Discussion**

The routine forms the triangular factor *T* of a real/complex block reflector *H* of order > *n*, which is defined as a product of *k* elementary reflectors. If *direct* = 'F',  $H = H(1) H(2) \dots H(k)$  and *T* is upper triangular. If *direct* = 'B',  $H = H(k) \dots H(2) H(1)$  and T is lower triangular. If *storev* = 'C', the vector which defines the elementary reflector H(i) is stored in the *i*-th column of the array *v*, and H = I - V * T * V'If *storev* = 'R', the vector which defines the elementary reflector H(i) is stored in the *i*-th row of the array *v*, and H = I - V' * T * VCurrently, only *storev* = 'R' and *direct* = 'B' are supported.

direct	CHARACTER*1. Specifies the order in which the elementary reflectors are multiplied to form the block reflector:
	If direct = 'F': $H = H(1) H(2) \dots H(k)$ (forward, not supported yet) If direct = 'B': $H = H(k) \dots H(2) H(1)$ (backward)
storev	CHARACTER*1. Specifies how the vectors which define the elementary reflectors are stored (see also <i>Application Notes</i> below): If <i>storev</i> = 'C': column-wise (not supported yet) If <i>storev</i> = 'R': row-wise

n	<b>INTEGER</b> . The order of the block reflector <i>H</i> . $n \ge 0$ .
k	<b>INTEGER.</b> The order of the triangular factor <i>T</i> (equal to the number of elementary reflectors). $k \ge 1$ .
V	REAL for slarzt DOUBLE PRECISION for dlarzt COMPLEX for clarzt COMPLEX*16 for zlarzt Array, DIMENSION ( <i>ldv</i> , <i>k</i> ) if storev = 'C' ( <i>ldv</i> , <i>n</i> ) if storev = 'R' The matrix <i>V</i> .
ldv	<b>INTEGER.</b> The leading dimension of the array v. If $storev = 'C'$ , $ldv \ge max(1,n)$ ; if $storev = 'R'$ , $ldv \ge k$ .
tau	REAL for slarzt DOUBLE PRECISION for dlarzt COMPLEX for clarzt COMPLEX*16 for zlarzt Array, DIMENSION (k). tau(i) must contain the scalar factor of the elementary reflector $H(i)$ .
ldt	<b>INTEGER.</b> The leading dimension of the output array $t$ . $ldt \ge k$ .
Output Parama	tors

t	REAL for slarzt
	DOUBLE PRECISION for dlarzt
	COMPLEX for clarzt
	COMPLEX*16 for zlarzt
	Array, DIMENSION (1dt,k). The k-by-k triangular factor
	T of the block reflector. If $direct = 'F'$ , T is upper
	triangular; if $direct = 'B'$ , T is lower triangular. The rest
	of the array is not used.
v	The matrix V. See Application Notes below.

### **Application Notes**

The shape of the matrix V and the storage of the vectors which define the H(i) is best illustrated by the following example with n = 5 and k = 3. The elements equal to 1 are not stored; the corresponding array elements are modified but restored on exit. The rest of the array is not used.

*direct* = 'F' and *storev* = 'C': direct = 'F' and storev = 'R':  $V = \begin{bmatrix} v_1 & v_2 & v_3 \\ v_1 & v_2 & v_3 \end{bmatrix}$  $\begin{bmatrix} v_1 & v_1 & v_1 & v_1 & v_1 & \dots & 1 \\ v_2 & v_2 & v_2 & v_2 & v_2 & \dots & 1 \\ v_3 & v_3 & v_3 & v_3 & v_3 & \dots & 1 \end{bmatrix}$ . . . 1. 1. 1 *direct* = 'B' and *storev* = 'C': direct = 'B' and storev = 'R': 1 ____V____ . 1 . . 1  $\begin{bmatrix} 1 & \dots & v_1 & v_1 & v_1 & v_1 & v_1 \\ \dots & 1 & \dots & v_2 & v_2 & v_2 & v_2 \\ \dots & 1 & \dots & v_3 & v_3 & v_3 & v_3 \end{bmatrix}$  $V = \begin{bmatrix} v_1 & v_2 & v_3 \\ v_1 & v_2 & v_3 \\ v_1 & v_2 & v_3 \\ v_1 & v_2 & v_3 \end{bmatrix}$ 

## ?las2

*Computes singular values of a 2-by-2 triangular matrix.* 

call slas2 ( f, g, h, ssmin, ssmax )
call dlas2 ( f, g, h, ssmin, ssmax )

### **Discussion**

The routine **?las2** computes the singular values of the 2-by-2 matrix

On return, *ssmin* is the smaller singular value and *ssmax* is the larger singular value.

#### **Input Parameters**

f, g, h	REAL for slas2
	DOUBLE PRECISION for dlas2
	The $(1,1)$ , $(1,2)$ and $(2,2)$ elements of the 2-by-2 matrix,
	respectively.

### **Output Parameters**

ssmin, ssmax REAL for slas2 DOUBLE PRECISION for dlas2 The smaller and the larger singular values, respectively.

### **Application Notes**

Barring over/underflow, all output quantities are correct to within a few units in the last place (*ulps*), even in the absence of a guard digit in addition/subtraction.

In IEEE arithmetic, the code works correctly if one matrix element is infinite.

Overflow will not occur unless the largest singular value itself overflows, or is within a few ulps of overflow. (On machines with partial overflow, like the Cray, overflow may occur if the largest singular value is within a factor of 2 of overflow.)

Underflow is harmless if underflow is gradual. Otherwise, results may correspond to a matrix modified by perturbations of size near the underflow threshold.

## ?lascl

Multiplies a general rectangular matrix by a real scalar defined as  $c_{to}/c_{from}$ .

call sl	lascl (	type,	kl,	ku,	cfrom,	cto,	m,	n,	a,	lda,	info	)
call dl	lascl (	type,	kl,	ku,	cfrom,	cto,	m,	n,	a,	lda,	info	)
call cl	lascl (	type,	kl,	ku,	cfrom,	cto,	m,	n,	a,	lda,	info	)
call zl	lascl (	type,	kl,	ku,	cfrom,	cto,	m,	n,	a,	lda,	info	)

### **Discussion**

The routine ?lasc1 multiplies the *m*-by-*n* real/complex matrix *A* by the real scalar cto/cfrom. The operation is performed without over/underflow as long as the final result cto*A(i,j)/cfrom does not over/underflow. type specifies that *A* may be full, upper triangular, lower triangular, upper Hessenberg, or banded.

### **Input Parameters**

type

## CHARACTER*1. *type* indices the storage *type* of the input matrix. = 'G': A is a full matrix. = 'L': A is a lower triangular matrix.

- = 'U': A is an upper triangular matrix.
- = 'H': A is an upper Hessenberg matrix.
- = 'B': A is a symmetric band matrix with lower

bandwidth kl and upper bandwidth ku and with the

	<ul> <li>only the lower half stored</li> <li>= 'Q': A is a symmetric band matrix with lower</li> <li>bandwidth k1 and upper bandwidth ku and with the</li> <li>only the upper half stored.</li> <li>= 'Z': A is a band matrix with lower bandwidth k1 and</li> <li>upper bandwidth ku.</li> </ul>
kl	<b>INTEGER.</b> The lower bandwidth of <i>A</i> . Referenced only if $type = 'B', 'Q'$ or 'Z'.
ku	<b>INTEGER.</b> The upper bandwidth of <i>A</i> . Referenced only if $type = 'B', 'Q'$ or 'Z'.
cfrom, cto	REAL for slascl/clascl DOUBLE PRECISION for dlascl/zlascl
	The matrix A is multiplied by $cto/cfrom$ . $A(i,j)$ is computed without over/underflow if the final result cto*A(i,j)/cfrom can be represented without over/underflow. $cfrom$ must be nonzero.
m	<b>INTEGER.</b> The number of rows of the matrix A. $m \ge 0$ .
п	<b>INTEGER.</b> The number of columns of the matrix <i>A</i> . $n \ge 0$ .
a	REAL for slasc1 DOUBLE PRECISION for dlasc1 COMPLEX for clasc1 COMPLEX*16 for zlasc1 Array, DIMENSION ( <i>lda</i> , <i>m</i> ). The matrix to be multiplied by <i>cto/cfrom</i> . See <i>type</i> for the storage type.
lda	<b>INTEGER.</b> The leading dimension of the array <i>a</i> . $1da \ge max(1,m)$ .

а	The multiplied matrix A.
info	INTEGER. If <i>info</i> = 0 - successful exit If <i>info</i> = - <i>i</i> < 0, the <i>i</i> -th argument had an illegal value.

# ?lasd0

Computes the singular values of a real upper bidiagonal n-by-m matrix B with diagonal d and off-diagonal e. Used by ?bdsdc.

#### **Discussion**

Using a divide and conquer approach, the routine ?lasd0 computes the singular value decomposition (SVD) of a real upper bidiagonal *n*-by-*m* matrix *B* with diagonal *d* and offdiagonal *e*, where m = n + sqre.

The algorithm computes orthogonal matrices U and VT such that B = U * S * VT. The singular values S are overwritten on d.

A related subroutine, **?lasda**, computes only the singular values, and optionally, the singular vectors in compact form.

n	<b>INTEGER.</b> On entry, the row dimension of the upper bidiagonal matrix. This is also the dimension of the main diagonal array $d$ .
sqre	<b>INTEGER.</b> Specifies the column dimension of the bidiagonal matrix. If $sqre = 0$ : The bidiagonal matrix has column dimension $m = n$ ; If $sqre = 1$ : The bidiagonal matrix has column dimension $m = n+1$ ;

d	REAL for slasd0 DOUBLE PRECISION for dlasd0 Array, DIMENSION ( <i>n</i> ). On entry, <i>d</i> contains the main diagonal of the bidiagonal matrix.
e	REAL for slasd0 DOUBLE PRECISION for dlasd0 Array, DIMENSION ( <i>m</i> -1). Contains the subdiagonal entries of the bidiagonal matrix. On exit, <i>e</i> is destroyed.
ldu	<b>INTEGER.</b> On entry, leading dimension of the output array <i>u</i> .
ldvt	<b>INTEGER.</b> On entry, leading dimension of the output array <i>vt</i> .
smlsiz	<b>INTEGER.</b> On entry, maximum size of the subproblems at the bottom of the computation tree.
iwork	INTEGER. Workspace array, DIMENSION must be at least (8 <i>n</i> ).
work	REAL for slasd0 DOUBLE PRECISION for dlasd0 Workspace array, DIMENSION must be at least $(3m^2 + 2m)$ .
Output Parame	ters
d	On exit $d$ , if <u>info</u> = 0, contains singular values of the bidiagonal matrix.
u	REAL for slasd0

REAL for slasd0 DOUBLE PRECISION for dlasd0 Array, DIMENSION at least (*ldq*, *n*). On exit, *u* contains the left singular vectors.

vt

contains the right singular vectors.
Array, DIMENSION at least ( <i>ldvt</i> , <i>m</i> ). On exit, <i>vt</i> '
DOUBLE PRECISION for dlasd0
REAL for slasd0

info

INTEGER.
If info = 0: successful exit.
If info = -i < 0, the i-th argument had an illegal
value.
If info = 1, an singular value did not converge.</pre>

## ?lasd1

Computes the SVD of an upper bidiagonal matrix B of the specified size. Used by ?bdsdc.

### **Discussion**

This routine computes the SVD of an upper bidiagonal *n*-by-*m* matrix *B*, where n = nl + nr + 1 and m = n + sqre. The routine ?lasd1 is called from ?lasd0.

A related subroutine **?lasd7** handles the case in which the singular values (and the singular vectors in factored form) are desired.

**?lasd1** computes the SVD as follows:

 $B = U(in) * \begin{bmatrix} D1(in) & 0 & 0 \\ Z1' & a & Z2' & b \\ 0 & 0 & D2(in) & 0 \end{bmatrix} * VT(in)$ = U(out) * (D(out) & 0) * VT(out)

where Z' = (ZI' a ZZ' b) = u' VT', and u is a vector of dimension m with *alpha* and *beta* in the *nl*+1 and *nl*+2 -th entries and zeros elsewhere; and the entry b is empty if *sqre* = 0.

The left singular vectors of the original matrix are stored in u, and the transpose of the right singular vectors are stored in vt, and the singular values are in d. The algorithm consists of three stages:

The first stage consists of deflating the size of the problem when there are multiple singular values or when there are zeros in the *Z* vector. For each such occurrence the dimension of the secular equation problem is reduced by one. This stage is performed by the routine ?lasd2.

The second stage consists of calculating the updated singular values. This is done by finding the square roots of the roots of the secular equation via the routine ?lasd4 (as called by ?lasd3). This routine also calculates the singular vectors of the current problem.

The final stage consists of computing the updated singular vectors directly using the updated singular values. The singular vectors for the current problem are multiplied with the singular vectors from the overall problem.

nl	<b>INTEGER</b> . The row dimension of the upper block. $nl \ge 1$ .
nr	<b>INTEGER</b> . The row dimension of the lower block. $nr \ge 1$ .
sqre	<b>INTEGER.</b> If <i>sqre</i> = 0: the lower block is an <i>nr</i> -by- <i>nr</i> square matrix. If <i>sqre</i> = 1: the lower block is an <i>nr</i> -by-( <i>nr</i> +1) rectangular matrix. The bidiagonal matrix has row dimension $n = nl + nr + 1$ , and column dimension $m = n + sqre$ .
đ	REAL for slasd1 DOUBLE PRECISION for dlasd1 Array, DIMENSION ( $n = nl+nr+1$ ). On entry d(1:nl,1:nl) contains the singular values of the upper block; and $d(nl+2:n)$ contains the singular values of the lower block.

alpha	REAL for slasd1 DOUBLE PRECISION for dlasd1 Contains the diagonal element associated with the added row.
beta	REAL for slasd1 DOUBLE PRECISION for dlasd1 Contains the off-diagonal element associated with the added row.
и	REAL for slasd1 DOUBLE PRECISION for dlasd1 Array, DIMENSION ( <i>ldu</i> , <i>n</i> ). On entry u(1:n1, 1:n1) contains the left singular vectors of the upper block; u(n1+2:n, n1+2:n) contains the left singular vectors of the lower block.
ldu	<b>INTEGER.</b> The leading dimension of the array $u$ . $1du \ge \max(1, n)$ .
vt	<pre>REAL for slasd1 DOUBLE PRECISION for dlasd1 Array, DIMENSION (ldvt, m), where m = n + sqre. On entry vt(1:nl+1, 1:nl+1)' contains the right singular vectors of the upper block; vt(nl+2:m, nl+2:m)' contains the right singular vectors of the lower block.</pre>
ldvt	<b>INTEGER.</b> The leading dimension of the array $vt$ . $ldvt \ge max(1, m)$ .
iwork	INTEGER. Workspace array, DIMENSION (4n).
work	REAL for slasd1 DOUBLE PRECISION for dlasd1 Workspace array, DIMENSION $(3m^2 + 2m)$ .

d

On exit d(1:n) contains the singular values of the modified matrix.

u	On exit <i>u</i> contains the left singular vectors of the bidiagonal matrix.
vt	On exit $vt'$ contains the right singular vectors of the bidiagonal matrix.
idxq	<b>INTEGER</b> Array, <b>DIMENSION</b> ( <i>n</i> ). Contains the permutation which will reintegrate the subproblem just solved back into sorted order, that is, $d(idxq(i = 1, n))$ will be in ascending order.
info	<pre>INTEGER. If info = 0: successful exit. If info = -i &lt; 0, the i-th argument had an illegal value. If info = 1, an singular value did not converge.</pre>

## ?lasd2

Merges the two sets of singular values together into a single sorted set. Used by ?bdsdc.

### **Discussion**

The routine **?lasd2** merges the two sets of singular values together into a single sorted set. Then it tries to deflate the size of the problem. There are two ways in which deflation can occur: when two or more singular values are close together or if there is a tiny entry in the *Z* vector. For each such occurrence the order of the related secular equation problem is reduced by one.

The routine **?lasd2** is called from **?lasd1**.

nl	<b>INTEGER.</b> The row dimension of the upper block. $nl \ge 1$ .
nr	<b>INTEGER.</b> The row dimension of the lower block. $nr \ge 1$ .
sqre	INTEGER. If sqre = 0: the lower block is an <i>nr</i> -by- <i>nr</i> square matrix If sqre = 1: the lower block is an <i>nr</i> -by-( <i>nr</i> +1) rectangular matrix. The bidiagonal matrix has $n = nl + nr + 1$ rows and $m = n + sqre \ge n$ columns.
d	REAL for slasd2 DOUBLE PRECISION for dlasd2 Array, DIMENSION (n). On entry d contains the singular values of the two submatrices to be combined.
alpha	REAL for slasd2 DOUBLE PRECISION for dlasd2 Contains the diagonal element associated with the added row.
beta	REAL for slasd2 DOUBLE PRECISION for dlasd2 Contains the off-diagonal element associated with the added row.
u	REAL for slasd2 DOUBLE PRECISION for dlasd2 Array, DIMENSION ( $ldu$ , $n$ ). On entry $u$ contains the left singular vectors of two submatrices in the two square blocks with corners at (1,1), ( $n1$ , $n1$ ), and ( $n1+2$ , $n1+2$ ), ( $n$ , $n$ ).
ldu	<b>INTEGER.</b> The leading dimension of the array $u$ . $1du \ge n$ .

ldu2	<b>INTEGER.</b> The leading dimension of the output array $u^2$ . $ldu^2 \ge n$ .
vt	REAL for slasd2 DOUBLE PRECISION for dlasd2 Array, DIMENSION ( <i>ldvt</i> , <i>m</i> ). On entry <i>vt</i> ' contains the right singular vectors of two submatrices in the two square blocks with corners at (1,1), ( <i>n1</i> +1, <i>n1</i> +1), and ( <i>n1</i> +2, <i>n1</i> +2), ( <i>m</i> , <i>m</i> ).
ldvt	<b>INTEGER</b> . The leading dimension of the array $vt$ . $ldvt \ge m$ .
ldvt2	<b>INTEGER.</b> The leading dimension of the output array $vt2$ . $ldvt2 \ge m$ .
idxp	INTEGER. Workspace array, DIMENSION ( <i>n</i> ). This will contain the permutation used to place deflated values of <i>d</i> at the end of the array. On output $idxp(2:k)$ points to the nondeflated <i>d</i> -values and $idxp(k+1:n)$ points to the deflated singular values.
idx	<b>INTEGER.</b> Workspace array, <b>DIMENSION</b> ( <i>n</i> ). This will contain the permutation used to sort the contents of <i>d</i> into ascending order.
coltyp	<pre>INTEGER. Workspace array, DIMENSION (n). As workspace, this will contain a label which will indicate which of the following types a column in the u2 matrix or a row in the vt2 matrix is: 1 : non-zero in the upper half only 2 : non-zero in the lower half only 3 : dense 4 : deflated.</pre>
idxq	<b>INTEGER.</b> Array, <b>DIMENSION</b> ( <i>n</i> ). This contains the permutation which separately sorts the two sub-problems in <i>d</i> into ascending order. Note that entries in the first half of this

permutation must first be moved one position backward; and entries in the second half must first have nl+1 added to their values.

### **Output Parameters**

k	<b>INTEGER.</b> Contains the dimension of the non-deflated matrix, This is the order of the related secular equation. $1 \leq \leq 1$ .
d	On exit <i>d</i> contains the trailing ( <i>n</i> - <i>k</i> ) updated singular values (those which were deflated) sorted into increasing order.
u	On exit $u$ contains the trailing $(n-k)$ updated left singular vectors (those which were deflated) in its last $n-k$ columns.
Z	REAL for slasd2 DOUBLE PRECISION for dlasd2 Array, DIMENSION (n). On exit z contains the updating row vector in the secular equation.
dsigma	REAL for slasd2 DOUBLE PRECISION for dlasd2 Array, DIMENSION ( <i>n</i> ). Contains a copy of the diagonal elements ( <i>k</i> -1 singular values and one zero) in the secular equation.
u2	REAL for slasd2 DOUBLE PRECISION for dlasd2 Array, DIMENSION ( <i>ldu2</i> , <i>n</i> ). Contains a copy of the first <i>k</i> -1 left singular vectors which will be used by ?lasd3 in a matrix multiply (?gemm) to solve for the new left singular vectors. <i>u2</i> is arranged into four blocks. The first block contains a column with 1 at <i>n1</i> +1 and zero everywhere else; the second block contains non-zero entries only at and above <i>n1</i> ; the third contains non-zero entries only below <i>n1</i> +1; and the fourth is dense.

vt	On exit $vt'$ contains the trailing $(n-k)$ updated right singular vectors (those which were deflated) in its last n-k columns. In case sqre =1, the last row of $vt$ spans the right null space.
vt2	REAL for slasd2 DOUBLE PRECISION for dlasd2 Array, DIMENSION $(ldvt2, n)$ . $vt2'$ contains a copy of the first $k$ right singular vectors which will be used by ?lasd3 in a matrix multiply (?gemm) to solve for the new right singular vectors. $vt2$ is arranged into three blocks. The first block contains a row that corresponds to the special 0 diagonal element in <i>sigma</i> ; the second block contains non-zeros only at and before $n1 + 1$ ; the third block contains non-zeros only at and after $n1 + 2$ .
idxc	INTEGER. Array, DIMENSION ( <i>n</i> ). This will contain the permutation used to arrange the columns of the deflated <i>U</i> matrix into three groups: the first group contains non-zero entries only at and above <i>n1</i> , the second contains non-zero entries only below <i>n1</i> +2, and the third is dense.
coltyp	On exit, it is an array of dimension 4, with <i>coltyp(i)</i> being the dimension of the <i>i</i> -th type columns.
info	<b>INTEGER.</b> If <i>info</i> = 0: successful exit If <i>info</i> = $-i$ < 0, the <i>i</i> -th argument had an illegal value.

# ?lasd3

Finds all square roots of the roots of the secular equation, as defined by the values in D and Z, and then updates the singular vectors by matrix multiplication. Used by ?bdsdc.

#### **Discussion**

The routine **?lasd3** finds all the square roots of the roots of the secular equation, as defined by the values in *D* and *Z*. It makes the appropriate calls to **?lasd4** and then updates the singular vectors by matrix multiplication.

The routine **?lasd3** is called from **?lasd1**.

nl	<b>INTEGER.</b> The row dimension of the upper block. $nl \ge 1$ .
nr	<b>INTEGER.</b> The row dimension of the lower block. $nr \ge 1$ .
sqre	<b>INTEGER.</b> If <i>sqre</i> = 0: the lower block is an <i>nr</i> -by- <i>nr</i> square matrix. If <i>sqre</i> = 1: the lower block is an <i>nr</i> -by-( <i>nr</i> +1) rectangular matrix. The bidiagonal matrix has $n = n1 + nr + 1$ rows and $m = n + sqre \ge n$ columns.
k	<b>INTEGER</b> . The size of the secular equation, $1 \leq \leq n$ .

q	REAL for slasd3 DOUBLE PRECISION for dlasd3 Workspace array, DIMENSION at least ( <i>ldg</i> , <i>k</i> ).
ldq	<b>INTEGER.</b> The leading dimension of the array $q$ . $ldq \ge k$ .
dsigma	REAL for slasd3 DOUBLE PRECISION for dlasd3 Array, DIMENSION ( <i>k</i> ). The first <i>k</i> elements of this array contain the old roots of the deflated updating problem. These are the poles of the secular equation.
u	REAL for slasd3 DOUBLE PRECISION for dlasd3 Array, DIMENSION ( $ldu$ , $n$ ). The last $n - k$ columns of this matrix contain the deflated left singular vectors.
ldu	<b>INTEGER.</b> The leading dimension of the array $u$ . $ldu \ge n$ .
u2	REAL for slasd3 DOUBLE PRECISION for dlasd3 Array, DIMENSION ( <i>ldu2</i> , <i>n</i> ). The first <i>k</i> columns of this matrix contain the non-deflated left singular vectors for the split problem.
ldu2	<b>INTEGER.</b> The leading dimension of the array $u^2$ . $ldu^2 \ge n$ .
vt	REAL for slasd3 DOUBLE PRECISION for dlasd3 Array, DIMENSION ( <i>ldvt</i> , <i>m</i> ). The last <i>m</i> - <i>k</i> columns of <i>vt</i> ' contain the deflated right singular vectors.
ldvt	<b>INTEGER.</b> The leading dimension of the array $vt$ . $ldvt \ge n$ .
vt2	REAL for slasd3 DOUBLE PRECISION for dlasd3 Array, DIMENSION ( <i>ldvt2</i> , <i>n</i> ). The first <i>k</i> columns of <i>vt2</i> ' contain the non-deflated right singular vectors for the split problem.

ldvt2	<b>INTEGER.</b> The leading dimension of the array $vt2$ . $ldvt2 \ge n$ .
idxc	INTEGER. Array, DIMENSION $(n)$ . The permutation used to arrange the columns of $u$ (and rows of $vt$ ) into three groups: the first group contains non-zero entries only at and above (or before) $nl$ +1; the second contains non-zero entries only at and below (or after) $nl$ +2; and the third is dense. The first column of $u$ and the row of $vt$ are treated separately, however. The rows of the singular vectors found by ?lasd4 must be likewise permuted before the matrix multiplies can take place.
ctot	INTEGER. Array, DIMENSION (4). A count of the total number of the various types of columns in $u$ (or rows in $vt$ ), as described in <i>idxc</i> . The fourth column type is any column which has been deflated.
Ζ	REAL for slasd3 DOUBLE PRECISION for dlasd3 Array, DIMENSION ( $k$ ). The first $k$ elements of this array contain the components of the deflation-adjusted updating row vector.
Output Param	eters
d	REAL for slasd3 DOUBLE PRECISION for dlasd3 Array, DIMENSION (k). On exit the square roots of the roots of the secular equation, in ascending order.
info	INTEGER.

If *info* = 0: successful exit.

If *info* = -*i* < 0, the *i*-th argument had an illegal value. If *info* = 1, an singular value did not converge.

## **Application Notes**

This code makes very mild assumptions about floating point arithmetic. It will work on machines with a guard digit in add/subtract, or on those binary machines without guard digits which subtract like the Cray XMP, Cray YMP, Cray C 90, or Cray 2. It could conceivably fail on hexadecimal or decimal machines without guard digits, but we know of none.

# ?lasd4

Computes the square root of the i-th updated eigenvalue of a positive symmetric rank-one modification to a positive diagonal matrix. Used by ?bdsdc.

call slasd4 ( n, i, d, z, delta, rho, sigma, work, info )
call dlasd4 ( n, i, d, z, delta, rho, sigma, work, info )

## **Discussion**

This routine computes the square root of the *i*-th updated eigenvalue of a positive symmetric rank-one modification to a positive diagonal matrix whose entries are given as the squares of the corresponding entries in the array *d*, and that  $0 \le d(i) < d(j)$  for i < j and that rho > 0. This is arranged by the calling routine, and is no loss in generality. The rank-one modified system is thus

diag(d)* diag(d) + *rho* **Z* * *Z*_transpose where we assume the Euclidean norm of *Z* is 1. The method consists of approximating the rational functions in the secular equation by simpler interpolating rational functions.

## **Input Parameters**

n

**INTEGER**. The length of all arrays.

i	<b>INTEGER.</b> The index of the eigenvalue to be computed. $1 \leq i \leq n$ .
d	REAL for slasd4 DOUBLE PRECISION for dlasd4 Array, DIMENSION ( <i>n</i> ). The original eigenvalues. It is assumed that they are in order, $0 \leq d(i) < d(j)$ for $i < j$ .
Ζ	REAL for slasd4 DOUBLE PRECISION for dlasd4 Array, DIMENSION ( <i>n</i> ). The components of the updating vector.
rho	REAL for slasd4 DOUBLE PRECISION for dlasd4 The scalar in the symmetric updating formula.
work	<b>REAL</b> for slasd4 <b>DOUBLE PRECISION</b> for dlasd4 Workspace array, <b>DIMENSION</b> $(n$ ). If $n \neq 1$ , work contains $(d(j) + sigma_i)$ in its $j$ -th component. If $n = 1$ , then work $(1) = 1$ .

# **Output Parameters**

delta	REAL for slasd4 DOUBLE PRECISION for dlasd4 Array, DIMENSION (n). If $n \neq 1$ , delta contains $(d(j) - sigma_i)$ in its j-th component. If $n = 1$ , then delta $(1) = 1$ . The vector delta contains the information necessary to construct the (singular) eigenvectors.
sigma	REAL for slasd4 DOUBLE PRECISION for dlasd4 The computed $\lambda_i$ , the <i>i</i> -th updated eigenvalue.
info	<pre>INTEGER. = 0: successful exit &gt; 0: if info = 1, the updating process failed.</pre>

# ?lasd5

Computes the square root of the *i*-th eigenvalue of a positive symmetric rank-one modification of a 2-by-2 diagonal matrix.Used by ?bdsdc.

call slasd5 ( i, d, z, delta, rho, dsigma, work )
call dlasd5 ( i, d, z, delta, rho, dsigma, work )

#### **Discussion**

This routine computes the square root of the i-th eigenvalue of a positive symmetric rank-one modification of a 2-by-2 diagonal matrix

diag(d) * diag(d) + rho *Z * Z_transpose

The diagonal entries in the array *d* are assumed to satisfy  $0 \le d(i) < d(j)$  for i < j. We also assume rho > 0 and that the Euclidean norm of the vector *Z* is one.

i	<b>INTEGER.</b> The index of the eigenvalue to be computed. i = 1 or $i = 2$ .
d	REAL for slasd5 DOUBLE PRECISION for dlasd5 Array, DIMENSION (2). The original eigenvalues. We assume $0 \le d(1) < d(2)$ .
Ζ	REAL for slasd5 DOUBLE PRECISION for dlasd5 Array, DIMENSION (2). The components of the updating vector.
rho	REAL for slasd5 DOUBLE PRECISION for dlasd5 The scalar in the symmetric updating formula.

work	<b>REAL</b> for slasd5 <b>DOUBLE PRECISION</b> for dlasd5. Workspace array, <b>DIMENSION</b> (2). Contains $(d(j) + sigma_i)$ in its <i>j</i> -th component.
Output Par	rameters
delta	REAL for slasd5 DOUBLE PRECISION for dlasd5. Array, DIMENSION (2). Contains $(d(j) - \lambda_i)$ in its <i>j</i> -th component. The vector <i>delta</i> contains the information necessary to construct the eigenvectors.
dsigma	REAL for slasd5 DOUBLE PRECISION for dlasd5. The computed $\lambda_i$ , the <i>i</i> -th updated eigenvalue.

# ?lasd6

Computes the SVD of an updated upper bidiagonal matrix obtained by merging two smaller ones by appending a row. Used by ?bdsdc.

call slasd6 ( icompq, nl, nr, sqre, d, vf, vl, alpha,
beta, idxq, perm, givptr, givcol, ldgcol,
givnum, ldgnum, poles, difl, difr, z, k, c,
s, work, iwork, info)
call dlasd6 ( icompq, nl, nr, sqre, d, vf, vl, alpha,
beta, idxq, perm, givptr, givcol, ldgcol,
givnum, ldgnum, poles, difl, difr, z, k, c,
s, work, iwork, info)

#### Discussion

The routine 2 lasd 6 computes the *SVD* of an updated upper bidiagonal matrix *B* obtained by merging two smaller ones by appending a row. This routine is used only for the problem which requires all singular values and optionally singular vector matrices in factored form. *B* is an *n*-by-*m* matrix with

n = nl + nr + 1 and m = n + sqre. A related subroutine, ?lasd1, handles the case in which all singular values and singular vectors of the bidiagonal matrix are desired. ?lasd6 computes the *SVD* as follows:

$$B = U(in) * \begin{bmatrix} D1(in) & 0 & 0 \\ Z1' & a & Z2' & b \\ 0 & 0 & D2(in) & 0 \end{bmatrix} * VT(in)$$

$$= U(out)*(D(out) \ 0)*VT(out)$$

where Z' = (ZI' a Z2' b) = u' VT', and u is a vector of dimension m with *alpha* and *beta* in the *nl*+1 and *nl*+2 -th entries and zeros elsewhere; and the entry b is empty if *sqre* = 0.

The singular values of *B* can be computed using *D1*, *D2*, the first components of all the right singular vectors of the lower block, and the last components of all the right singular vectors of the upper block. These components are stored and updated in vf and v1, respectively, in ?lasd6. Hence *U* and *VT* are not explicitly referenced.

The singular values are stored in D. The algorithm consists of two stages: the first stage consists of deflating the size of the problem when there are multiple singular values or if there is a zero in the Z vector. For each such occurrence the dimension of the secular equation problem is reduced by one. This stage is performed by the routine ?lasd7.

The second stage consists of calculating the updated singular values. This is done by finding the roots of the secular equation via the routine <code>?lasd4</code> (as called by <code>?lasd8</code>). This routine also updates *vf* and *vl* and computes the distances between the updated singular values and the old singular values. <code>?lasd6</code> is called from <code>?lasda</code>.

icompq	<ul> <li>INTEGER. Specifies whether singular vectors are to be computed in factored form:</li> <li>= 0: Compute singular values only</li> <li>= 1: Compute singular vectors in factored form as well.</li> </ul>
nl	<b>INTEGER</b> . The row dimension of the upper block. $nl \ge 1$ .
nr	<b>INTEGER</b> . The row dimension of the lower block. $nr \ge 1$ .
sqre	<ul> <li>INTEGER.</li> <li>= 0: the lower block is an <i>nr</i>-by-<i>nr</i> square matrix.</li> <li>= 1: the lower block is an <i>nr</i>-by-(<i>nr</i>+1) rectangular matrix.</li> <li>The bidiagonal matrix has row dimension <i>n</i>=<i>n</i>1+<i>nr</i>+1, and column dimension <i>m</i> = <i>n</i> + <i>sqre</i>.</li> </ul>
đ	REAL for slasd6 DOUBLE PRECISION for dlasd6 Array, DIMENSION ( $nl+nr+1$ ). On entry $d(1:nl,1:nl)$ contains the singular values of the upper block, and d(nl+2:n) contains the singular values of the lower block.
vf	REAL for slasd6 DOUBLE PRECISION for dlasd6 Array, DIMENSION ( $m$ ). On entry, $vf(1:nl+1)$ contains the first components of all right singular vectors of the upper block; and $vf(nl+2:m)$ contains the first components of all right singular vectors of the lower block.
vl	REAL for slasd6 DOUBLE PRECISION for dlasd6 Array, DIMENSION (m). On entry, v1(1:n1+1) contains the last components of all right singular vectors of the upper block; and v1(n1+2:m) contains the last components of all right singular vectors of the lower block.

alpha	REAL for slasd6 DOUBLE PRECISION for dlasd6 Contains the diagonal element associated with the added row.
beta	<b>REAL</b> for slasd6 <b>DOUBLE PRECISION</b> for dlasd6 Contains the off-diagonal element associated with the added row.
ldgcol	<b>INTEGER.</b> The leading dimension of the output array $givcol$ , must be at least $n$ .
ldgnum	<b>INTEGER.</b> The leading dimension of the output arrays <i>givnum</i> and <i>poles</i> , must be at least <i>n</i> .
work	REAL for slasd6 DOUBLE PRECISION for dlasd6 Workspace array, DIMENSION (4m).
iwork	INTEGER Workspace array, DIMENSION (3n).
Output Par	ameters
d	On exit $d(1:n)$ contains the singular values of the modified matrix.
vf	On exit, <i>vf</i> contains the first components of all right singular vectors of the bidiagonal matrix.
vl	On exit, v1 contains the last components of all right singular vectors of the bidiagonal matrix.
idxq	INTEGER. Array, DIMENSION ( <i>n</i> ). This contains the permutation

which will reintegrate the subproblem just solved back into sorted order, that is, d(idxq(i = 1, n)) will be in ascending order.

# permINTEGER.Array, DIMENSION (n). The permutations (from<br/>deflation and sorting) to be applied to each block. Not<br/>referenced if *icompq* = 0.

givptr	<b>INTEGER.</b> The number of Givens rotations which took place in this subproblem. Not referenced if $icompq = 0$ .
givcol	<b>INTEGER.</b> Array, <b>DIMENSION</b> ( $1dgcol$ , 2). Each pair of numbers indicates a pair of columns to take place in a Givens rotation. Not referenced if $icompq = 0$ .
givnum	<b>REAL</b> for slasd6 <b>DOUBLE PRECISION</b> for dlasd6 Array, <b>DIMENSION</b> ( <i>ldgnum</i> , 2). Each number indicates the <i>C</i> or <i>S</i> value to be used in the corresponding Givens rotation. Not referenced if <i>icompq</i> = 0.
poles	<b>REAL</b> for slasd6 <b>DOUBLE PRECISION</b> for dlasd6 Array, <b>DIMENSION</b> ( <i>ldgnum</i> , 2). On exit, <i>poles</i> (1,*) is an array containing the new singular values obtained from solving the secular equation, and <i>poles</i> (2,*) is an array containing the poles in the secular equation. Not referenced if <i>icompq</i> = 0.
difl	<b>REAL</b> for slasd6 <b>DOUBLE PRECISION</b> for dlasd6 Array, <b>DIMENSION</b> ( <i>n</i> ). On exit, $difl(i)$ is the distance between <i>i</i> -th updated (undeflated) singular value and the <i>i</i> -th (undeflated) old singular value.
difr	REAL for slasd6 DOUBLE PRECISION for dlasd6 Array, DIMENSION ( $ldgnum, 2$ ) if $icompq = 1$ and DIMENSION ( $n$ ) if $icompq = 0$ . On exit, $difr(i, 1)$ is the distance between <i>i</i> -th updated (undeflated) singular value and the <i>i</i> +1-th (undeflated) old singular value. If $icompq = 1$ , $difr(1:k, 2)$ is an array containing the normalizing factors for the right singular vector matrix. See ?lasd8 for details on $difl$ and $difr$ .

Z	REAL for slasd6
	DOUBLE PRECISION for dlasd6
	Array, DIMENSION (m).
	The first elements of this array contain the components of the deflation-adjusted updating row vector.
k	<b>INTEGER.</b> Contains the dimension of the non-deflated matrix. This is the order of the related secular equation. $1 \leq k \leq n$ .
С	REAL for slasd6
	DOUBLE PRECISION for dlasd6
	<i>c</i> contains garbage if <i>sqre</i> =0 and the <i>C</i> -value of a
	Givens rotation related to the right null space if
	sqre = 1.
S	REAL for slasd6
	DOUBLE PRECISION for dlasd6
	s contains garbage if sqre =0 and the S-value of a
	Givens rotation related to the right null space if
	<i>sqre</i> = 1.
info	INTEGER.
	= 0: successful exit.
	< 0: if <i>info</i> = - <i>i</i> , the <i>i</i> -th argument had an illegal value.
	>0:if <i>info</i> = 1, an singular value did not converge

# ?lasd7

Merges the two sets of singular values together into a single sorted set. Then it tries to deflate the size of the problem. Used by ?bdsdc.

## **Discussion**

The routine 2lasd7 merges the two sets of singular values together into a single sorted set. Then it tries to deflate the size of the problem. There are two ways in which deflation can occur: when two or more singular values are close together or if there is a tiny entry in the *Z* vector. For each such occurrence the order of the related secular equation problem is reduced by one. 2lasd7 is called from 2lasd6.

icompq	<ul> <li>INTEGER.Specifies whether singular vectors are to be computed in compact form, as follows:</li> <li>= 0: Compute singular values only.</li> <li>= 1: Compute singular vectors of upper bidiagonal matrix in compact form.</li> </ul>
nl	<b>INTEGER</b> . The row dimension of the upper block. $nl \ge 1$ .
nr	<b>INTEGER</b> . The row dimension of the lower block. $nr \ge 1$ .
sqre	<b>INTEGER.</b> = 0: the lower block is an <i>nr</i> -by- <i>nr</i> square matrix. = 1: the lower block is an <i>nr</i> -by-( <i>nr</i> +1) rectangular matrix. The bidiagonal matrix has $n = nl + nr + 1$ rows and $m = n + sqre \ge n$ columns.
d	REAL for slasd7 DOUBLE PRECISION for dlasd7 Array, DIMENSION (n). On entry <i>d</i> contains the singular values of the two submatrices to be combined.
ZW	REAL for slasd7 DOUBLE PRECISION for dlasd7 Array, DIMENSION (m). Workspace for z.

vf	REAL for slasd7 DOUBLE PRECISION for dlasd7 Array, DIMENSION ( $m$ ). On entry, $vf(1:nl+1)$ contains the first components of all right singular vectors of the upper block; and $vf(nl+2:m)$ contains the first components of all right singular vectors of the lower block.
vfw	REAL for slasd7 DOUBLE PRECISION for dlasd7 Array, DIMENSION ( m ). Workspace for vf.
vl	REAL for slasd7 DOUBLE PRECISION for dlasd7 Array, DIMENSION ( $m$ ). On entry, $v1(1:n1+1)$ contains the last components of all right singular vectors of the upper block; and $v1(n1+2:m)$ contains the last components of all right singular vectors of the lower block.
vlw	REAL for slasd7 DOUBLE PRECISION for dlasd7 Array, DIMENSION (m). Workspace for v1.
alpha	REAL for slasd7 DOUBLE PRECISION for dlasd7. Contains the diagonal element associated with the added row.
beta	REAL for slasd7 DOUBLE PRECISION for dlasd7 Contains the off-diagonal element associated with the added row.
idx	INTEGER. Workspace array, DIMENSION $(n)$ . This will contain the permutation used to sort the contents of $d$ into ascending order.

vf

vl

idxp	INTEGER. Workspace array, DIMENSION $(n)$ . This will contain the permutation used to place deflated values of $d$ at the end of the array.
idxq	INTEGER. Array, DIMENSION ( <i>n</i> ). This contains the permutation which separately sorts the two sub-problems in <i>d</i> into ascending order. Note that entries in the first half of this permutation must first be moved one position backward; and entries in the second half must first have $nl+1$ added to their values.
ldgcol	<b>INTEGER</b> . The leading dimension of the output array $givcol$ , must be at least $n$ .
ldgnum	<b>INTEGER</b> . The leading dimension of the output array <i>givnum</i> , must be at least <i>n</i> .
Output Para	ameters
k	<b>INTEGER.</b> Contains the dimension of the non-deflated matrix, this is the order of the related secular equation. $1 \leq s$ .
d	On exit, $d$ contains the trailing $(n-k)$ updated singular values (those which were deflated) sorted into increasing order.
Z	REAL for slasd7 DOUBLE PRECISION for dlasd7. Array, DIMENSION (m). On exit, z contains the

updating row vector in the secular equation. On exit, *vf* contains the first components of all right singular vectors of the bidiagonal matrix.

On exit, vl contains the last components of all right singular vectors of the bidiagonal matrix.

dsigma	REAL for slasd7 DOUBLE PRECISION for dlasd7. Array, DIMENSION ( <i>n</i> ). Contains a copy of the diagonal elements ( <i>k</i> -1 singular values and one zero) in the secular equation.
idxp	On output, $idxp(2:k)$ points to the nondeflated <i>d</i> -values and $idxp(k+1:n)$ points to the deflated singular values.
perm	<b>INTEGER.</b> Array, <b>DIMENSION</b> ( <i>n</i> ). The permutations (from deflation and sorting) to be applied to each singular block. Not referenced if $i compq = 0$ .
givptr	<b>INTEGER</b> . The number of Givens rotations which took place in this subproblem. Not referenced if $icompq = 0$ .
givcol	<b>INTEGER.</b> Array, <b>DIMENSION</b> ( $1dgco1$ , 2). Each pair of numbers indicates a pair of columns to take place in a Givens rotation. Not referenced if $icompq = 0$ .
givnum	<b>REAL</b> for slasd7 <b>DOUBLE PRECISION</b> for dlasd7. Array, <b>DIMENSION</b> ( <i>ldgnum</i> , 2). Each number indicates the <i>C</i> or <i>S</i> value to be used in the corresponding Givens rotation. Not referenced if <i>icompq</i> = 0.
С	REAL for slasd7. DOUBLE PRECISION for dlasd7. <i>c</i> contains garbage if <i>sqre</i> =0 and the <i>C</i> -value of a Givens rotation related to the right null space if <i>sqre</i> = 1.
5	REAL for slasd7. DOUBLE PRECISION for dlasd7. s contains garbage if sqre =0 and the S-value of a Givens rotation related to the right null space if sqre = 1.

info

INTEGER.

= 0: successful exit.
< 0: if *info* = -*i*, the *i*-th argument had an illegal value.

# ?lasd8

Finds the square roots of the roots of the secular equation, and stores, for each element in D, the distance to its two nearest poles. Used by ?bdsdc.

## **Discussion**

The routine **?lasd8** finds the square roots of the roots of the secular equation, as defined by the values in *dsigma* and *z*. It makes the appropriate calls to **?lasd4**, and stores, for each element in *d*, the distance to its two nearest poles (elements in *dsigma*). It also updates the arrays *vf* and *vl*, the first and last components of all the right singular vectors of the original bidiagonal matrix. **?lasd8** is called from **?lasd6**.

icompq	<ul> <li>INTEGER. Specifies whether singular vectors are to be computed in factored form in the calling routine:</li> <li>= 0: Compute singular values only.</li> <li>= 1: Compute singular vectors in factored form as well.</li> </ul>
k	<b>INTEGER.</b> The number of terms in the rational function to be solved by <b>?lasd4</b> . $k \ge 1$ .

Z	REAL for slasd8 DOUBLE PRECISION for dlasd8. Array, DIMENSION ( <i>k</i> ). The first <i>k</i> elements of this array contain the components of the deflation-adjusted updating row vector.	
vf	REAL for slasd8 DOUBLE PRECISION for dlasd8. Array, DIMENSION ( k ). On entry, vf contains information passed through dbede8.	
vl	REAL for slasd8 DOUBLE PRECISION for dlasd8. Array, DIMENSION ( k ).On entry, vl contains information passed through dbede8.	
lddifr	<b>INTEGER.</b> The leading dimension of the output array $difr$ , must be at least $k$ .	
dsigma	REAL for slasd8 DOUBLE PRECISION for dlasd8. Array, DIMENSION ( k ). The first k elements of this array contain the old roots of the deflated updating problem. These are the poles of the secular equation.	
work	REAL for slasd8 DOUBLE PRECISION for dlasd8. Workspace array, DIMENSION at least (3k).	
Output Parameters		
d	REAL for slasd8 DOUBLE PRECISION for dlasd8. Array, DIMENSION ( k ). On output, d contains the updated singular values.	
vf	On exit, <i>vf</i> contains the first <i>k</i> components of the first components of all right singular vectors of the bidiagonal matrix.	
vl	On exit, $v1$ contains the first $k$ components of the last components of all right singular vectors of the bidiagonal matrix.	

difl	REAL for slasd8 DOUBLE PRECISION for dlasd8. Array, DIMENSION ( $k$ ). On exit, $difl(i) = d(i) - dsigma(i)$ .
difr	<pre>REAL for slasd8 DOUBLE PRECISION for dlasd8. Array, DIMENSION ( lddifr, 2 ) if icompq = 1 and DIMENSION ( k ) if icompq = 0. On exit, difr(i,1) = d(i) - dsigma(i+1), difr(k,1) is not defined and will not be referenced. If icompq = 1, difr(1:k,2) is an array containing the normalizing factors for the right singular vector matrix.</pre>
info	<ul> <li>INTEGER.</li> <li>= 0: successful exit.</li> <li>&lt; 0: if <i>info</i> = -<i>i</i>, the <i>i</i>-th argument had an illegal value.</li> <li>&gt; 0: if <i>info</i> = 1, an singular value did not converge.</li> </ul>

# ?lasd9

Finds the square roots of the roots of the secular equation, and stores, for each element in D, the distance to its two nearest poles. Used by ?bdsdc.

#### **Discussion**

The routine **?lasd9** finds the square roots of the roots of the secular equation, as defined by the values in *dsigma* and *z*. It makes the appropriate calls to **?lasd4**, and stores, for each element in *d*, the distance

to its two nearest poles (elements in dsigma). It also updates the arrays vf and vl, the first and last components of all the right singular vectors of the original bidiagonal matrix. ?lasd9 is called from ?lasd7.

icompq	INTEGER.Specifies whether singular vectors are to be computed in factored form in the calling routine: If <i>icompq</i> = 0, compute singular values only; If <i>icompq</i> = 1, compute singular vector matrices in factored form also.
k	<b>INTEGER.</b> The number of terms in the rational function to be solved by slasd4. $k \ge 1$ .
dsigma	REAL for slasd9 DOUBLE PRECISION for dlasd9. Array, DIMENSION(k). The first k elements of this array contain the old roots of the deflated updating problem. These are the poles of the secular equation.
Ζ	REAL for slasd9 DOUBLE PRECISION for dlasd9. Array, DIMENSION ( <i>k</i> ). The first <i>k</i> elements of this array contain the components of the deflation-adjusted updating row vector.
vf	REAL for slasd9 DOUBLE PRECISION for dlasd9. Array, DIMENSION(k). On entry, vf contains information passed through sbede8.
vl	REAL for slasd9 DOUBLE PRECISION for dlasd9. Array, DIMENSION(k). On entry, v1 contains information passed through sbede8.
work	REAL for slasd9 DOUBLE PRECISION for dlasd9. Workspace array, DIMENSION at least (3k).

# **Output Parameters**

d	<b>REAL</b> for slasd9 <b>DOUBLE PRECISION</b> for dlasd9. Array, <b>DIMENSION</b> $(k)$ . $d(i)$ contains the updated singular values.
vf	On exit, $vf$ contains the first $k$ components of the first components of all right singular vectors of the bidiagonal matrix.
vl	On exit, <b>v1</b> contains the first <i>k</i> components of the last components of all right singular vectors of the bidiagonal matrix.
difl	REAL for slasd9 DOUBLE PRECISION for dlasd9. Array, DIMENSION (k). On exit, $difl(i) = d(i) - dsigma(i)$ .
difr	<pre>REAL for slasd9 DOUBLE PRECISION for dlasd9. Array, DIMENSION (ldu, 2) if icompq =1 and DIMENSION (k) if icompq = 0. On exit, difr(i, 1) = d(i) - dsigma(i+1), difr(k, 1) is not defined and will not be referenced. If icompq = 1, difr(1:k, 2) is an array containing the normalizing factors for the right singular vector matrix.</pre>
info	<pre>INTEGER. = 0: successful exit. &lt; 0: if info = -i, the i-th argument had an illegal value. &gt; 0: if info = 1, an singular value did not converge</pre>

# ?lasda

Computes the singular value decomposition (SVD) of a real upper bidiagonal matrix with diagonal d and off-diagonal e. Used by ?bdsdc.

## **Discussion**

Using a divide and conquer approach, ?lasda computes the singular value decomposition (SVD) of a real upper bidiagonal *n*-by-*m* matrix *B* with diagonal *d* and off-diagonal *e*, where m = n + sqre. The algorithm computes the singular values in the SVD B = U*S*VT. The orthogonal matrices *U* and *VT* are optionally computed in compact form. A related subroutine, ?lasd0, computes the singular values and the singular vectors in explicit form.

icompq	<b>INTEGER</b> . Specifies whether singular vectors are to be
	computed in compact form, as follows:
	= 0: Compute singular values only.
	= 1: Compute singular vectors of upper bidiagonal
	matrix in compact form.
smlsiz	<b>INTEGER</b> . The maximum size of the subproblems at the
	bottom of the computation tree.

n	<b>INTEGER</b> . The row dimension of the upper bidiagonal matrix. This is also the dimension of the main diagonal array <i>d</i> .
sqre	<b>INTEGER.</b> Specifies the column dimension of the bidiagonal matrix. If sqre = 0: The bidiagonal matrix has column dimension $m = n$ ; If sqre = 1: The bidiagonal matrix has column dimension $m = n + 1$ .
d	REAL for slasda DOUBLE PRECISION for dlasda. Array, DIMENSION ( <i>n</i> ). On entry <i>d</i> contains the main diagonal of the bidiagonal matrix.
е	REAL for slasda DOUBLE PRECISION for dlasda. Array, DIMENSION ( <i>m</i> -1). Contains the subdiagonal entries of the bidiagonal matrix. On exit, <i>e</i> has been destroyed.
ldu	<b>INTEGER.</b> The leading dimension of arrays $u$ , $vt$ , difl, difr, poles, givnum, and z. $ldu \ge n$ .
ldgcol	<b>INTEGER</b> . The leading dimension of arrays <i>givcol</i> and <i>perm</i> . $ldgcol \ge n$ .
work	REAL for slasda DOUBLE PRECISION for dlasda. Workspace array, DIMENSION $(6n + (smlsiz + 1)^2)$ .
iwork	INTEGER. Workspace array, DIMENSION must be at least (7 <i>n</i> ).
Output Parameters	
d	On exit $d$ , if <i>info</i> = 0, contains the singular values of the bidiagonal matrix.
u	REAL for slasda DOUBLE PRECISION for dlasda.

Array, DIMENSION (*ldu*, *smlsiz*) if *icompq* = 1.

	Not referenced if $icompq = 0$ . If $icompq = 1$ , on exit, <i>u</i> contains the left singular vector matrices of all subproblems at the bottom level.
vt	REAL for slasda DOUBLE PRECISION for dlasda. Array, DIMENSION ( <i>ldu</i> , <i>smlsiz</i> +1) if <i>icompq</i> = 1, and not referenced if <i>icompq</i> = 0. If <i>icompq</i> = 1, on exit, <i>vt</i> contains the right singular vector matrices of all subproblems at the bottom level.
k	INTEGER. Array, DIMENSION (n) if $icompq = 1$ and DIMENSION (1) if $icompq = 0$ . If $icompq = 1$ , on exit, $k(i)$ is the dimension of the <i>i</i> -th secular equation on the computation tree.
difl	REAL for slasda DOUBLE PRECISION for dlasda. Array, DIMENSION ( $ldu$ , $nlvl$ ), where $nlvl = floor (log_2 (n/smlsiz)))$ .
difr	REAL for slasda DOUBLE PRECISION for dlasda. Array, DIMENSION ( $1du$ , 2 $nlv1$ ) if $icompq = 1$ and DIMENSION (n) if $icompq = 0$ . If $icompq = 1$ , on exit, $dif1(1:n, i)$ and $difr(1:n, 2i-1)$ record distances between singular values on the <i>i</i> -th level and singular values on the ( <i>i</i> -1)-th level, and difr(1:n, 2i) contains the normalizing factors for the right singular vector matrix. See ?lasd8 for details.
Ζ	REAL for slasda DOUBLE PRECISION for dlasda. Array, DIMENSION ( $1du$ , $nlv1$ ) if $icompq = 1$ and DIMENSION ( $n$ ) if $icompq = 0$ .

The first k elements of z(1, i) contain the components of the deflation-adjusted updating row vector for subproblems on the i-th level. REAL for slasda poles DOUBLE PRECISION for dlasda Array, DIMENSION (1du, 2*nlv1) if icompg = 1, and not referenced if icompg = 0. If icompg = 1, on exit, poles(1, 2i - 1) and poles(1, 2i) contain the new and old singular values involved in the secular equations on the *i*-th level. INTEGER. givptr Array, DIMENSION (*n*) if icompq = 1, and not referenced if icompg = 0. If icompg = 1, on exit, givptr(i) records the number of Givens rotations performed on the *i*-th problem on the computation tree. givcol INTEGER. Array, DIMENSION (ldgcol, 2*nlvl) if icompg = 1, and not referenced if icompq = 0. If icompq = 1, on exit, for each i, givcol(1, 2i - 1) and givcol(1, 2i)record the locations of Givens rotations performed on the *i*-th level on the computation tree. INTEGER. perm Array, DIMENSION (ldgcol, nlvl) if icompg = 1, and not referenced if icompg = 0. If icompg = 1, on exit, <u>perm</u> (1, i) records permutations done on the *i*-th level of the computation tree. REAL for slasda givnum DOUBLE PRECISION for dlasda. Array DIMENSION (1du, 2*nlv1) if icompg = 1, and not referenced if icompq = 0. If icompq = 1, on exit, for each i, givnum(1, 2i - 1) and givnum(1, 2i) record the C- and S-values of Givens rotations performed on the *i*-th level on the computation tree.

С	REAL for slasda
	DOUBLE PRECISION for dlasda.
	Array,
	DIMENSION (n) if $icompq = 1$ , and
	DIMENSION (1) if $icompq = 0$ .
	If $icompq = 1$ and the <i>i</i> -th subproblem is not square, on exit, $c(i)$ contains the <i>C</i> -value of a Givens rotation related to the right null space of the <i>i</i> -th subproblem.
S	REAL for slasda
	DOUBLE PRECISION for dlasda.
	Array,
	DIMENSION $(n)$ icompq = 1, and
	DIMENSION (1) if $icompq = 0$ .
	If $i compq = 1$ and the <i>i</i> -th subproblem is not square, on exit, $s(i)$ contains the <i>S</i> -value of a Givens rotation related to the right null space of the <i>i</i> -th subproblem.
info	INTEGER.
	= 0: successful exit.
	< 0: if $info = -i$ , the <i>i</i> -th argument had an illegal value
	> 0: if <i>info</i> = 1, an singular value did not converge

# ?lasdq

Computes the SVD of a real bidiagonal matrix with diagonal d and off-diagonal e. Used by ?bdsdc.

# Discussion

The routine **?lasdq** computes the singular value decomposition (*SVD*) of a real (upper or lower) bidiagonal matrix with diagonal *d* and off-diagonal *e*, accumulating the transformations if desired. Letting *B* denote the input bidiagonal matrix, the algorithm computes orthogonal matrices *Q* and *P* such that B = Q S P'(P') denotes the transpose of *P*). The singular values *S* are overwritten on *d*.

The input matrix U is changed to UQ if desired.

The input matrix VT is changed to P'VT if desired.

The input matrix C is changed to Q'C if desired.

uplo	CHARACTER*1. On entry, <i>uplo</i> specifies whether the input bidiagonal matrix is upper or lower bidiagonal. If $uplo = 'U'$ or 'u', <i>B</i> is upper bidiagonal; If $uplo = 'L'$ or '1', <i>B</i> is lower bidiagonal.
sqre	INTEGER. = 0: then the input matrix is <i>n</i> -by- <i>n</i> . = 1: then the input matrix is <i>n</i> -by- $(n+1)$ if $uplu = 'U'$ and $(n+1)$ -by- <i>n</i> if $uplu = 'L'$ . The bidiagonal matrix has $n = nl + nr + 1$ rows and $m = n + sqre \ge n$ columns.
n	<b>INTEGER.</b> On entry, $n$ specifies the number of rows and columns in the matrix. $n$ must be at least 0.
ncvt	<b>INTEGER.</b> On entry, <i>ncvt</i> specifies the number of columns of the matrix <i>VT</i> . <i>ncvt</i> must be at least 0.
nru	<b>INTEGER.</b> On entry, <i>nru</i> specifies the number of rows of the matrix <i>U</i> . <i>nru</i> must be at least 0.
ncc	<b>INTEGER.</b> On entry, <i>ncc</i> specifies the number of columns of the matrix $C$ . <i>ncc</i> must be at least 0.
d	REAL for slasdq DOUBLE PRECISION for dlasdq. Array, DIMENSION ( <i>n</i> ). On entry, <i>d</i> contains the diagonal entries of the bidiagonal matrix whose <i>SVD</i> is desired.

e	REAL for slasdq DOUBLE PRECISION for dlasdq. Array, DIMENSION is $(n-1)$ if sqre = 0 and n if sqre = 1. On entry, the entries of e contain the off-diagonal entries of the bidiagonal matrix whose SVD is desired.
vt	<b>REAL</b> for slasdq <b>DOUBLE PRECISION</b> for dlasdq. Array, <b>DIMENSION</b> ( <i>ldvt</i> , <i>ncvt</i> ). On entry, contains a matrix which on exit has been premultiplied by <i>P</i> ', dimension <i>n</i> -by- <i>ncvt</i> if <i>sqre</i> = 0 and ( <i>n</i> +1)-by- <i>ncvt</i> if <i>sqre</i> = 1 (not referenced if <i>ncvt</i> =0).
ldvt	INTEGER. On entry, <i>ldvt</i> specifies the leading dimension of <i>vt</i> as declared in the calling (sub) program. <i>ldvt</i> must be at least 1. If <i>ncvt</i> is nonzero, <i>ldvt</i> must also be at least <i>n</i> .
u	REAL for slasdq DOUBLE PRECISION for dlasdq. Array, DIMENSION ( <i>ldu</i> , <i>n</i> ). On entry, contains a matrix which on exit has been postmultiplied by $Q$ , dimension <i>nru</i> -by- <i>n</i> if <i>sqre</i> = 0 and <i>nru</i> -by-( <i>n</i> +1) if <i>sqre</i> = 1 (not referenced if <i>nru</i> =0).
ldu	<b>INTEGER.</b> On entry, <i>ldu</i> specifies the leading dimension of <i>u</i> as declared in the calling (sub) program. <i>ldu</i> must be at least max( $1, nru$ ).
С	REAL for slasdq DOUBLE PRECISION for dlasdq. Array, DIMENSION ( <i>ldc</i> , <i>ncc</i> ). On entry, contains an <i>n</i> -by- <i>ncc</i> matrix which on exit has been premultiplied by $Q'$ , dimension <i>n</i> -by- <i>ncc</i> if <i>sqre</i> = 0 and ( <i>n</i> +1)-by- <i>ncc</i> if <i>sqre</i> = 1 (not referenced if <i>ncc</i> =0).
ldc	<b>INTEGER.</b> On entry, <i>ldc</i> specifies the leading dimension of $c$ as declared in the calling (sub) program. <i>ldc</i> must be at least 1. If <i>ncc</i> is non-zero, <i>ldc</i> must also be at least <i>n</i> .

work	REAL for slasdq DOUBLE PRECISION for dlasdq. Array, DIMENSION $(4n)$ . This is a workspace array. Only referenced if one of <i>ncvt</i> , <i>nru</i> , or <i>ncc</i> is nonzero, and if <i>n</i> is at least 2.	
Output Parameters		
d	On normal exit, <i>d</i> contains the singular values in ascending order.	
e	On normal exit, e will contain 0. If the algorithm does not converge, d and e will contain the diagonal and superdiagonal entries of a bidiagonal matrix orthogonally equivalent to the one given as input.	
vt	On exit, the matrix has been premultiplied by $P'$ .	
u	On exit, the matrix has been postmultiplied by $Q$ .	
С	On exit, the matrix has been premultiplied by $Q'$ .	
info	<b>INTEGER.</b> On exit, a value of 0 indicates a successful exit. If <i>info</i> < 0, argument number <i>-info</i> is illegal. If <i>info</i> > 0, the algorithm did not converge, and <i>info</i> specifies how many superdiagonals did not converge.	

# ?lasdt

Creates a tree of subproblems for bidiagonal divide and conquer. Used by ?bdsdc.

call slasdt ( n, lvl, nd, inode, ndiml, ndimr, msub )
call dlasdt ( n, lvl, nd, inode, ndiml, ndimr, msub )

#### **Discussion**

The routine creates a tree of subproblems for bidiagonal divide and conquer.

## **Input Parameters**

n	<b>INTEGER.</b> On entry, the number of diagonal elements of the bidiagonal matrix.
msub	<b>INTEGER.</b> On entry, the maximum row dimension each subproblem at the bottom of the tree can be of.
Output Parame	ters
lvl	<b>INTEGER.</b> On exit, the number of levels on the computation tree.
nd	INTEGER. On exit, the number of nodes on the tree.
inode	<b>INTEGER</b> . Array, <b>DIMENSION</b> ( <i>n</i> ). On exit, centers of subproblems.
ndiml	<b>INTEGER</b> . Array, <b>DIMENSION</b> ( <i>n</i> ). On exit, row dimensions of left children.
ndimr	<b>INTEGER</b> . Array, <b>DIMENSION</b> ( <i>n</i> ). On exit, row dimensions of right children.

# ?laset

Initializes the off-diagonal elements and the diagonal elements of a matrix to given values.

call slaset ( uplo, m, n, alpha, beta, a, lda )
call dlaset ( uplo, m, n, alpha, beta, a, lda )
call claset ( uplo, m, n, alpha, beta, a, lda )
call zlaset ( uplo, m, n, alpha, beta, a, lda )

# Discussion

The routine initializes an *m*-by-*n* matrix A to *beta* on the diagonal and *alpha* on the off-diagonals.

# Input parameters

uplo	CHARACTER*1. Specifies the part of the matrix A to be set. If $uplo = 'U'$ , upper triangular part is set; the strictly lower triangular part of A is not changed. If $uplo = 'L'$ : lower triangular part is set; the strictly upper triangular part of A is not changed. Otherwise: all of the matrix A is set.
m	<b>INTEGER.</b> The number of rows of the matrix A. $m \ge 0$ .
п	<b>INTEGER.</b> The number of columns of the matrix <i>A</i> . $n \ge 0$ .
alpha, beta	REAL for slaset DOUBLE PRECISION for dlaset COMPLEX for claset COMPLEX*16 for zlaset. The constants to which the off-diagonal and diagonal elements are to be set, respectively.
a	REAL for slaset DOUBLE PRECISION for dlaset COMPLEX for claset COMPLEX*16 for zlaset. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the <i>m</i> -by- <i>n</i> matrix <i>A</i> .
lda	<b>INTEGER.</b> The leading dimension of the array <i>A</i> . $lda \ge max(1,m)$ .
Output Param	otors

Output Parameters

а	On exit, the leading <i>m</i> -by- <i>n</i> subr	matrix of A is set as
	follows:	
	if $uplo = 'U', A(i,j) = alpha,$	$1 \le i \le j$ -1, $1 \le j \le n$ ,
	if $uplo = 'L', A(i,j) = alpha,$	$j+1 \le i \le m, 1 \le j \le n$

otherwise, A(i,j) = alpha,  $1 \le i \le m$ ,  $1 \le j \le n$ ,  $i \ne j$ ,

and, for all uplo,  $A(i,i) = beta, 1 \le i \le \min(m, n)$ .

# ?lasq1

Computes the singular values of a real square bidiagonal matrix. Used by ?bdsqr.

```
call slasq1 ( n, d, e, work, info )
call dlasq1 ( n, d, e, work, info )
```

#### **Discussion**

The routine 2lasq1 computes the singular values of a real *n*-by-*n* bidiagonal matrix with diagonal *d* and off-diagonal *e*. The singular values are computed to high relative accuracy, in the absence of denormalization, underflow and overflow.

n	<b>INTEGER.</b> The number of rows and columns in the matrix. $n \ge 0$ .
đ	REAL for slasq1 DOUBLE PRECISION for dlasq1. Array, DIMENSION ( <i>n</i> ). On entry, <i>d</i> contains the diagonal elements of the bidiagonal matrix whose <i>SVD</i> is desired.
e	REAL for slasq1 DOUBLE PRECISION for dlasq1. Array, DIMENSION ( <i>n</i> ). On entry, elements <i>e</i> (1: <i>n</i> -1) contain the off-diagonal elements of the bidiagonal matrix whose <i>SVD</i> is desired.

work REAL for slasq1 DOUBLE PRECISION for dlasq1. Workspace array, DIMENSION (4n).

#### **Output Parameters**

d	On normal exit, <i>d</i> contains the singular values in decreasing order.
е	On exit, e is overwritten.
info	<pre>INTEGER. = 0: successful exit; &lt; 0: if info = -i, the i-th argument had an illegal value; &gt; 0: the algorithm failed: = 1, a split was marked by a positive value in e; = 2, current block of z not diagonalized after 30*n iterations (in inner while loop); = 3, termination criterion of outer while loop not met (program created more than n unreduced blocks.</pre>

# ?lasq2

Computes all the eigenvalues of the symmetric positive definite tridiagonal matrix associated with the qd array z to high relative accuracy. Used by ?bdsqr and ?stegr.

```
call slasq2 ( n, z, info )
call dlasq2 ( n, z, info )
```

## **Discussion**

The routine **?lasq2** computes all the eigenvalues of the symmetric positive definite tridiagonal matrix associated with the qd array z to high relative accuracy, in the absence of denormalization, underflow and overflow.

To see the relation of z to the tridiagonal matrix, let L be a unit lower bidiagonal matrix with subdiagonals z(2,4,6,...) and let U be an upper bidiagonal matrix with 1's above and diagonal z(1,3,5,...). The tridiagonal is LU or, if you prefer, the symmetric tridiagonal to which it is similar.

## **Input Parameters**

n	INTEGER. The number of rows and columns in the
	matrix. $n \geq 0$ .
Z	REAL for slasq2
	DOUBLE PRECISION for dlasq2.
	Array, DIMENSION $(4n)$ . On entry, <i>z</i> holds the <i>qd</i> array.

## **Output Parameters**

Z

On exit, entries 1 to *n* hold the eigenvalues in decreasing order, z(2n+1) holds the trace, and z(2n+2)holds the sum of the eigenvalues. If n > 2, then z(2n+3) holds the iteration count, z(2n+4) holds ndivs/nin², and z(2n+5) holds the percentage of shifts that failed. INTEGER. info = 0: successful exit; < 0: if the *i*-th argument is a scalar and had an illegal value, then info = -i, if the *i*-th argument is an array and the *j*-entry had an illegal value, then *info* = -(i * 100 + j);> 0: the algorithm failed: = 1, a split was marked by a positive value in *e*; = 2, current block of z not diagonalized after 30*niterations (in inner while loop); = 3, termination criterion of outer while loop not met (program created more than n unreduced blocks).

# **Application Notes**

The routine **?lasq2** defines a logical variable, *ieee*, which is **.TRUE**. on machines which follow IEEE-754 floating-point standard in their handling of infinities and NaNs, and **.FALSE**. otherwise. This variable is passed to **?lasq3**.

# ?lasq3

Checks for deflation, computes a shift and calls dqds. Used by ?bdsqr.

## **Discussion**

The routine 2lasq3 checks for deflation, computes a shift (tau) and calls dqds. In case of failure, it changes shifts, and tries again until output is positive.

i0	INTEGER. First index.
<i>n0</i>	INTEGER. Last index.
Ζ	REAL for slasq3 DOUBLE PRECISION for dlasq3. Array, DIMENSION (4 <i>n</i> ). <i>z</i> holds the <i>qd</i> array.
pp	INTEGER. <i>pp</i> =0 for ping, <i>pp</i> =1 for pong.
desig	REAL for slasq3 DOUBLE PRECISION for dlasq3. Lower order part of <i>sigma</i> .

qmax	REAL for slasq3 DOUBLE PRECISION for dlasq3. Maximum value of $q$ .
ieee	LOGICAL. Flag for IEEE or non-IEEE arithmetic (passed to ?lasq5).
Output Parame	ters
dmin	REAL for slasq3 DOUBLE PRECISION for dlasq3. Minimum value of $d$ .
sigma	REAL for slasq3 DOUBLE PRECISION for dlasq3. Sum of shifts used in current segment.
desig	Lower order part of <i>sigma</i> .
nfail	<b>INTEGER</b> . Number of times shift was too big.
iter	<b>INTEGER</b> . Number of iterations.
ndiv	INTEGER. Number of divisions.
ttype	INTEGER. Shift type.

# ?lasq4

Computes an approximation to the smallest eigenvalue using values of d from the previous transform. Used by ?bdsqr.

# Discussion

The routine computes an approximation tau to the smallest eigenvalue using values of d from the previous transform.

i0	INTEGER. First index.
<i>n0</i>	INTEGER. Last index.
Z	REAL for slasq4 DOUBLE PRECISION for dlasq4. Array, DIMENSION (4 $n$ ). $z$ holds the $qd$ array.
рр	<b>INTEGER</b> . <i>pp</i> =0 for ping, <i>pp</i> =1 for pong.
noin	<b>INTEGER.</b> The value of <i>n0</i> at start of eigtest.
dmin	REAL for slasq4 DOUBLE PRECISION for dlasq4. Minimum value of $d$ .
dmin1	REAL for slasq4 DOUBLE PRECISION for dlasq4. Minimum value of $d$ , excluding $d(n0)$ .
dmin2	<b>REAL</b> for slasq4 DOUBLE PRECISION for dlasq4. Minimum value of $d$ , excluding $d(n0)$ and $d(n0-1)$ .
dn	REAL for slasq4 DOUBLE PRECISION for dlasq4. Contains $d(n)$ .
dn1	REAL for slasq4 DOUBLE PRECISION for dlasq4. Contains $d(n-1)$ .
dn2	REAL for slasq4 DOUBLE PRECISION for dlasq4. Contains $d(n-2)$ .

#### **Output Parameters**

tau	REAL for slasq4			
	DOUBLE PRECISION for dlasq4.			
	This is the shift.			
ttype	INTEGER. Shift type.			

# ?lasq5

Computes one dqds transform in ping-pong form. Used by ?bdsqr and ?stegr.

#### **Discussion**

The routine computes one dqds transform in ping-pong form, one version for IEEE machines another for non-IEEE machines.

iO	INTEGER First index.
<i>n0</i>	INTEGER Last index.
Ζ	REAL for slasq5 DOUBLE PRECISION for dlasq5. Array, DIMENSION (4 <i>n</i> ). <i>z</i> holds the <i>qd</i> array. <i>emin</i> is stored in $z(4*n0)$ to avoid an extra argument.
pp	<b>INTEGER</b> . <i>pp</i> =0 for ping, <i>pp</i> =1 for pong.
tau	REAL for slasq5 DOUBLE PRECISION for dlasq5. This is the shift.

	ameters
dmin	REAL for slasq5
	DOUBLE PRECISION for dlasq5
	Minimum value of $d$ .
dmin1	REAL for slasq5
	DOUBLE PRECISION for dlasq5.
	Minimum value of $d$ , excluding $d(n0)$ .
dmin2	REAL for slasq5
	DOUBLE PRECISION for dlasq5.
	Minimum value of $d$ , excluding $d(n0)$ and $d(n0-1)$ .
dn	REAL for slasq5
	DOUBLE PRECISION for dlasq5.
	Contains $d(no)$ , the last value of $d$ .
dnm1	REAL for slasq5
	DOUBLE PRECISION for dlasq5.
	Contains $d(no-1)$ .
dnm2	REAL for slasq5
	DOUBLE PRECISION for dlasq5.
	Contains $d(n0-2)$ .

## *ieee* LOGICAL. Flag for IEEE or non-IEEE arithmetic.

# ?lasq6

Computes one dqds transform in ping-pong form. Used by ?bdsqr and ?stegr.

### Discussion

The routine 2lasq6 computes one dqd (shift equal to zero) transform in ping-pong form, with protection against underflow and overflow.

### **Input Parameters**

i0	INTEGER. First index.
<i>n0</i>	INTEGER. Last index.
Z	REAL for slasq6 DOUBLE PRECISION for dlasq6. Array, DIMENSION (4n). $z$ holds the $qd$ array. <i>emin</i> is stored in $z(4*n0)$ to avoid an extra argument.
pp	<b>INTEGER</b> . <i>pp</i> =0 for ping, <i>pp</i> =1 for pong.

## **Output Parameters**

dmin	REAL for slasq6 DOUBLE PRECISION for dlasq6. Minimum value of $d$ .
dminl	REAL for slasq6 DOUBLE PRECISION for dlasq6. Minimum value of $d$ , excluding $d(n0)$ .
dmin2	REAL for slasq6 DOUBLE PRECISION for dlasq6. Minimum value of $d$ , excluding $d(n0)$ and $d(n0-1)$ .
dn	REAL for slasq6 DOUBLE PRECISION for dlasq6. Contains $d(n0)$ , the last value of $d$ .
drim1	REAL for slasq6 DOUBLE PRECISION for dlasq6. Contains $d(n0-1)$ .
drım2	REAL for slasq6 DOUBLE PRECISION for dlasq6. Contains $d(n0-2)$ .

# ?lasr

Applies a sequence of plane rotations to a general rectangular matrix.

```
call slasr ( side, pivot, direct, m, n, c, s, a, lda )
call dlasr ( side, pivot, direct, m, n, c, s, a, lda )
call clasr ( side, pivot, direct, m, n, c, s, a, lda )
call zlasr ( side, pivot, direct, m, n, c, s, a, lda )
```

#### **Discussion**

The routine performs the transformation:

A := PA, when *side* = 'L' or 'l' (Left-hand side) A := A P', when *side* = 'R' or 'r' (Right-hand side)

where *A* is an *m*-by-*n* real matrix and *P* is an orthogonal matrix, consisting of a sequence of plane rotations determined by the parameters *pivot* and *direct* as follows (z = m when *side* = 'L' or 'l' and z = n when *side* = 'R' or 'r'):

When direct = 'F' or 'f' (Forward sequence) then  $P = P(z - 1) \dots P(2) P(1)$ , and when direct = 'B' or 'b' (Backward sequence) then  $P = P(1) P(2) \dots P(z - 1)$ ,

where P(k) is a plane rotation matrix for the following planes:

when pivot = 'V' or 'v' (Variable pivot), the plane (k, k + 1)when pivot = 'T' or 't' (Top pivot), the plane (1, k + 1)when pivot = 'B' or 'b' (Bottom pivot), the plane (k, z)

c(k) and s(k) must contain the cosine and sine that define the matrix P(k). The 2-by-2 plane rotation part of the matrix P(k), R(k), is assumed to be of the form:

$$R(k) = \begin{bmatrix} c(k) & s(k) \\ -s(k) & c(k) \end{bmatrix}$$

side	CHARACTER*1. Specifies whether the plane rotation matrix <i>P</i> is applied to <i>A</i> on the left or the right. = 'L': Left, compute <i>A</i> := <i>P A</i> = 'R': Right, compute <i>A</i> := <i>A P</i> '
direct	CHARACTER*1. Specifies whether <i>P</i> is a forward or backward sequence of plane rotations. = 'F': Forward, $P = P(z - 1) \dots P(2) P(1)$ = 'B': Backward, $P = P(1) P(2) \dots P(z - 1)$
pivot	CHARACTER*1. Specifies the plane for which $P(k)$ is a plane rotation matrix. = 'v': Variable pivot, the plane $(k, k+1)$ = 'T': Top pivot, the plane $(1, k+1)$ = 'B': Bottom pivot, the plane $(k, z)$
m	<b>INTEGER.</b> The number of rows of the matrix <i>A</i> . If $m \leq 1$ , an immediate return is effected.
п	<b>INTEGER.</b> The number of columns of the matrix <i>A</i> . If $n \leq 1$ , an immediate return is effected.
C, S	<pre>REAL for slasr/clasr DOUBLE PRECISION for dlasr/zlasr. Arrays, DIMENSION (m-1) if side = 'L', (n-1) if side = 'R'. c(k) and s(k) contain the cosine and sine that define the matrix P(k) as described above.</pre>
a	REAL for slasr DOUBLE PRECISION for dlasr COMPLEX for clasr COMPLEX*16 for zlasr. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). The <i>m</i> -by- <i>n</i> matrix <i>A</i> .
lda	<b>INTEGER.</b> The leading dimension of the array <i>A</i> . $1da \ge \max(1,m)$ .

#### **Output Parameters**

а

On exit, A is overwritten by PA if side = 'R' or by AP' if side = 'L'.

# ?lasrt

Sorts numbers in increasing or decreasing order.

```
call slasrt ( id, n, d, info )
call dlasrt ( id, n, d, info )
```

#### **Discussion**

The routine ?lasrt sorts the numbers in *d* in increasing order (if id = 'I') or in decreasing order (if id = 'D'). It uses Quick Sort, reverting to Insertion Sort on arrays of size  $\leq 0$ . Dimension of stack limits *n* to about  $2^{32}$ .

#### **Input Parameters**

id	CHARACTER*1. = 'I': sort <i>d</i> in increasing order; = 'D': sort <i>d</i> in decreasing order.
п	<b>INTEGER</b> . The length of the array <i>d</i> .
d	REAL for slasrt
	DOUBLE PRECISION for dlasrt.
	On entry, the array to be sorted.

#### **Output Parameters**

d	On exit, $d$ has been sorted into increasing order $(d(1) \leq \leq d(n))$ or into decreasing order $(d(1) \geq \geq d(n))$ , depending on <i>id</i> .
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -i, the i-th argument had an illegal value.</pre>

# ?lassq

Updates a sum of squares represented in scaled form.

call slassq ( n, x, incx, scale, sumsq )
call dlassq ( n, x, incx, scale, sumsq )
call classq ( n, x, incx, scale, sumsq )
call zlassq ( n, x, incx, scale, sumsq )

#### **Discussion**

The real routines slassq/dlassq return the values *scl* and *smsq* such that

$$scl^{2} * smsq = x(1)^{2} + ... + x(n)^{2} + scale^{2} * sumsq,$$

where x(i) = x(1 + (i - 1) incx).

The value of *sumsq* is assumed to be non-negative and *scl* returns the value

 $scl = \max(scale, abs(x(i))).$ 

Values *scale* and *sumsq* must be supplied in *scale* and *sumsq*, and *scl* and *smsq* are overwritten on *scale* and *sumsq*, respectively.

The complex routines classq/zlassq return the values *scl* and *ssq* such that

$$scl^{2} * ssq = x(1)^{2} + ... + x(n)^{2} + scale^{2} * sumsq,$$

where x(i) = abs (x(1 + (i - 1) incx)).

The value of *sumsq* is assumed to be at least unity and the value of *ssq* will then satisfy

 $1.0 \leq ssq \leq sumsq + 2n$ 

scale is assumed to be non-negative and scl returns the value

 $scl = \max(scale, abs(real(x(i))), abs(aimag(x(i)))).$ 

Values *scale* and *sumsq* must be supplied in *scale* and *sumsq*, and *scl* and *ssq* are overwritten on *scale* and *sumsq*, respectively.

All routines **?lassq** make only one pass through the vector *x*.

## **Input Parameters**

n	<b>INTEGER.</b> The number of elements to be used from the vector $\mathbf{x}$ .
x	REAL for slassq DOUBLE PRECISION for dlassq COMPLEX for classq COMPLEX*16 for zlassq. The vector for which a scaled sum of squares is computed: $x(i) = x(1 + (i - 1) incx), 1 \le \le n$ .
incx	<b>INTEGER</b> . The increment between successive values of the vector $\mathbf{x}$ . <i>incx</i> > 0.
scale	REAL for slassq/classq DOUBLE PRECISION for dlassq/zlassq. On entry, the value <i>scale</i> in the equation above.
sumsq	REAL for slassq/classq DOUBLE PRECISION for dlassq/zlassq. On entry, the value <i>sumsq</i> in the equation above.

# **Output Parameters**

scale	On exit, <i>scale</i> is overwritten with <i>scl</i> , the scaling factor for the sum of squares.
sumsq	<ul> <li>For real flavors:</li> <li>On exit, sumsq is overwritten with the value smsq in the equation above.</li> <li>For complex flavors:</li> <li>On exit, sumsq is overwritten with the value ssq in the equation above.</li> </ul>

# ?lasv2

Computes the singular value decomposition of a 2-by-2 triangular matrix

call slasv2 ( f, g, h, ssmin, ssmax, snr, csr, snl, csl )
call dlasv2 ( f, g, h, ssmin, ssmax, snr, csr, snl, csl )

#### **Discussion**

The routine **?lasv2** computes the singular value decomposition of a 2-by-2 triangular matrix

On return, abs(ssmax) is the larger singular value, abs(ssmin) is the smaller singular value, and (csl,snl) and (csr,snr) are the left and right singular vectors for abs(ssmax), giving the decomposition

1	csl	snl	fg	9	csr	-snr	=	ssmax 0	0
	-snl	csl	0	h	snr	csr		0	ssmin

#### **Input Parameters**

f, g, h
REAL for slasv2
DOUBLE PRECISION for dlasv2.
The (1,1), (1,2) and (2,2) elements of the 2-by-2 matrix, respectively.

#### **Output Parameters**

ssmin, ssmax REAL for slasv2
DOUBLE PRECISION for dlasv2.
abs(ssmin) and abs(ssmax) is the smaller and the
larger singular value, respectively.

snl, csl	REAL for slasv2 DOUBLE PRECISION for dlasv2. The vector ( <i>csl</i> , <i>snl</i> ) is a unit left singular vector for the singular value abs( <i>ssmax</i> ).
snr, csr	REAL for slasv2 DOUBLE PRECISION for dlasv2. The vector ( <i>csr</i> , <i>snr</i> ) is a unit right singular vector for the singular value abs( <i>ssmax</i> ).

### **Application Notes**

Any input parameter may be aliased with any output parameter. Barring over/underflow and assuming a guard digit in subtraction, all output quantities are correct to within a few units in the last place (ulps).

In IEEE arithmetic, the code works correctly if one matrix element is infinite.

Overflow will not occur unless the largest singular value itself overflows or is within a few ulps of overflow. (On machines with partial overflow, like the Cray, overflow may occur if the largest singular value is within a factor of 2 of overflow.)

Underflow is harmless if underflow is gradual. Otherwise, results may correspond to a matrix modified by perturbations of size near the underflow threshold.

# ?laswp

Performs a series of row interchanges on a general rectangular matrix.

call slaswp ( n, a, lda, k1, k2, ipiv, incx )
call dlaswp ( n, a, lda, k1, k2, ipiv, incx )
call claswp ( n, a, lda, k1, k2, ipiv, incx )
call zlaswp ( n, a, lda, k1, k2, ipiv, incx )

### Discussion

The routine performs a series of row interchanges on the matrix A. One row interchange is initiated for each of rows k1 through k2 of A.

### **Input Parameters**

n	<b>INTEGER</b> . The number of columns of the matrix A.
a	<ul> <li>REAL for slaswp</li> <li>DOUBLE PRECISION for dlaswp</li> <li>COMPLEX for claswp</li> <li>COMPLEX*16 for zlaswp.</li> <li>Array, DIMENSION (<i>lda</i>, <i>n</i>).</li> <li>On entry, the matrix of column dimension <i>n</i> to which the row interchanges will be applied.</li> </ul>
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> .
k1	<b>INTEGER.</b> The first element of <i>ipiv</i> for which a row interchange will be done.
k2	<b>INTEGER.</b> The last element of <i>ipiv</i> for which a row interchange will be done.
ipiv	<pre>INTEGER. Array, DIMENSION (m * abs(incx)). The vector of pivot indices. Only the elements in positions k1 through k2 of ipiv are accessed. ipiv(k) = l implies rows k and l are to be interchanged</pre>
incx	<b>INTEGER.</b> The increment between successive values of <i>ipiv</i> . If <i>ipiv</i> is negative, the pivots are applied in reverse order.

### **Output Parameters**

a On exit, the permuted matrix	а	On exit, the	permuted	matrix
--------------------------------	---	--------------	----------	--------

# ?lasy2

Solves the Sylvester matrix equation where the matrices are of order 1 or 2.

#### **Discussion**

The routine solves for the *n*1-by-*n*2 matrix *X*,  $1 \le n1, n2 \le 2$ , in

op(TL) * X + isgn * X * op(TR) = scale *B,

where

*TL* is n1-by-n1, *TR* is n2- by-n2, *B* is n1-by-n2, and isgn = 1 or -1. op(T) = T or *T*, where *T* denotes the transpose of *T*.

ltranl	LOGICAL. On entry, <i>ltranl</i> specifies the op( $TL$ ): = .FALSE., op( $TL$ ) = $TL$ , = .TRUE., op( $TL$ ) = $TL'$ .
ltranr	LOGICAL. On entry, <i>ltranr</i> specifies the op( <i>TR</i> ): = .FALSE., op( <i>TR</i> ) = <i>TR</i> , = .TRUE., op( <i>TR</i> ) = <i>TR</i> '.
isgn	<b>INTEGER</b> . On entry, <i>isgn</i> specifies the sign of the equation as described before. <i>isgn</i> may only be 1 or -1.
nl	<b>INTEGER</b> . On entry, <i>n1</i> specifies the order of matrix <i>TL</i> . <i>n1</i> may only be 0, 1 or 2.

n2	INTEGER. On entry, <i>n2</i> specifies the order of matrix <i>TR</i> . <i>n2</i> may only be 0, 1 or 2.
tl	REAL for slasy2 DOUBLE PRECISION for dlasy2. Array, DIMENSION ( <i>ldt1</i> ,2). On entry, <i>t1</i> contains an <i>n1</i> -by- <i>n1</i> matrix <i>TL</i> .
ldtl	<b>INTEGER.</b> The leading dimension of the matrix $t1$ . $ldt1 \ge max(1,n1)$ .
tr	REAL for slasy2 DOUBLE PRECISION for dlasy2. Array, DIMENSION ( <i>ldtr</i> ,2). On entry, <i>tr</i> contains an <i>n</i> 2-by- <i>n</i> 2 matrix <i>TR</i> .
ldtr	INTEGER. The leading dimension of the matrix $tr$ . $ldtr \ge max(1,n2)$ .
b	REAL for slasy2 DOUBLE PRECISION for dlasy2. Array, DIMENSION ( <i>ldb</i> ,2). On entry, the <i>n1</i> -by- <i>n2</i> matrix <i>b</i> contains the right-hand side of the equation.
ldb	INTEGER. The leading dimension of the matrix <i>b</i> . $1db \ge max(1,n1)$ .
ldx	INTEGER. The leading dimension of the output matrix x. $1dx \ge max(1,n1)$ .
Output Parameters	

scale	REAL for slasy2
	DOUBLE PRECISION for dlasy2.
	On exit, <i>scale</i> contains the scale factor.
	scale is chosen less than or equal to 1 to prevent the
	solution overflowing.

x	<b>REAL</b> for slasy2 DOUBLE PRECISION for dlasy2. Array, DIMENSION ( <i>ldx</i> ,2). On exit, x contains the <i>n1</i> -by- <i>n2</i> solution.
xnorm	REAL for slasy2 DOUBLE PRECISION for dlasy2. On exit, <i>xnorm</i> is the infinity-norm of the solution.
info	<ul> <li>INTEGER. On exit, <i>info</i> is set to</li> <li>0: successful exit.</li> <li>1: <i>TL</i> and <i>TR</i> have too close eigenvalues, so <i>TL</i> or <i>TR</i> is perturbed to get a nonsingular equation.</li> </ul>



**NOTE.** *In the interests of speed, this routine does not check the inputs for errors.* 

# ?lasyf

Computes a partial factorization of a real/complex symmetric matrix, using the diagonal pivoting method.

call slasyf ( uplo, n, nb, kb, a, lda, ipiv, w, ldw, info) call dlasyf ( uplo, n, nb, kb, a, lda, ipiv, w, ldw, info) call clasyf ( uplo, n, nb, kb, a, lda, ipiv, w, ldw, info) call zlasyf ( uplo, n, nb, kb, a, lda, ipiv, w, ldw, info)

#### **Discussion**

The routine **?lasyf** computes a partial factorization of a real/complex symmetric matrix *A* using the Bunch-Kaufman diagonal pivoting method. The partial factorization has the form:

$$A = \begin{bmatrix} I & U_{12} \\ 0 & U_{22} \end{bmatrix} \begin{bmatrix} A_{11} & 0 \\ 0 & D \end{bmatrix} \begin{bmatrix} I & 0 \\ U_{12}' & U_{22}' \end{bmatrix} \text{ if } uplo = 'U', \text{ or}$$
$$A = \begin{bmatrix} L_{11} & 0 \\ L_{21} & I \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} L_{11}' & L_{21}' \\ 0 & I \end{bmatrix} \text{ if } uplo = 'L'$$

where the order of D is at most nb. The actual order is returned in the argument kb, and is either nb or nb-1, or n if  $n \leq nb$ .

This is an auxiliary routine called by ?sytrf. It uses blocked code (calling Level 3 BLAS) to update the submatrix  $A_{11}$  (if uplo = 'U') or  $A_{22}$  (if uplo = 'L').

uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the symmetric matrix <i>A</i> is stored: = 'U': Upper triangular = 'L': Lower triangular
п	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ .
nb	<b>INTEGER.</b> The maximum number of columns of the matrix <i>A</i> that should be factored. <i>nb</i> should be at least 2 to allow for 2-by-2 pivot blocks.
a	REAL for slasyf DOUBLE PRECISION for dlasyf COMPLEX for clasyf COMPLEX*16 for zlasyf. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the symmetric matrix <i>A</i> . If <i>uplo</i> = 'U', the leading <i>n</i> -by- <i>n</i> upper triangular part of <i>a</i> contains the upper triangular part of the matrix <i>A</i> , and the strictly lower triangular part of <i>a</i> is not referenced. If <i>uplo</i> = 'L', the leading <i>n</i> -by- <i>n</i> lower

triangular part of a contains the lower triangular part of the matrix A, and the strictly upper triangular part of a is not referenced.

lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $1 \text{da} \ge \max(1, n)$ .
W	REAL for slasyf DOUBLE PRECISION for dlasyf COMPLEX for clasyf COMPLEX*16 for zlasyf. Workspace array, DIMENSION ( <i>ldw</i> , <i>nb</i> ).
ldw	<b>INTEGER.</b> The leading dimension of the array w. $1dw \ge max(1,n)$ .

### **Output Parameters**

kb	<b>INTEGER.</b> The number of columns of <i>A</i> that were actually factored <i>kb</i> is either <i>nb</i> -1 or <i>nb</i> , or <i>n</i> if $n \leq nb$ .
a	On exit, a contains details of the partial factorization.
ipiv	<pre>INTEGER. Array, DIMENSION (n). Details of the interchanges and the block structure of D. If uplo = 'U', only the last kb elements of ipiv are set; if uplo = 'L', only the first kb elements are set.</pre>
	If $ipiv(k) > 0$ , then rows and columns $k$ and $ipiv(k)$ were interchanged and $D(k,k)$ is a 1-by-1 diagonal block. If $uplo = 'U'$ and $ipiv(k) = ipiv(k-1) < 0$ , then rows and columns $k$ -1 and $-ipiv(k)$ were interchanged and D(k-1:k, k-1:k) is a 2-by-2 diagonal block. If $uplo = 'L'$ and $ipiv(k) = ipiv(k+1) < 0$ , then rows and columns $k+1$ and $-ipiv(k)$ were interchanged and D(k:k+1, k:k+1) is a 2-by-2 diagonal block.

infoINTEGER.= 0: successful exit> 0: if info = k, D(k,k) is exactly zero. Thefactorization has been completed, but the block diagonalmatrix D is exactly singular.

# ?lahef

Computes a partial factorization of a complex Hermitian indefinite matrix, using the diagonal pivoting method.

call clahef ( uplo, n, nb, kb, a, lda, ipiv, w, ldw, info)
call zlahef ( uplo, n, nb, kb, a, lda, ipiv, w, ldw, info)

#### **Discussion**

The routine **?lahef** computes a partial factorization of a complex Hermitian matrix *A*, using the Bunch-Kaufman diagonal pivoting method. The partial factorization has the form:

$$A = \begin{bmatrix} I & U_{12} \\ 0 & U_{22} \end{bmatrix} \begin{bmatrix} A_{11} & 0 \\ 0 & D \end{bmatrix} \begin{bmatrix} I & 0 \\ U_{12}' & U_{22}' \end{bmatrix} \text{ if } uplo = 'U', \text{ or}$$
$$A = \begin{bmatrix} L_{11} & 0 \\ L_{21} & I \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} L_{11}' & L_{21}' \\ 0 & I \end{bmatrix} \text{ if } uplo = 'L'$$

where the order of *D* is at most *nb*. The actual order is returned in the argument *kb*, and is either *nb* or *nb*-1, or *n* if  $n \leq nb$ . Note that U' denotes the conjugate transpose of *U*.

This is an auxiliary routine called by ?hetrf. It uses blocked code (calling Level 3 BLAS) to update the submatrix  $A_{11}$  (if uplo = 'U') or  $A_{22}$  (if uplo = 'L').

### **Input Parameters**

uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the Hermitian matrix <i>A</i> is stored: = ' <b>u</b> ': Upper triangular = ' <b>L</b> ': Lower triangular	
п	INTEGER. The order of the matrix A. $n \ge 0$ .	
nb	<b>INTEGER.</b> The maximum number of columns of the matrix <i>A</i> that should be factored. <i>nb</i> should be at least 2 to allow for 2-by-2 pivot blocks.	
a	COMPLEX for clahef COMPLEX*16 for zlahef. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the Hermitian matrix <i>A</i> . If <i>uplo</i> = 'U', the leading <i>n</i> -by- <i>n</i> upper triangular part of <i>a</i> contains the upper triangular part of the matrix <i>A</i> , and the strictly lower triangular part of <i>a</i> is not referenced. If <i>uplo</i> = 'L', the leading <i>n</i> -by- <i>n</i> lower triangular part of <i>a</i> contains the lower triangular part of the matrix <i>A</i> , and the strictly upper triangular part of <i>a</i> is not referenced.	
lda	<b>INTEGER.</b> The leading dimension of the array <i>a</i> . $1 da \ge max(1,n)$ .	
W	COMPLEX for clahef COMPLEX*16 for zlahef. Workspace array, DIMENSION ( <i>ldw</i> , <i>nb</i> ).	
ldw	INTEGER. The leading dimension of the array w. $ldw \ge max(1,n)$ .	
Output Parameters		

#### kb

INTEGER. The number of columns of A that were actually factored kb is either nb-1 or nb, or n if  $n \leq nb$ .

а	On exit, a contains details of the partial factorization.
ipiv	INTEGER. Array, DIMENSION ( <i>n</i> ). Details of the interchanges and the block structure of <i>D</i> . If $uplo = 'U'$ , only the last <i>kb</i> elements of <i>ipiv</i> are set; if $uplo = 'L'$ , only the first <i>kb</i> elements are set.
	If $ipiv(k) > 0$ , then rows and columns $k$ and $ipiv(k)$ were interchanged and $D(k,k)$ is a 1-by-1 diagonal block. If $uplo = 'U'$ and $ipiv(k) = ipiv(k-1) < 0$ , then rows and columns $k$ -1and $-ipiv(k)$ were interchanged and D(k-1:k, k-1:k) is a 2-by-2 diagonal block. If $uplo = 'L'$ and $ipiv(k) = ipiv(k+1) < 0$ , then rows and columns $k+1$ and $-ipiv(k)$ were interchanged and D(k:k+1, k:k+1) is a 2-by-2 diagonal block.
info	<b>INTEGER.</b> = 0: successful exit > 0: if <i>info</i> = $k$ , $D(k,k)$ is exactly zero. The factorization has been completed, but the block diagonal matrix $D$ is exactly singular.

# ?latbs

Solves a triangular banded system of equations.

### **Discussion**

The routine solves one of the triangular systems

Ax = s b or  $A^{T}x = s b$  or  $A^{H}x = s b$  (for complex flavors)

with scaling to prevent overflow, where *A* is an upper or lower triangular band matrix. Here  $A^{T}$  denotes the transpose of *A*,  $A^{H}$  denotes the conjugate transpose of *A*, *x* and *b* are *n*-element vectors, and *s* is a scaling factor, usually less than or equal to 1, chosen so that the components of *x* will be less than the overflow threshold. If the unscaled problem will not cause overflow, the Level 2 BLAS routine ?tbsv is called. If the matrix *A* is singular (A(j, j) = 0 for some *j*), then *s* is set to 0 and a non-trivial solution to Ax = 0 is returned.

uplo	CHARACTER*1. Specifies whether the matrix <i>A</i> is upper or lower triangular. = 'U': Upper triangular = 'L': Lower triangular
trans	CHARACTER*1. Specifies the operation applied to A. = 'N': Solve $Ax = s b$ (no transpose) = 'T': Solve $A^{T}x = s b$ (transpose) = 'C': Solve $A^{H}x = s b$ (conjugate transpose)
diag	CHARACTER*1. Specifies whether or not the matrix <i>A</i> is unit triangular = 'N': Non-unit triangular = 'U': Unit triangular
normin	CHARACTER*1. Specifies whether <i>cnorm</i> has been set or not. = 'Y': <i>cnorm</i> contains the column norms on entry; = 'N': <i>cnorm</i> is not set on entry. On exit, the norms will be computed and stored in <i>cnorm</i> .
п	<b>INTEGER</b> . The order of the matrix A. $n \ge 0$ .

kd	<b>INTEGER.</b> The number of subdiagonals or superdiagonals in the triangular matrix $A$ . $kd \ge 0$ .
ab	REAL for slatbs POUBLE PRECISION for dlatbs COMPLEX for clatbs COMPLEX *16 for zlatbs. Array, DIMENSION ( <i>ldab</i> , <i>n</i> ). The upper or lower triangular band matrix <i>A</i> , stored in the first <i>kd</i> +1 rows of the array. The <i>j</i> -th column of <i>A</i> is stored in the <i>j</i> -th column of the array <i>ab</i> as follows: if <i>uplo</i> = 'U', <i>ab</i> ( <i>kd</i> +1+ <i>i</i> - <i>j</i> , <i>j</i> ) = $A(i,j)$ for max(1, <i>j</i> - <i>kd</i> ) $\leq i \leq j$ ; if <i>uplo</i> = 'L', <i>ab</i> (1+ <i>i</i> - <i>j</i> , <i>j</i> ) = $A(i,j)$ for $j \leq i \leq \min(n, j+kd)$ .
ldab	<b>INTEGER.</b> The leading dimension of the array <i>ab</i> . $1dab \ge kd+1$ .
x	REAL for slatbs DOUBLE PRECISION for dlatbs COMPLEX for clatbs COMPLEX*16 for zlatbs. Array, DIMENSION (n). On entry, the right hand side b of the triangular system.
CIOTM	REAL for slatbs/clatbs DOUBLE PRECISION for dlatbs/zlatbs. Array, DIMENSION (n). If normin = 'Y', cnorm is an input argument and cnorm(j) contains the norm of the off-diagonal part of the j-th column of A. If trans = 'N', cnorm(j) must be greater than or equal to the infinity-norm, and if trans = 'T' or 'C', cnorm(j) must be greater than or equal to the 1-norm.

#### **Output Parameters**

scale	<b>REAL</b> for slatbs/clatbs <b>DOUBLE PRECISION</b> for dlatbs/zlatbs. The scaling factor <i>s</i> for the triangular system as described above. If <i>scale</i> = 0, the matrix <i>A</i> is singular or badly scaled, and the vector <i>x</i> is an exact or approximate solution to Ax = 0.
cnorm	If $normin = 'N'$ , <i>cnorm</i> is an output argument and <i>cnorm</i> ( <i>j</i> ) returns the 1-norm of the off-diagonal part of the <i>j</i> -th column of <i>A</i> .
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -k, the k-th argument had an illegal value</pre>

# ?latdf

Uses the LU factorization of the n-by-n matrix computed by ?getc2 and computes a contribution to the reciprocal Dif-estimate.

call slatdf ( ijob, n, z, ldz, rhs, rdsum, rdscal, ipiv, jpiv )
call dlatdf ( ijob, n, z, ldz, rhs, rdsum, rdscal, ipiv, jpiv )
call clatdf ( ijob, n, z, ldz, rhs, rdsum, rdscal, ipiv, jpiv )
call zlatdf ( ijob, n, z, ldz, rhs, rdsum, rdscal, ipiv, jpiv )

#### **Discussion**

The routine **?latdf** uses the *LU* factorization of the *n*-by-*n* matrix *Z* computed by **?getc2** and computes a contribution to the reciprocal Dif-estimate by solving Zx = b for *x*, and choosing the right-hand side *b* such that the norm of *x* is as large as possible. On entry *rhs* = *b* holds the contribution from earlier solved sub-systems, and on return *rhs* = *x*.

The factorization of Z returned by ?getc2 has the form Z = P L U Q, where P and Q are permutation matrices. L is lower triangular with unit diagonal elements and U is upper triangular.

ijob	<b>INTEGER.</b> <i>i job</i> = 2: First compute an approximative null-vector <i>e</i> of <i>Z</i> using ?gecon, <i>e</i> is normalized, and solve for $Zx = \pm e - f$ with the sign giving the greater value of 2-norm( <i>x</i> ). This option is about 5 times as expensive as default. <i>i job</i> $\neq$ 2 (default): Local look ahead strategy where all entries of the right-hand side <i>b</i> is chosen as either +1 or -1.
n	<b>INTEGER.</b> The number of columns of the matrix <i>Z</i> .
Ζ	REAL for slatdf/clatdf DOUBLE PRECISION for dlatdf/zlatdf. Array, DIMENSION ( $ldz$ , $n$ ) On entry, the $LU$ part of the factorization of the <i>n</i> -by- <i>n</i> matrix <i>Z</i> computed by ?getc2: $Z = PL UQ$ .
ldz	<b>INTEGER.</b> The leading dimension of the array <i>z</i> . $1 da \ge max(1, n)$ .
rhs	REAL for slatdf/clatdf DOUBLE PRECISION for dlatdf/zlatdf. Array, DIMENSION (n). On entry, <i>rhs</i> contains contributions from other subsystems.
rdsum	REAL for slatdf/clatdf DOUBLE PRECISION for dlatdf/zlatdf. On entry, the sum of squares of computed contributions to the <i>D</i> if-estimate under computation by ?tgsyl, where the scaling factor <i>rdscal</i> has been factored out.

	If trans = 'T', rdsum is not touched. Note that rdsum only makes sense when ?tgsy2 is called by ?tgsy1.
rdscal	REAL for slatdf/clatdf DOUBLE PRECISION for dlatdf/zlatdf. On entry, scaling factor used to prevent overflow in <i>rdsum</i> . If <i>trans</i> = T', <i>rdscal</i> is not touched. Note that <i>rdscal</i> only makes sense when ?tgsy2 is called by ?tgsy1.
ipiv	<b>INTEGER.</b> Array, <b>DIMENSION</b> ( <i>n</i> ). The pivot indices; for $1 \leq i \leq n$ , row <i>i</i> of the matrix has been interchanged with row $ipiv(i)$ .
jpiv	<b>INTEGER.</b> Array, <b>DIMENSION</b> ( <i>n</i> ). The pivot indices; for $1 \leq j \leq n$ , column <i>j</i> of the matrix has been interchanged with column $jpiv(j)$ .
Output Parameters	
rhs	On exit, <i>rhs</i> contains the solution of the subsystem with

rhs	On exit, <i>rhs</i> contains the solution of the subsystem with entries according to the value of <i>ijob</i> .
rdsum	On exit, the corresponding sum of squares updated with the contributions from the current sub-system. If <i>trans</i> = 'T', <i>rdsum</i> is not touched.
rdscal	On exit, <i>rdscal</i> is updated with respect to the current contributions in <i>rdsum</i> . If <i>trans</i> = 'T', <i>rdscal</i> is not touched.

# ?latps

Solves a triangular system of equations with the matrix held in packed storage.

```
call slatps (uplo, trans, diag, normin, n, ap, x, scale, cnorm, info)
call dlatps (uplo, trans, diag, normin, n, ap, x, scale, cnorm, info)
call clatps (uplo, trans, diag, normin, n, ap, x, scale, cnorm, info)
call zlatps (uplo, trans, diag, normin, n, ap, x, scale, cnorm, info)
```

#### **Discussion**

The routine **?latps** solves one of the triangular systems

Ax = s b or  $A^{T}x = s b$  or  $A^{H}x = s b$  (for complex flavors)

with scaling to prevent overflow, where *A* is an upper or lower triangular matrix stored in packed form. Here  $A^{T}$  denotes the transpose of *A*,  $A^{H}$  denotes the conjugate transpose of *A*, *x* and *b* are *n*-element vectors, and *s* is a scaling factor, usually less than or equal to 1, chosen so that the components of *x* will be less than the overflow threshold. If the unscaled problem will not cause overflow, the Level 2 BLAS routine ?tpsv is called. If the matrix *A* is singular (A(j, j) = 0 for some *j*), then *s* is set to 0 and a non-trivial solution to Ax = 0 is returned.

uplo	CHARACTER*1. Specifies whether the matrix <i>A</i> is upper or lower triangular. = 'U': Upper triangular = 'L': Lower triangular
trans	CHARACTER*1. Specifies the operation applied to A. = 'N': Solve $Ax = s b$ (no transpose) = 'T': Solve $A^{T}x = s b$ (transpose) = 'C': Solve $A^{H}x = s b$ (conjugate transpose)

diag	CHARACTER*1. Specifies whether or not the matrix <i>A</i> is unit triangular. = 'N': Non-unit triangular = 'U': Unit triangular
normin	CHARACTER*1. Specifies whether <i>cnorm</i> has been set or not. = 'Y': <i>cnorm</i> contains the column norms on entry; = 'N': <i>cnorm</i> is not set on entry. On exit, the norms will be computed and stored in <i>cnorm</i> .
n	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ .
ap	REAL for slatps DOUBLE PRECISION for dlatps COMPLEX for clatps COMPLEX*16 for zlatps. Array, DIMENSION $(n(n+1)/2)$ . The upper or lower triangular matrix $A$ , packed columnwise in a linear array. The <i>j</i> -th column of $A$ is stored in the array <i>ap</i> as follows: if <i>uplo</i> = 'U', <i>ap</i> ( <i>i</i> + ( <i>j</i> -1) <i>j</i> /2) = $A(i,j)$ for $1 \le i \le j$ ; if <i>uplo</i> = 'L', <i>ap</i> ( <i>i</i> + ( <i>j</i> -1)(2 <i>n</i> - <i>j</i> )/2) = $A(i,j)$ for $j \le \le$ .
x	REAL for slatps DOUBLE PRECISION for dlatps COMPLEX for clatps COMPLEX*16 for zlatps. Array, DIMENSION (n) On entry, the right hand side b of the triangular system.
СЛОГТ	REAL for slatps/clatps DOUBLE PRECISION for dlatps/zlatps. Array, DIMENSION (n). If normin = 'Y', cnorm is an input argument and cnorm(j) contains the norm of the off-diagonal part of the j-th column of A. If trans = 'N', cnorm(j) must be greater than or equal to the infinity-norm, and if trans = 'T' or 'C', cnorm(j) must be greater than or equal to the 1-norm.

#### **Output Parameters**

x	On exit, $\mathbf{x}$ is overwritten by the solution vector $x$ .
scale	<b>REAL</b> for slatps/clatps <b>DOUBLE PRECISION</b> for dlatps/zlatps. The scaling factor <i>s</i> for the triangular system as described above. If <i>scale</i> = 0, the matrix <i>A</i> is singular or badly scaled, and the vector <i>x</i> is an exact or approximate solution to Ax = 0.
cnorm	If $normin = 'N'$ , <i>cnorm</i> is an output argument and <i>cnorm(j)</i> returns the 1-norm of the off-diagonal part of the <i>j</i> -th column of <i>A</i> .
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -k, the k-th argument had an illegal value</pre>

# ?latrd

Reduces the first nb rows and columns of a symmetric/Hermitian matrix A to real tridiagonal form by an orthogonal/unitary similarity transformation.

call slatrd ( uplo, n, nb, a, lda, e, tau, w, ldw )
call dlatrd ( uplo, n, nb, a, lda, e, tau, w, ldw )
call clatrd ( uplo, n, nb, a, lda, e, tau, w, ldw )
call zlatrd ( uplo, n, nb, a, lda, e, tau, w, ldw )

#### **Discussion**

The routine **?latrd** reduces *nb* rows and columns of a real symmetric or complex Hermitian matrix A to symmetric/Hermitian tridiagonal form by an orthogonal/unitary similarity transformation Q' A Q, and returns the

matrices V and W which are needed to apply the transformation to the unreduced part of A.

If uplo = 'U', ?latrd reduces the last *nb* rows and columns of a matrix, of which the upper triangle is supplied;

if uplo = L', ?latrd reduces the first *nb* rows and columns of a matrix, of which the lower triangle is supplied.

This is an auxiliary routine called by ?sytrd/?hetrd.

uplo	CHARACTER Specifies whether the upper or lower triangular part of the symmetric/Hermitian matrix <i>A</i> is stored: = ' <b>u</b> ': Upper triangular = ' <b>L</b> ': Lower triangular
n	<b>INTEGER</b> . The order of the matrix <i>A</i> .
nb	<b>INTEGER.</b> The number of rows and columns to be reduced.
a	REAL for slatrd DOUBLE PRECISION for dlatrd COMPLEX for clatrd COMPLEX*16 for zlatrd. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the symmetric/Hermitian matrix <i>A</i> If $uplo = 'U'$ , the leading <i>n</i> -by- <i>n</i> upper triangular part of <i>a</i> contains the upper triangular part of the matrix <i>A</i> , and the strictly lower triangular part of <i>a</i> is not referenced. If $uplo = 'L'$ , the leading <i>n</i> -by- <i>n</i> lower triangular part of <i>a</i> contains the lower triangular part of the matrix <i>A</i> , and the strictly upper triangular part of <i>a</i> is not referenced.
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $1 da \ge (1, n)$ .

ldw INTEGER. The leading dimension of the output array w.  $1 dw \geq max(1.n)$ . **Output Parameters** On exit, if uplo = 'U', the last *nb* columns have been а reduced to tridiagonal form, with the diagonal elements overwriting the diagonal elements of a; the elements above the diagonal with the array tau, represent the orthogonal/unitary matrix Q as a product of elementary reflectors: if uplo = L', the first *nb* columns have been reduced to tridiagonal form, with the diagonal elements overwriting the diagonal elements of *a*; the elements below the diagonal with the array tau, represent the orthogonal/unitary matrix Q as a product of elementary reflectors. REAL for slatrd/clatrd е DOUBLE PRECISION for dlatrd/zlatrd. If uplo = 'U', e(n-nb:n-1) contains the superdiagonal elements of the last *nb* columns of the reduced matrix; if uplo = L', e(1:nb) contains the subdiagonal elements of the first *nb* columns of the reduced matrix. REAL for slatrd tau DOUBLE PRECISION for dlatrd COMPLEX for clatrd COMPLEX*16 for zlatrd. Array, DIMENSION (*lda*, *n*). The scalar factors of the elementary reflectors, stored in tau(n-nb:n-1) if uplo = 'U', and in tau(1:nb) if uplo= 'L'. REAL for slatrd W DOUBLE PRECISION for dlatrd COMPLEX for clatrd

COMPLEX*16 for zlatrd.

Array, DIMENSION (*lda*, *n*).

The *n*-by-*nb* matrix *W* required to update the unreduced part of *A*.

#### **Application Notes**

If uplo = 'U', the matrix Q is represented as a product of elementary reflectors

 $Q = H(n) H(n-1) \dots H(n-nb+1)$ 

Each H(i) has the form

H(i) = I - tau * v * v'

where tau is a real/complex scalar, and v is a real/complex vector with v(i:n) = 0 and v(i-1) = 1; v(1:i-1) is stored on exit in a(1:i-1, i), and tau in tau(i-1).

If uplo = L', the matrix Q is represented as a product of elementary reflectors

$$Q = H(1) H(2) \dots H(nb)$$

Each H(i) has the form

H(i) = I - tau * v * v'

where tau is a real/complex scalar, and v is a real/complex vector with v(1:i) = 0 and v(i+1) = 1; v(i+1:n) is stored on exit in a(i+1:n, i), and tau in tau(i).

The elements of the vectors *v* together form the *n*-by-*nb* matrix *V* which is needed, with *W*, to apply the transformation to the unreduced part of the matrix, using a symmetric/Hermitian rank-2k update of the form: A := A - VW - WV.

The contents of *a* on exit are illustrated by the following examples with n = 5 and nb = 2:

if uplo = 'U':
 if uplo = 'L':

 
$$\begin{bmatrix} a & a & v_4 & v_5 \\ a & a & v_4 & v_5 \\ a & 1 & v_5 \\ d & 1 \\ d \end{bmatrix}$$
 $\begin{bmatrix} d \\ 1 & d \\ v_1 & 1 & a \\ v_1 & v_2 & a & a \\ v_1 & v_2 & a & a \end{bmatrix}$ 

where d denotes a diagonal element of the reduced matrix, a denotes an element of the original matrix that is unchanged, and  $v_i$  denotes an element of the vector defining H(i).

## ?latrs

Solves a triangular system of equations with the scale factor set to prevent overflow.

#### **Discussion**

The routine solves one of the triangular systems

Ax = s b or  $A^{T}x = s b$  or  $A^{H}x = s b$  (for complex flavors)

with scaling to prevent overflow. Here A is an upper or lower triangular matrix,  $A^{T}$  denotes the transpose of A,  $A^{H}$  denotes the conjugate transpose of A, x and b are *n*-element vectors, and s is a scaling factor, usually less than or equal to 1, chosen so that the components of x will be less than the overflow threshold. If the unscaled problem will not cause overflow, the Level 2 BLAS routine ?trsv is called. If the matrix A is singular (A(j, j) = 0 for some j), then s is set to 0 and a non-trivial solution to Ax = 0 is returned.

CHARACTER*1. Specifies whether the matrix <i>A</i> is upper or lower triangular. = ' <b>u</b> ': Upper triangular = ' <b>L</b> ': Lower triangular
CHARACTER*1. Specifies the operation applied to A. = 'N': Solve $Ax = s b$ (no transpose) = 'T': Solve $A^{T}x = s b$ (transpose) = 'C': Solve $A^{H}x = s b$ (conjugate transpose)
CHARACTER*1. Specifies whether or not the matrix <i>A</i> is unit triangular. = 'N': Non-unit triangular = 'U': Unit triangular
CHARACTER*1. Specifies whether <i>cnorm</i> has been set or not. = 'Y': <i>cnorm</i> contains the column norms on entry; = 'N': <i>cnorm</i> is not set on entry. On exit, the norms will be computed and stored in <i>cnorm</i> .
<b>INTEGER.</b> The order of the matrix A. $n \ge 0$
<ul> <li>REAL for slatrs</li> <li>DOUBLE PRECISION for dlatrs</li> <li>COMPLEX for clatrs</li> <li>COMPLEX*16 for zlatrs.</li> <li>Array, DIMENSION (<i>lda</i>, <i>n</i>). Contains the triangular matrix <i>A</i>. If <i>uplo</i> = 'U', the leading <i>n</i>-by-<i>n</i> upper triangular part of the array <i>a</i> contains the upper triangular matrix, and the strictly lower triangular part of <i>a</i> is not referenced. If <i>uplo</i> = 'L', the leading <i>n</i>-by-<i>n</i> lower triangular part of the array <i>a</i> contains the lower triangular matrix, and the strictly upper triangular part of <i>a</i> is not referenced. If <i>uplo</i> = 'L', the leading <i>n</i>-by-<i>n</i> lower triangular matrix, and the strictly upper triangular part of <i>a</i> is not referenced. If <i>diag</i> = 'U', the diagonal elements of <i>a</i> are also not referenced and are assumed to be 1.</li> </ul>

lda	INTEGER.	
	The leading dimension of the array <b>a</b> . $1 \text{da} \ge \max(1, n)$ .	
x	REAL for slatrs	
	DOUBLE PRECISION for dlatrs	
	COMPLEX for clatrs	
	COMPLEX*16 for zlatrs.	
	Array, DIMENSION $(n)$ . On entry, the right hand side $b$	
	of the triangular system.	
cnorm	REAL for slatrs/clatrs)	
	DOUBLE PRECISION for dlatrs/zlatrs.	
	Array, DIMENSION (n). If normin = 'Y', cnorm is an	
	input argument and <u>cnorm</u> (j) contains the norm of the	
	off-diagonal part of the <i>j</i> -th column of <i>A</i> . If <i>trans</i> =	
	'N', <i>cnorm</i> ( <i>j</i> ) must be greater than or equal to the	
	infinity-norm, and if <i>trans</i> = 'T' or 'C', <i>cnorm</i> ( <i>j</i> ) must	
	be greater than or equal to the 1-norm.	
Output Parameters		
x	On exit, $\mathbf{x}$ is overwritten by the solution vector $x$ .	
x scale	On exit, $\mathbf{x}$ is overwritten by the solution vector $x$ . REAL for slatrs/clatrs)	
	•	
	REAL for slatrs/clatrs)	
	REAL for slatrs/clatrs) DOUBLE PRECISION for dlatrs/zlatrs.	
	REAL for slatrs/clatrs) DOUBLE PRECISION for dlatrs/zlatrs. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). The scaling factor <i>s</i> for the	
	REAL for slatrs/clatrs ) DOUBLE PRECISION for dlatrs/zlatrs. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). The scaling factor <i>s</i> for the triangular system as described above.	
	<pre>REAL for slatrs/clatrs ) DOUBLE PRECISION for dlatrs/zlatrs. Array, DIMENSION (<i>lda</i>, <i>n</i>). The scaling factor <i>s</i> for the triangular system as described above. If <i>scale</i> = 0, the matrix <i>A</i> is singular or badly scaled,</pre>	
	<b>REAL</b> for slatrs/clatrs ) <b>DOUBLE PRECISION</b> for dlatrs/zlatrs. Array, <b>DIMENSION</b> ( <i>lda</i> , <i>n</i> ). The scaling factor <i>s</i> for the triangular system as described above. If <i>scale</i> = 0, the matrix <i>A</i> is singular or badly scaled, and the vector <i>x</i> is an exact or approximate solution to	
scale	<b>REAL</b> for slatrs/clatrs ) <b>DOUBLE PRECISION</b> for dlatrs/zlatrs. Array, <b>DIMENSION</b> ( <i>lda</i> , <i>n</i> ). The scaling factor <i>s</i> for the triangular system as described above. If <i>scale</i> = 0, the matrix <i>A</i> is singular or badly scaled, and the vector <i>x</i> is an exact or approximate solution to $Ax = 0$ .	
scale	<b>REAL</b> for slatrs/clatrs ) <b>DOUBLE PRECISION</b> for dlatrs/zlatrs. Array, <b>DIMENSION</b> ( <i>lda</i> , <i>n</i> ). The scaling factor <i>s</i> for the triangular system as described above. If <i>scale</i> = 0, the matrix <i>A</i> is singular or badly scaled, and the vector <i>x</i> is an exact or approximate solution to $Ax = 0$ . If <i>normin</i> = ' <i>N</i> ', <i>cnorm</i> is an output argument and	
scale	REAL for slatrs/clatrs ) DOUBLE PRECISION for dlatrs/zlatrs. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). The scaling factor <i>s</i> for the triangular system as described above. If <i>scale</i> = 0, the matrix <i>A</i> is singular or badly scaled, and the vector <i>x</i> is an exact or approximate solution to Ax = 0. If <i>normin</i> = ' <i>N</i> ', <i>cnorm</i> is an output argument and <i>cnorm</i> ( <i>j</i> ) returns the 1-norm of the off-diagonal part of	

= 0: successful exit

< 0: if *info* = -*k*, the *k*-th argument had an illegal value

## **Application Notes**

A rough bound on x is computed; if that is less than overflow, 2trsv is called, otherwise, specific code is used which checks for possible overflow or divide-by-zero at every operation.

A columnwise scheme is used for solving Ax = b. The basic algorithm if A is lower triangular is

x[1:n] := b[1:n]for j = 1, ..., nx(j) := x(j) / A(j,j)x[j+1:n] := x[j+1:n] - x(j)*A[j+1:n,j]end

Define bounds on the components of x after j iterations of the loop:

M(j) = bound on x[1:j] G(j) = bound on x[j+1:n]Initially, let M(0) = 0 and  $G(0) = \max\{x(i), i=1,...,n\}$ .

Then for iteration j+1 we have

$$\begin{split} \mathbf{M}(j+1) &\leq \mathbf{G}(j) / |A(j+1,j+1)| \\ G(j+1) &\leq \mathbf{G}(j) + M(j+1) * |A[j+2:n,j+1]| \\ &\leq \mathbf{G}(j) \left(1 + \textit{cnorm}(j+1) / |A(j+1,j+1)|\right), \end{split}$$

where cnorm(j+1) is greater than or equal to the infinity-norm of column j+1 of A, not counting the diagonal. Hence

$$G(j) \leq G(0) \prod_{1 \leq i \leq j} (1 + \operatorname{cnorm}(i) / |A(i,i)|)$$

and

$$|x(j)| \le (G(0)/|A(j,j)|) \prod_{1 \le i \le j} (1 + cnorm(i)/|A(i,i)|)$$

Since  $|x(j)| \leq M(j)$ , we use the Level 2 BLAS routine ?trsv if the reciprocal of the largest M(j), j=1,..,n, is larger than max(*underflow*, 1/*overflow*).

The bound on x(j) is also used to determine when a step in the columnwise method can be performed without fear of overflow. If the computed bound

is greater than a large constant, x is scaled to prevent overflow, but if the bound overflows, x is set to 0, x(j) to 1, and scale to 0, and a non-trivial solution to Ax = 0 is found.

Similarly, a row-wise scheme is used to solve  $A^{T}x = b$  or  $A^{H}x = b$ . The basic algorithm for A upper triangular is

for j = 1, ..., nx(j) := (b(j) - A[1:j-1,j]' x[1:j-1]) / A(j,j)end

We simultaneously compute two bounds

G(j) = bound on  $(b(i) - A[1:i-1,i]' * x[1:i-1]), 1 \le i \le j$ 

M(j) = bound on  $x(i), 1 \le i \le j$ 

The initial values are G(0) = 0,  $M(0) = \max\{b(i), i=1,..,n\}$ , and we add the constraint  $G(j) \ge G(j-1)$  and  $M(j) \ge M(j-1)$  for  $j \ge 1$ .

Then the bound on x(j) is

 $M(j) \le M(j-1) * (1 + cnorm(j)) / |A(j,j)|$ 

$$\leq M(0) \prod_{1 \leq i \leq j} (1 + \operatorname{cnorm}(i) / |A(i,i)|)$$

and we can safely call ?trsv if 1/M(n) and 1/G(n) are both greater than max(*underflow*, 1/overflow).

# ?latrz

Factors an upper trapezoidal matrix by means of orthogonal/unitary transformations.

call slatrz ( m, n, l, a, lda, tau, work )
call dlatrz ( m, n, l, a, lda, tau, work )
call clatrz ( m, n, l, a, lda, tau, work )
call zlatrz ( m, n, l, a, lda, tau, work )

### Discussion

The routine <code>?latrz</code> factors the <code>m-by-(m+1)</code> real/complex upper trapezoidal matrix

 $[A1 \ A2] = [A(1:m, 1:m) \ A(1:m, n-1+1:n)]$ 

as  $(R \ 0) \times Z$ , by means of orthogonal/unitary transformations. *Z* is an (m+1)-by-(m+1) orthogonal/unitary matrix and *R* and *A*1 are *m*-by-*m* upper triangular matrices.

m	<b>INTEGER.</b> The number of rows of the matrix <i>A</i> . $m \ge 0$ .
п	<b>INTEGER.</b> The number of columns of the matrix A. $n \ge 0$ .
1	<b>INTEGER.</b> The number of columns of the matrix <i>A</i> containing the meaningful part of the Householder vectors. $n-m \ge 1 \ge 0.$
a	REAL for slatrz DOUBLE PRECISION for dlatrz COMPLEX for clatrz COMPLEX*16 for zlatrz. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the leading <i>m</i> -by- <i>n</i> upper trapezoidal part of the array <i>a</i> must contain the matrix to be factorized.
lda	<b>INTEGER</b> . The leading dimension of the array <i>a</i> . $1 da \ge max(1,m)$ .
work	REAL for slatrz DOUBLE PRECISION for dlatrz COMPLEX for clatrz COMPLEX*16 for zlatrz. Workspace array, DIMENSION (m).

a	On exit, the leading <i>m</i> -by- <i>m</i> upper triangular part of <i>a</i> contains the upper triangular matrix <i>R</i> , and elements $n-1+1$ to <i>n</i> of the first <i>m</i> rows of <i>a</i> , with the array <i>tau</i> , represent the orthogonal/unitary matrix <i>Z</i> as a product of <i>m</i> elementary reflectors.
tau	REAL for slatrz DOUBLE PRECISION for dlatrz COMPLEX for clatrz COMPLEX*16 for zlatrz.

Array, **DIMENSION** (*m*). The scalar factors of the elementary reflectors.

### **Application Notes**

The factorization is obtained by Householder's method. The *k*-th transformation matrix, Z(k), which is used to introduce zeros into the (m - k + 1)-th row of *A*, is given in the form

$$Z(k) = \begin{bmatrix} I & 0 \\ 0 & T(k) \end{bmatrix}$$

where

$$T(k) = I - tau * u(k) * u(k)', \quad u(k) = \begin{vmatrix} 1 \\ 0 \\ z(k) \end{vmatrix}$$

*tau* is a scalar and z(k) is an *l*-element vector. *tau* and z(k) are chosen to annihilate the elements of the *k*-th row of A2. The scalar *tau* is returned in the *k*-th element of *tau* and the vector u(k) in the *k*-th row of A2, such that the elements of z(k) are in a(k, l+1), ..., a(k, n). The elements of *R* are returned in the upper triangular part of A1.

Z is given by

 $Z = Z(1) Z(2) \dots Z(m).$ 

# ?lauu2

Computes the product  $UU^H$  or  $L^HL$ , where U and L are upper or lower triangular matrices (unblocked algorithm).

call	slauu2	(	uplo,	n,	a,	lda,	info	)
call	dlauu2	(	uplo,	n,	a,	lda,	info	)
call	clauu2	(	uplo,	n,	a,	lda,	info	)
call	zlauu2	(	uplo,	n,	a,	lda,	info	)

## Discussion

The routine ?lauu2 computes the product UU' or L'L, where the triangular factor U or L is stored in the upper or lower triangular part of the array a. If uplo = 'U' or 'u', then the upper triangle of the result is stored, overwriting the factor U in a. If uplo = 'L' or 'l', then the lower triangle of the result is stored, overwriting the factor L in a.

This is the unblocked form of the algorithm, calling Level 2 BLAS.

uplo	CHARACTER*1. Specifies whether the triangular factor stored in the array a is upper or lower triangular: = 'U': Upper triangular = 'L': Lower triangular
n	<b>INTEGER.</b> The order of the triangular factor <i>U</i> or <i>L</i> . $n \ge 0$ .
a	REAL for slauu2 DOUBLE PRECISION for dlauu2 COMPLEX for clauu2

	COMPLEX*16 for zlauu2. Array, DIMENSION ( <i>lda</i> , <i>n</i> ).On entry, the triangular factor $U$ or $L$ .		
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $1 da \ge max(1,n)$ .		
Output Parameters			
a	On exit, if $uplo = 'U'$ , the upper triangle of <i>a</i> is overwritten with the upper triangle of the product $UU'$ ; if $uplo = 'L'$ , the lower triangle of <i>a</i> is overwritten with the lower triangle of the product $L'L$ .		
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -k, the k-th argument had an illegal value</pre>		

# ?lauum

Computes the product  $UU^H$  or  $L^HL$ , where U and L are upper or lower triangular matrices.

call slauum ( uplo, n, a, lda, info )
call dlauum ( uplo, n, a, lda, info )
call clauum ( uplo, n, a, lda, info )
call zlauum ( uplo, n, a, lda, info )

# Discussion

The routine **?lauum** computes the product UU' or L'L, where the triangular factor U or L is stored in the upper or lower triangular part of the array **a**.

If uplo = 'U' or 'u', then the upper triangle of the result is stored, overwriting the factor U in **a**.

If uplo = 'L' or 'l', then the lower triangle of the result is stored, overwriting the factor L in **a**.

This is the blocked form of the algorithm, calling Level 3 BLAS.

# **Input Parameters**

uplo	CHARACTER*1. Specifies whether the triangular factor stored in the array <i>a</i> is upper or lower triangular: = ' <b>u</b> ': Upper triangular = ' <b>L</b> ': Lower triangular
п	<b>INTEGER.</b> The order of the triangular factor $U$ or $L$ . $n \ge 0$ .
a	REAL for slauum DOUBLE PRECISION for dlauum COMPLEX for clauum COMPLEX*16 for zlauum. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the triangular factor <i>U</i> or <i>L</i> .
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $1 da \ge max(1,n)$ .

# **Output Parameters**

a	On exit, if $uplo = 'U'$ , the upper triangle of <i>a</i> is overwritten with the upper triangle of the product $UU'$ ; if $uplo = 'L'$ , the lower triangle of <i>a</i> is overwritten with the lower triangle of the product $L'L$ .
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -k, the k-th argument had an illegal value</pre>

# ?org2l/?ung2l

Generates all or part of the orthogonal/unitary matrix Q from a QL factorization determined by ?geqlf (unblocked algorithm).

call sorg2l ( m, n, k, a, lda, tau, work, info )
call dorg2l ( m, n, k, a, lda, tau, work, info )
call cung2l ( m, n, k, a, lda, tau, work, info )
call zung2l ( m, n, k, a, lda, tau, work, info )

#### **Discussion**

The routine  $\operatorname{corg2l}/\operatorname{corg2l}$  generates an *m*-by-*n* real/complex matrix *Q* with orthonormal columns, which is defined as the last *n* columns of a product of *k* elementary reflectors of order *m*:

 $Q = H(k) \dots H(2) H(1)$  as returned by ?geqlf.

m	<b>INTEGER.</b> The number of rows of the matrix $Q. m \ge 0$ .
п	<b>INTEGER.</b> The number of columns of the matrix $Q. m \ge n \ge 0$ .
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $Q$ . $n \ge k \ge 0$ .
a	REAL for sorg21 DOUBLE PRECISION for dorg21 COMPLEX for cung21 COMPLEX*16 for zung21. Array, DIMENSION ( $lda, n$ ). On entry, the ( $n-k+i$ )-th column must contain the vector

	which defines the elementary reflector $H(i)$ , for $i = 1, 2,, k$ , as returned by ?geqlf in the last k columns of its array argument a.
lda	<b>INTEGER</b> . The first dimension of the array $a$ . $1 da \ge max(1,m)$ .
tau	REAL for sorg21 DOUBLE PRECISION for dorg21 COMPLEX for cung21 COMPLEX*16 for zung21. Array, DIMENSION (k). tau(i) must contain the scalar factor of the elementary reflector $H(i)$ , as returned by ?geqlf.
work	REAL for sorg21 DOUBLE PRECISION for dorg21 COMPLEX for cung21 COMPLEX*16 for zung21. Workspace array, DIMENSION (n).

а	On exit, the <i>m</i> -by- <i>n</i> matrix $Q$ .
info	INTEGER.
	= 0: successful exit
	< 0: if <u>info</u> = -i, the i-th argument has an illegal value

# ?org2r/?ung2r

Generates all or part of the orthogonal/unitary matrix Q from a QR factorization determined by ?geqrf (unblocked algorithm).

call sorg2r ( m, n, k, a, lda, tau, work, info )
call dorg2r ( m, n, k, a, lda, tau, work, info )

```
call cung2r ( m, n, k, a, lda, tau, work, info )
call zung2r ( m, n, k, a, lda, tau, work, info )
```

## **Discussion**

The routine  $\operatorname{corg2r}/\operatorname{curg2r}$  generates an *m*-by-*n* real/complex matrix Q with orthonormal columns, which is defined as the first *n* columns of a product of *k* elementary reflectors of order *m* 

 $Q = H(1) H(2) \dots H(k)$ 

as returned by ?geqrf.

· · ·	
m	<b>INTEGER.</b> The number of rows of the matrix $Q. m \ge 0$ .
п	<b>INTEGER.</b> The number of columns of the matrix $Q. m \ge n \ge 0$ .
k	INTEGER. The number of elementary reflectors whose product defines the matrix $Q$ . $n \ge k \ge 0$ .
a	REAL for sorg2r DOUBLE PRECISION for dorg2r COMPLEX for cung2r COMPLEX*16 for zung2r. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the <i>i</i> -th column must contain the vector which defines the elementary reflector $H(i)$ , for $i = 1, 2,, k$ , as returned by ?geqrf in the first <i>k</i> columns of its array argument <i>a</i> .
lda	INTEGER. The first DIMENSION of the array a. $1 da \ge max(1,m)$ .
tau	REAL for sorg2r DOUBLE PRECISION for dorg2r COMPLEX for cung2r COMPLEX*16 for zung2r.

	Array, DIMENSION (k). tau(i) must contain the scalar factor of the elementary reflector $H(i)$ , as returned by ?geqrf.
work	REAL for sorg2r
	DOUBLE PRECISION for dorg2r
	COMPLEX for cung2r
	COMPLEX*16 for zung2r.
	Workspace array, DIMENSION (n).
Output Para	imeters
a	On exit, the <i>m</i> -by- <i>n</i> matrix $Q$ .
info	<b>INTEGER.</b> = 0: successful exit

< 0: if <u>info</u> = -<u>i</u>, the <u>i</u>-th argument has an illegal value

# ?orgl2/?ungl2

Generates all or part of the orthogonal/unitary matrix Q from an LQ factorization determined by ?gelqf (unblocked algorithm).

call sorgl2 ( m, n, k, a, lda, tau, work, info )
call dorgl2 ( m, n, k, a, lda, tau, work, info )
call cungl2 ( m, n, k, a, lda, tau, work, info )
call zungl2 ( m, n, k, a, lda, tau, work, info )

#### **Discussion**

The routine  $\operatorname{corgl2/?ungl2}$  generates a *m*-by-*n* real/complex matrix *Q* with orthonormal rows, which is defined as the first *m* rows of a product of *k* elementary reflectors of order *n* 

 $Q = H(k) \dots H(2) H(1)$  or  $Q = H(k)' \dots H(2)' H(1)'$ 

as returned by ?gelqf.

# **Input Parameters**

m	INTEGER. The number of rows of the matrix $Q.m \ge 0$ .
n	<b>INTEGER.</b> The number of columns of the matrix $Q$ . $n \ge m$ .
k	INTEGER. The number of elementary reflectors whose product defines the matrix $Q. m \ge k \ge 0$ .
a	REAL for sorg12 DOUBLE PRECISION for dorg12 COMPLEX for cung12 COMPLEX*16 for zung12. Array, DIMENSION ( <i>1da</i> , <i>n</i> ). On entry, the <i>i</i> -th row must contain the vector which defines the elementary reflector $H(i)$ , for $i = 1, 2,, k$ , as returned by ?gelqf in the first <i>k</i> rows of its array argument <i>a</i> .
lda	INTEGER. The first dimension of the array $a$ . $lda \ge max(1,m)$ .
tau	REAL for sorg12 DOUBLE PRECISION for dorg12 COMPLEX for cung12 COMPLEX*16 for zung12. Array, DIMENSION $(k)$ . tau(i) must contain the scalar factor of the elementary reflector H $(i)$ , as returned by ?gelqf.
work	REAL for sorgl2 DOUBLE PRECISION for dorgl2 COMPLEX for cungl2 COMPLEX*16 for zungl2. Workspace array, DIMENSION (m).
Output Barama	toro

#### **Output Parameters**

a On exit, the m-by-n matrix Q.

info

INTEGER.

= 0: successful exit

< 0: if *info* = -*i*, the *i*-th argument has an illegal value.

# ?orgr2/?ungr2

Generates all or part of the orthogonal/unitary matrix Q from an RQ factorization determined by ?gerqf (unblocked algorithm).

call	sorgr2	(	m,	n,	k,	a,	lda,	tau,	work,	info	)
call	dorgr2	(	m,	n,	k,	a,	lda,	tau,	work,	info	)
call	cungr2	(	m,	n,	k,	a,	lda,	tau,	work,	info	)
call	zungr2	(	m,	n,	k,	a,	lda,	tau,	work,	info	)

## **Discussion**

The routine ?orgr2/?ungr2 generates an *m*-by-*n* real matrix Q with orthonormal rows, which is defined as the last *m* rows of a product of *k* elementary reflectors of order *n*  $Q = H(1) H(2) \dots H(k)$  or  $Q = H(1)' H(2)' \dots H(k)'$ 

as returned by ?gerqf.

m	<b>INTEGER.</b> The number of rows of the matrix $Q. m \ge 0$ .
n	<b>INTEGER.</b> The number of columns of the matrix $Q. n \ge m$ .
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $Q.m \ge k \ge 0$ .
a	REAL for sorgr2 DOUBLE PRECISION for dorgr2 COMPLEX for cungr2

	COMPLEX*16 for zungr2. Array, DIMENSION ( <i>lda</i> , <i>n</i> ).On entry, the ( <i>m</i> - <i>k</i> + <i>i</i> )-th row must contain the vector which defines the elementary reflector $H(i)$ , for $i = 1, 2,, k$ , as returned by ?gerqf in the last <i>k</i> rows of its array argument <i>a</i> .
lda	<b>INTEGER</b> . The first dimension of the array $a$ . $1da \ge max(1,m)$ .
tau	REAL for sorgr2 DOUBLE PRECISION for dorgr2 COMPLEX for cungr2 COMPLEX*16 for zungr2. Array, DIMENSION $(k)$ .tau $(\dot{i})$ must contain the scalar factor of the elementary reflector $H(\dot{i})$ , as returned by ?gerqf.
work	REAL for sorgr2 DOUBLE PRECISION for dorgr2 COMPLEX for cungr2 COMPLEX*16 for zungr2. Workspace array, DIMENSION (m).

а	On exit, the <i>m</i> -by- <i>n</i> matrix $Q$ .
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -i, the i-th argument has an illegal value</pre>

# ?orm2l/?unm2l

Multiplies a general matrix by the orthogonal/unitary matrix from a QL factorization determined by ?geqlf (unblocked algorithm).

call sorm21	(	side,	trans,	m,	n,	k,	a,	lda,	tau,	с,	ldc,	work,	info	)
call dorm21	(	side,	trans,	m,	n,	k,	a,	lda,	tau,	с,	ldc,	work,	info	)
call cunm2l	(	side,	trans,	m,	n,	k,	a,	lda,	tau,	с,	ldc,	work,	info	)
call zunm21	(	side,	trans,	m,	n,	k,	a,	lda,	tau,	с,	ldc,	work,	info	)

## **Discussion**

The routine  $\operatorname{corm2l/?unm2l}$  overwrites the general real/complex *m*-by-*n* matrix *C* with

Q*C if side = 'L' and trans = 'N', or Q'*C if side = 'L' and trans = 'T' (for real flavors) or trans = 'C' (for complex flavors), or C*Q if side = 'R' and trans = 'N', or C*Q' if side = 'R' and trans = 'T' (for real flavors) or trans = 'C' (for complex flavors)

where Q is a real orthogonal or complex unitary matrix defined as the product of k elementary reflectors

 $Q = H(\mathbf{k}) \dots H(2) H(1)$ 

as returned by ?geqlf. Q is of order *m* if *side* = 'L' and of order *n* if *side* = 'R'.

#### **Input Parameters**

side

CHARACTER*1. = 'L': apply Q or Q' from the left = 'R': apply Q or Q' from the right

trans	CHARACTER*1. = 'N': apply Q (No transpose) = 'T': apply Q' (Transpose, for real flavors) = 'C': apply Q' (Conjugate transpose, for complex flavors)
m	<b>INTEGER.</b> The number of rows of the matrix $C. m \ge 0$ .
n	INTEGER. The number of columns of the matrix $C. n \ge 0$ .
k	INTEGER. The number of elementary reflectors whose product defines the matrix Q. If <i>side</i> = 'L', $m \ge k \ge 0$ ; if <i>side</i> = 'R', $n \ge k \ge 0$ .
a	REAL for sorm21 DOUBLE PRECISION for dorm21 COMPLEX for cunm21 COMPLEX*16 for zunm21. Array, DIMENSION ( $1da,k$ ). The <i>i</i> -th column must contain the vector which defines the elementary reflector $H(i)$ , for $i = 1, 2,, k$ , as returned by ?geqlf in the last <i>k</i> columns of its array argument <i>a</i> . The array <i>a</i> is modified by the routine but restored on exit.
lda	INTEGER. The leading dimension of the array $a$ . If $side = 'L'$ , $1da \ge max(1, m)$ ; if $side = 'R'$ , $1da \ge max(1, n)$ .
tau	REAL for sorm21 DOUBLE PRECISION for dorm21 COMPLEX for cunm21 COMPLEX*16 for zunm21. Array, DIMENSION $(k)$ . $tau(i)$ must contain the scalar factor of the elementary reflector $H(i)$ , as returned by ?geqlf.

С	REAL for sorm21 DOUBLE PRECISION for dorm21
	COMPLEX for cunm21
	COMPLEX*16 for zunm21.
	Array, DIMENSION ( $ldc$ , $n$ ).On entry, the <i>m</i> -by- $n$ matrix <i>C</i> .
ldc	<b>INTEGER</b> . The leading dimension of the array <i>C</i> . $1dc \ge max(1,m)$ .
work	REAL for sorm21 DOUBLE PRECISION for dorm21 COMPLEX for cunm21 COMPLEX*16 for zunm21. Workspace array, DIMENSION: (n) if side = 'L', (m) if side = 'R'.

С	On exit, $c$ is overwritten by $QC$ or $Q'C$ or $CQ'$ or $CQ$ .
info	INTEGER.
	= 0: successful exit
	< 0: if <i>info</i> = - <i>i</i> , the <i>i</i> -th argument had an illegal value

# ?orm2r/?unm2r

Multiplies a general matrix by the orthogonal/unitary matrix from a QR factorization determined by ?geqrf (unblocked algorithm).

call sorm2r ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info ) call dorm2r ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info ) call cunm2r ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info ) call zunm2r ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info )

### **Discussion**

The routine ?orm2r/?unm2r overwrites the general real/complex *m*-by-*n* matrix *C* with

Q*C if side = 'L' and trans = 'N', or Q'*C if side = 'L' and trans = 'T' (for real flavors) or trans = 'C' (for complex flavors), or C*Q if side = 'R' and trans = 'N', or C*Q' if side = 'R' and trans = 'T' (for real flavors) or trans = 'C' (for complex flavors)

where Q is a real orthogonal or complex unitary matrix defined as the product of k elementary reflectors

 $Q = H(1) H(2) \dots H(k)$ 

as returned by ?geqrf. Q is of order m if side = 'L' and of order n if side = 'R'.

side	CHARACTER*1. = 'L': apply $Q$ or $Q'$ from the left = 'R': apply $Q$ or $Q'$ from the right
trans	CHARACTER*1. = 'N': apply Q (No transpose) = 'T': apply Q' (Transpose, for real flavors) = 'C': apply Q' (Conjugate transpose, for complex flavors)
m	<b>INTEGER.</b> The number of rows of the matrix $C. m \ge 0$ .
n	<b>INTEGER.</b> The number of columns of the matrix $C. n \ge 0$ .
k	INTEGER. The number of elementary reflectors whose product defines the matrix $Q$ . If $side = 'L', m \ge k \ge 0$ ; if $side = 'R', n \ge k \ge 0$ .

a	REAL for sorm2r
	DOUBLE PRECISION for dorm2r
	COMPLEX for cunm2r
	COMPLEX*16 for zunm2r.
	Array, DIMENSION ( $1da,k$ ). The <i>i</i> -th column must
	contain the vector which defines the elementary
	reflector $H(i)$ , for $i = 1, 2,, k$ , as returned by ?geqrf in
	the first $k$ columns of its array argument $a$ . The array $a$
	is modified by the routine but restored on exit.
lda	INTEGER.
	The leading dimension of the array a.
	If $side = 'L'$ , $1da \ge max(1, m)$ ;
	if $side = 'R'$ , $1da \ge max(1, n)$ .
tau	REAL for sorm2r
	DOUBLE PRECISION for dorm2r
	COMPLEX for cunm2r
	COMPLEX*16 for zunm2r.
	Array, DIMENSION (k).
	tau(i) must contain the scalar factor of the elementary
	reflector $H(i)$ , as returned by <b>?geqrf</b> .
С	REAL for sorm2r
	DOUBLE PRECISION for dorm2r
	COMPLEX for cunm2r
	COMPLEX*16 for zunm2r.
	Array, <b>DIMENSION</b> ( <i>ldc</i> , <i>n</i> ). On entry, the <i>m</i> -by- <i>n</i>
	matrix C.
ldc	INTEGER.
	The leading dimension of the array <i>C</i> . $1dc \ge max(1,m)$ .
work	REAL for sorm2r
	DOUBLE PRECISION for dorm2r
	COMPLEX for cunm2r
	COMPLEX*16 for zunm2r.
	Workspace array, DIMENSION
	(n) if $side = L'$ ,
	(m) if $side = 'R'$ .

С	On exit, $c$ is overwritten by $QC$ or $Q'C$ or $CQ'$ or $CQ$ .
info	<b>INTEGER.</b> = 0: successful exit < 0: if <i>info</i> = -i, the <i>i</i> -th argument had an illegal value

# ?orml2/?unml2

Multiplies a general matrix by the orthogonal/unitary matrix from a LQ factorization determined by ?gelqf (unblocked algorithm).

call sorml2 ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info ) call dorml2 ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info ) call cunml2 ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info ) call zunml2 ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info )

# **Discussion**

The routine  $\operatorname{corml2/2unml2}$  overwrites the general real/complex *m*-by-*n* matrix *C* with

 $Q^*C$  if side = 'L' and trans = 'N', or  $Q'^*C$  if side = 'L' and trans = 'T' (for real flavors) or trans = 'C' (for complex flavors), or  $C^*Q$  if side = 'R' and trans = 'N', or  $C^*Q'$  if side = 'R' and trans = 'T' (for real flavors) or trans = 'C' (for complex flavors)

where Q is a real orthogonal or complex unitary matrix defined as the product of k elementary reflectors

 $Q = H(k) \dots H(2) H(1)$  or  $Q = H(k)' \dots H(2)' H(1)'$ 

as returned by ?gelqf. Q is of order m if side = 'L' and of order n if side = 'R'.

side	CHARACTER*1. = 'L': apply $Q$ or $Q'$ from the left = 'R': apply $Q$ or $Q'$ from the right
trans	CHARACTER*1. = 'N': apply Q (No transpose) = 'T': apply Q' (Transpose, for real flavors) = 'C': apply Q' (Conjugate transpose, for complex flavors)
т	<b>INTEGER.</b> The number of rows of the matrix $C. m \ge 0$ .
п	<b>INTEGER.</b> The number of columns of the matrix $C$ . $n \ge 0$ .
k	<b>INTEGER.</b> The number of elementary reflectors whose product defines the matrix $Q$ . If <i>side</i> = 'L', $m \ge k \ge 0$ ; if <i>side</i> = 'R', $n \ge k \ge 0$ .
a	REAL for sorml2 DOUBLE PRECISION for dorml2 COMPLEX for cunml2 COMPLEX*16 for zunml2. Array, DIMENSION ( <i>lda</i> , <i>m</i> ) if <i>side</i> = 'L', ( <i>lda</i> , <i>n</i> ) if <i>side</i> = 'R' The <i>i</i> -th row must contain the vector which defines the elementary reflector $H(i)$ , for $i = 1, 2,, k$ , as returned by ?gelqf in the first <i>k</i> rows of its array argument <i>a</i> . The array <i>a</i> is modified by the routine but restored on exit.
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $1 da \ge max(1,k)$ .
tau	REAL for sorml2 DOUBLE PRECISION for dorml2 COMPLEX for cunml2 COMPLEX*16 for zunml2.

	Array, DIMENSION (k). tau(i) must contain the scalar factor of the elementary reflector $H(i)$ , as returned by ?gelqf.
С	REAL for sorm12 DOUBLE PRECISION for dorm12 COMPLEX for cunm12 COMPLEX*16 for zunm12. Array, DIMENSION ( <i>ldc</i> , <i>n</i> ) On entry, the <i>m</i> -by- <i>n</i> matrix <i>C</i> .
ldc	<b>INTEGER.</b> The leading dimension of the array $c$ . $ldc \ge max(1,m)$ .
work	REAL for sorm12 DOUBLE PRECISION for dorm12 COMPLEX for cunm12 COMPLEX*16 for zunm12. Workspace array, DIMENSION (n) if side = 'L', (m) if side = 'R'
Output Param	otors

С	On exit, $c$ is overwritten by $QC$ or $Q'C$ or $CQ'$ or $CQ$ .
info	INTEGER.
	= 0: successful exit
	< 0: if <i>info</i> = - <i>i</i> , the <i>i</i> -th argument had an illegal value

# ?ormr2/?unmr2

Multiplies a general matrix by the orthogonal/unitary matrix from a RQ factorization determined by ?gerqf (unblocked algorithm).

call sormr2 ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info )

call dormr2 ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info )
call cunmr2 ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info )
call zunmr2 ( side, trans, m, n, k, a, lda, tau, c, ldc, work, info )

#### Discussion

The routine ?ormr2/?unmr2 overwrites the general real/complex *m*-by-*n* matrix *C* with

Q * C if side = 'L' and trans = 'N', or Q'*C if side = 'L' and trans = 'T' (for real flavors) or trans = 'C' (for complex flavors), or C*Q if side = 'R' and trans = 'N', or C*Q' if side = 'R' and trans = 'T' (for real flavors) or trans = 'C' (for complex flavors)

where Q is a real orthogonal or complex unitary matrix defined as the product of k elementary reflectors

 $Q = H(1) H(2) \dots H(k)$  or  $Q = H(1)' H(2)' \dots H(k)'$ 

as returned by ?gerqf. Q is of order m if side = 'L' and of order n if side = 'R'.

side	CHARACTER*1. = 'L': apply $Q$ or $Q'$ from the left = 'R': apply $Q$ or $Q'$ from the right
trans	CHARACTER*1. = 'N': apply Q (No transpose) = 'T': apply Q' (Transpose, for real flavors) = 'C': apply Q' (Conjugate transpose, for complex flavors)
m	<b>INTEGER.</b> The number of rows of the matrix $C. m \ge 0$ .
n	<b>INTEGER.</b> The number of columns of the matrix $C$ . $n \ge 0$ .

k	INTEGER.
	The number of elementary reflectors whose product
	defines the matrix Q.
	If $side = L', m \ge k \ge 0;$
	if $side = 'R', n \ge k \ge 0$ .
a	REAL for sormr2
	DOUBLE PRECISION for dormr2
	COMPLEX for cunmr2
	COMPLEX*16 for zunmr2.
	Array, DIMENSION
	(1da, m) if side = 'L',
	(1da, n) if side = 'R'
	The $i$ -th row must contain the vector which defines the
	elementary reflector $H(i)$ , for $i = 1, 2,, k$ , as returned by
	<b>?gerqf</b> in the last <i>k</i> rows of its array argument <i>a</i> . The
	array a is modified by the routine but restored on exit.
lda	INTEGER.
	The leading dimension of the array a. $1 \text{da} \ge \max(1, k)$ .
tau	REAL for sormr2
	DOUBLE PRECISION for dormr2
	COMPLEX for cunmr2
	COMPLEX*16 for zunmr2.
	Array, DIMENSION (k).
	tau(i) must contain the scalar factor of the elementary
	reflector $H(i)$ , as returned by ?gerqf.
С	REAL for sormr2
	DOUBLE PRECISION for dormr2
	COMPLEX for cunmr2
	COMPLEX*16 for zunmr2.
	Array, DIMENSION (ldc, n).
	On entry, the <i>m</i> -by- <i>n</i> matrix $C$ .
ldc	INTEGER.
	The leading dimension of the array C. $1dc \ge max(1,m)$ .

work

REAL for sormr2 DOUBLE PRECISION for dormr2 COMPLEX for cunmr2 COMPLEX*16 for zunmr2. Workspace array, **DIMENSION** (n) if side = 'L', (m) if side = 'R'

#### **Output Parameters**

С	On exit, $c$ is overwritten by $QC$ or $Q'C$ or $CQ'$ or $CQ$ .
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -i, the i-th argument had an illegal value</pre>

# ?ormr3/?unmr3

Multiplies a general matrix by the orthogonal/unitary matrix from a RZ factorization determined by ?tzrzf (unblocked algorithm).

call sormr3 (side, trans, m, n, k, l, a, lda, tau, c, ldc, work, info) call dormr3 (side, trans, m, n, k, l, a, lda, tau, c, ldc, work, info) call cunmr3 (side, trans, m, n, k, l, a, lda, tau, c, ldc, work, info) call zunmr3 (side, trans, m, n, k, l, a, lda, tau, c, ldc, work, info)

### Discussion

The routine ?ormr3/?unmr3 overwrites the general real/complex m-by-n matrix C with

O*C if side = 'L' and trans = 'N', or Q' * C if side = 'L' and trans = 'T' (for real flavors) or trans = 'C' (for complex flavors), or C*Q if side = 'R' and trans = 'N', or C*Q' if side = 'R' and trans = 'T' (for real flavors) or trans = 'C' (for complex flavors)

where Q is a real orthogonal or complex unitary matrix defined as the product of k elementary reflectors

 $Q = H(1) H(2) \dots H(k)$ 

as returned by ?tzrzf. Q is of order m if side = 'L' and of order n if side = 'R'.

side	CHARACTER*1. = 'L': apply $Q$ or $Q$ ' from the left = 'R': apply $Q$ or $Q$ ' from the right
trans	CHARACTER*1. = 'N': apply Q (No transpose) = 'T': apply Q' (Transpose, for real flavors) = 'C': apply Q' (Conjugate transpose, for complex flavors)
m	<b>INTEGER.</b> The number of rows of the matrix $C. m \ge 0$ .
п	<b>INTEGER.</b> The number of columns of the matrix $C$ . $n \ge 0$ .
k	INTEGER. The number of elementary reflectors whose product defines the matrix $Q$ . If side = 'L', $m \ge k \ge 0$ ; if side = 'R', $n \ge k \ge 0$ .
1	INTEGER. The number of columns of the matrix A containing the meaningful part of the Householder reflectors. If $side = 'L', m \ge 1 \ge 0$ , if $side = 'R', n \ge 1 \ge 0$ .

a	REAL for sormr3
	DOUBLE PRECISION for dormr3
	COMPLEX for cunmr3
	COMPLEX*16 for zunmr3.
	Array, DIMENSION
	(1da, m) if side = 'L',
	(1da, n) if side = 'R'
	The <i>i</i> -th row must contain the vector which defines the elementary reflector $H(i)$ , for $i = 1, 2,, k$ , as returned by ?tzrzf in the last k rows of its array argument a. The array a is modified by the routine but restored on exit.
lda	INTEGER.
	The leading dimension of the array <b>a</b> . $1da \ge max(1,k)$ .
tau	REAL for sormr3
	DOUBLE PRECISION for dormr3
	COMPLEX for cunmr3
	COMPLEX*16 for zunmr3.
	Array, DIMENSION (k).
	$t_{au}(i)$ must contain the scalar factor of the elementary
	reflector $H(i)$ , as returned by ?tzrzf.
С	REAL for sormr3
	DOUBLE PRECISION for dormr3
	COMPLEX for cunmr3
	COMPLEX*16 for zunmr3.
	Array, DIMENSION (1dc, n).
	On entry, the <i>m</i> -by- <i>n</i> matrix <i>C</i> .
ldc	INTEGER.
	The leading dimension of the array $c$ . $ldc \ge max(1,m)$ .
work	REAL for sormr3
	DOUBLE PRECISION for dormr3
	COMPLEX for cunmr3
	COMPLEX*16 for zunmr3.
	Workspace array, DIMENSION
	(n) if $side = L'$ ,
	(m) if $side = 'R'$ .

С	On exit, $c$ is overwritten by $QC$ or $Q'C$ or $CQ'$ or $CQ$ .
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -i, the i-th argument had an illegal value</pre>

# ?pbtf2

Computes the Cholesky factorization of a symmetric/Hermitian positive definite band matrix (unblocked algorithm).

call spbtf2 ( uplo, n, kd, ab, ldab, info )
call dpbtf2 ( uplo, n, kd, ab, ldab, info )
call cpbtf2 ( uplo, n, kd, ab, ldab, info )
call zpbtf2 ( uplo, n, kd, ab, ldab, info )

### **Discussion**

The routine computes the Cholesky factorization of a real symmetric or complex Hermitian positive definite band matrix *A*. The factorization has the form

A = U' U, if uplo = 'U', or A = L L', if uplo = 'L',

where U is an upper triangular matrix, U' is the transpose of U, and L is lower triangular.

This is the unblocked version of the algorithm, calling Level 2 BLAS.

### **Input Parameters**

```
uplo
```

CHARACTER*1.

Specifies whether the upper or lower triangular part of the symmetric/Hermitian matrix *A* is stored:

- = '**U**': Upper triangular
- = 'L': Lower triangular

п	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ .
kd	INTEGER. The number of super-diagonals of the matrix A if $uplo = U$ , or the number of sub-diagonals if $uplo = L$ . $kd \ge 0$ .
ab	REAL for spbtf2 DOUBLE PRECISION for dpbtf2 COMPLEX for cpbtf2 COMPLEX*16 for zpbtf2. Array, DIMENSION ( <i>ldab</i> , <i>n</i> ). On entry, the upper or lower triangle of the symmetric/ Hermitian band matrix <i>A</i> , stored in the first <i>kd</i> +1 rows of the array. The <i>j</i> -th column of <i>A</i> is stored in the <i>j</i> -th column of the array <i>ab</i> as follows: if <i>uplo</i> = 'U', <i>ab</i> ( <i>kd</i> +1+ <i>i</i> - <i>j</i> , <i>j</i> ) = $A(i, j)$ for max(1, <i>j</i> - <i>kd</i> ) $\leq i \leq j$ ; if <i>uplo</i> = 'L', <i>ab</i> (1+ <i>i</i> - <i>j</i> , <i>j</i> ) = $A(i, j)$ for $j \leq i \leq \min(n, j+kd)$ .
ldab	<b>INTEGER.</b> The leading dimension of the array <i>ab.</i> $1dab \ge kd+1$ .
Output P	arameters
ab	On exit, if $info = 0$ , the triangular factor U or L from the Cholesky factorization $A = U' U$ or $A = L L'$ of the band matrix A, in the same storage format as A.
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -k, the k-th argument had an illegal value &gt; 0: if info = k, the leading minor of order k is not positive definite, and the factorization could not be completed.</pre>

# ?potf2

Computes the Cholesky factorization of a symmetric/Hermitian positive definite matrix (unblocked algorithm).

call spotf2 ( uplo, n, a, lda, info )
call dpotf2 ( uplo, n, a, lda, info )
call cpotf2 ( uplo, n, a, lda, info )
call zpotf2 ( uplo, n, a, lda, info )

## **Discussion**

The routine ?potf2 computes the Cholesky factorization of a real symmetric or complex Hermitian positive definite matrix A. The factorization has the form

A = U' U, if <u>uplo</u> = 'U', or

A = L L', if uplo = 'L',

where U is an upper triangular matrix and L is lower triangular.

This is the unblocked version of the algorithm, calling Level 2 BLAS.

uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the symmetric/Hermitian matrix <i>A</i> is stored. = ' <b>U</b> ': Upper triangular = ' <b>L</b> ': Lower triangular
п	<b>INTEGER.</b> The order of the matrix $A$ . $n \ge 0$ .
a	REAL for spotf2 DOUBLE PRECISION or dpotf2 COMPLEX for cpotf2 COMPLEX*16 for zpotf2. Array, DIMENSION ( <i>1da</i> , <i>n</i> ). On entry, the symmetric/Hermitian matrix <i>A</i> .

	If $uplo = 'U'$ , the leading <i>n</i> -by- <i>n</i> upper triangular part of <i>a</i> contains the upper triangular part of the matrix <i>A</i> , and the strictly lower triangular part of <i>a</i> is not referenced. If $uplo = 'L'$ , the leading <i>n</i> -by- <i>n</i> lower triangular part of <i>a</i> contains the lower triangular part of the matrix <i>A</i> , and the strictly upper triangular part of <i>a</i> is not referenced.		
lda	<b>INTEGER</b> . The leading dimension of the array <i>a</i> . $1 da \ge max(1,n)$ .		
Output Par	Output Parameters		
a	On exit, if $info = 0$ , the factor $U$ or $L$ from the Cholesky factorization $A = U'U$ or $A = LL'$ .		
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -k, the k-th argument had an illegal value &gt; 0: if info = k, the leading minor of order k is not positive definite, and the factorization could not be completed.</pre>		

# ?ptts2

Solves a tridiagonal system of the form AX=B using the  $L D L^H$  factorization computed by ?pttrf.

```
call sptts2 ( n, nrhs, d, e, b, ldb )
call dptts2 ( n, nrhs, d, e, b, ldb )
call cptts2 ( iuplo, n, nrhs, d, e, b, ldb )
call zptts2 ( iuplo, n, nrhs, d, e, b, ldb )
```

# **Discussion**

The routine ?ptts2 solves a tridiagonal system of the form A X = BReal flavors sptts2/dptts2 use the L D L factorization of A computed by spttrf/dpttrf, and complex flavors cptts2/zptts2 use the U'D U or L D L' factorization of A computed by cpttrf/zpttrf. D is a diagonal matrix specified in the vector d, U (or L) is a unit bidiagonal matrix whose superdiagonal (subdiagonal) is specified in the vector e, and X and B are n-by-nrhs matrices.

iuplo	<b>INTEGER.</b> Used with complex flavors only. Specifies the form of the factorization and whether the vector $e$ is the superdiagonal of the upper bidiagonal factor $U$ or the subdiagonal of the lower bidiagonal factor $L$ . = 1: $A = U'DU$ , $e$ is the superdiagonal of $U$ ; = 0: $A = LDL'$ , $e$ is the subdiagonal of $L$
п	<b>INTEGER.</b> The order of the tridiagonal matrix A. $n \ge 0$ .
nrhs	<b>INTEGER.</b> The number of right hand sides, that is, the number of columns of the matrix <i>B</i> . nrhs $\geq 0$ .
d	REAL for sptts2/cptts2 DOUBLE PRECISION for dptts2/zptts2. Array, DIMENSION $(n)$ . The <i>n</i> diagonal elements of the diagonal matrix <i>D</i> from the factorization of <i>A</i> .
e	REAL for sptts2 DOUBLE PRECISION for dptts2 COMPLEX for cptts2 COMPLEX*16 for zptts2. Array, DIMENSION ( <i>n</i> -1). Contains the ( <i>n</i> -1) subdiagonal elements of the unit bidiagonal factor <i>L</i> from the <i>LDL</i> ' factorization of <i>A</i> (for

b

real flavors, or for complex flavors when $iuplo = 0$ ).
For complex flavors when $iuplo = 1, e$ contains the
(n-1) superdiagonal elements of the unit bidiagonal
factor U from the factorization $A = U'DU$ .
REAL for sptts2/cptts2
DOUBLE PRECISION for dptts2/zptts2.
Array, DIMENSION (1db, nrhs).
On entry, the right hand side vectors <i>B</i> for the system of
linear equations.

1dbINTEGER.The leading dimension of the array B.  $1db \ge max(1,n)$ .

### **Output Parameters**

*b* On exit, the solution vectors, *X*.

# ?rscl

Multiplies a vector by the reciprocal of a real scalar.

call srscl ( n, sa, sx, incx )
call drscl ( n, sa, sx, incx )
call csrscl ( n, sa, sx, incx )
call zdrscl ( n, sa, sx, incx )

#### **Discussion**

The routine **?rscl** multiplies an *n*-element real/complex vector x by the real scalar 1/a. This is done without overflow or underflow as long as the final result x/a does not overflow or underflow.

#### **Input Parameters**

п

INTEGER.

The number of components of the vector *x*.

sa	REAL for srscl/csrscl
	DOUBLE PRECISION for drscl/zdrscl.
	The scalar <i>a</i> which is used to divide each component of
	the vector x. sa must be $\geq 0$ , or the subroutine will
	divide by zero.
sx	REAL for srscl
	DOUBLE PRECISION for drscl
	COMPLEX for csrscl
	COMPLEX*16 for zdrscl.
	Array, DIMENSION $(1+(n-1)*abs(incx))$ .
	The <i>n</i> -element vector <i>x</i> .
incx	INTEGER.
	The increment between successive values of the vector
	SX.
	If $incx > 0$ , $sx(1) = x(1)$ and
	$sx(1+(i-1)*incx) = x(i),  1 < i \leq n.$
	rameters

On exit, the result x/a. SX

# ?sygs2/?hegs2

Reduces a symmetric/Hermitian definite generalized eigenproblem to standard form, using the factorization results obtained from ?potrf (unblocked algorithm).

> call ssygs2 ( itype, uplo, n, a, lda, b, ldb, info ) call dsygs2 ( itype, uplo, n, a, lda, b, ldb, info ) call chegs2 ( itype, uplo, n, a, lda, b, ldb, info ) call zhegs2 ( itype, uplo, n, a, lda, b, ldb, info )

# **Discussion**

The routine ?sygs2/?hegs2 reduces a real symmetric-definite or a complex Hermitian-definite generalized eigenproblem to standard form. If itype = 1, the problem is

 $Ax = \lambda Bx$ ,

and A is overwritten by inv(U')*A*inv(U) or inv(L)*A*inv(L').

If itype = 2 or 3, the problem is

 $ABx = \lambda x$  or  $BAx = \lambda x$ ,

and A is overwritten by UAU' or L'AL. B must have been previously factorized as U'U or LL' by ?potrf.

### **Input Parameters**

itype	<b>INTEGER.</b> = 1: compute $inv(U')*A*inv(U)$ or $inv(L)*A*inv(L')$ ; = 2 or 3: compute $UAU'$ or $L'AL$ .
uplo	CHARACTER Specifies whether the upper or lower triangular part of the symmetric/Hermitian matrix <i>A</i> is stored, and how <i>B</i> has been factorized. = ' <b>u</b> ': Upper triangular = ' <b>L</b> ': Lower triangular
n	<b>INTEGER.</b> The order of the matrices <i>A</i> and <i>B</i> . $n \ge 0$ .
a	REAL for ssygs2 DOUBLE PRECISION for dsygs2 COMPLEX for chegs2 COMPLEX*16 for zhegs2. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the symmetric/Hermitian matrix <i>A</i> . If $uplo = 'U'$ , the leading <i>n</i> -by- <i>n</i> upper triangular part of <i>a</i> contains the upper triangular part of the matrix <i>A</i> , and the strictly lower triangular part of <i>a</i> is not referenced. If $uplo = 'L'$ , the leading <i>n</i> -by- <i>n</i> lower triangular part of <i>a</i> contains the lower triangular part of the matrix <i>A</i> , and the strictly upper triangular part of <i>a</i> is not referenced.

lda	INTEGER.
	The leading dimension of the array <b>a</b> . $1 \text{da} \ge \max(1, n)$ .
Ь	REAL for ssygs2 DOUBLE PRECISION for dsygs2 COMPLEX for chegs2 COMPLEX*16 for zhegs2. Array, DIMENSION ( <i>1db</i> , <i>n</i> ). The triangular factor from the Cholesky factorization of <i>B</i> as returned by ?potrf.
ldb	INTEGER.
	The leading dimension of the array <i>B</i> . $1db \ge max(1,n)$ .
Output Param	neters
a	On exit, if $info = 0$ , the transformed matrix, stored in the same format as A.
info	<pre>INTEGER. = 0: successful exit. &lt; 0: if info = -i, the i-th argument had an illegal</pre>

value.

# ?sytd2/?hetd2

Reduces a symmetric/Hermitian matrix to real symmetric tridiagonal form by an orthogonal/unitary similarity transformation (unblocked algorithm).

call	ssytd2	(	uplo,	n,	a,	lda,	d,	e,	tau,	info	)
call	dsytd2	(	uplo,	n,	a,	lda,	d,	e,	tau,	info	)
call	chetd2	(	uplo,	n,	a,	lda,	d,	e,	tau,	info	)
call	zhetd2	(	uplo,	n,	a,	lda,	d,	e,	tau,	info	)

## **Discussion**

The routine  $\frac{sytd2}{hetd2}$  reduces a real symmetric/complex Hermitian matrix *A* to real symmetric tridiagonal form *T* by an orthogonal/unitary similarity transformation: Q'AQ = T.

### **Input Parameters**

uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the symmetric/Hermitian matrix <i>A</i> is stored: = ' <b>u</b> ': Upper triangular = ' <b>L</b> ': Lower triangular
n	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ .
a	REAL for ssytd2 DOUBLE PRECISION for dsytd2 COMPLEX for chetd2 COMPLEX*16 for zhetd2. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the symmetric/Hermitian matrix <i>A</i> . If $uplo = 'U'$ , the leading <i>n</i> -by- <i>n</i> upper triangular part of <i>a</i> contains the upper triangular part of the matrix <i>A</i> , and the strictly lower triangular part of <i>a</i> is not referenced. If $uplo = 'L'$ , the leading <i>n</i> -by- <i>n</i> lower triangular part of <i>a</i> contains the lower triangular part of the matrix <i>A</i> , and the strictly upper triangular part of the matrix <i>A</i> , and the strictly upper triangular part of the matrix <i>A</i> , and the strictly upper triangular part of <i>a</i> is not referenced.
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $1 da \ge max(1,n)$ .

### **Output Parameters**

а

On exit, if uplo = 'U', the diagonal and first superdiagonal of *a* are overwritten by the corresponding elements of the tridiagonal matrix *T*, and the elements above the first superdiagonal, with the array tau, represent the orthogonal/unitary matrix *Q* as a product of elementary reflectors;

	if $uplo = L'$ , the diagonal and first subdiagonal of <i>a</i> are overwritten by the corresponding elements of the tridiagonal matrix <i>T</i> , and the elements below the first subdiagonal, with the array <i>tau</i> , represent the orthogonal/unitary matrix <i>Q</i> as a product of elementary reflectors.
d	REAL for ssytd2/chetd2 DOUBLE PRECISION for dsytd2/zhetd2. Array, DIMENSION ( <i>n</i> ). The diagonal elements of the tridiagonal matrix <i>T</i> : d(i) = a(i,i).
e	REAL for ssytd2/chetd2 DOUBLE PRECISION for dsytd2/zhetd2. Array, DIMENSION (n-1). The off-diagonal elements of the tridiagonal matrix T: e(i) = a(i,i+1) if uplo = 'U', e(i) = a(i+1,i) if uplo = 'L'.
tau	REAL for ssytd2 DOUBLE PRECISION for dsytd2 COMPLEX for chetd2 COMPLEX*16 for zhetd2. Array, DIMENSION ( <i>n</i> -1). The scalar factors of the elementary reflectors .
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -i, the i-th argument had an illegal value.</pre>

# ?sytf2

Computes the factorization of a real/complex symmetric indefinite matrix, using the diagonal pivoting method (unblocked algorithm).

call	ssytf2	(	uplo,	n,	a,	lda,	ipiv,	info	)
call	dsytf2	(	uplo,	n,	a,	lda,	ipiv,	info	)
call	csytf2	(	uplo,	n,	a,	lda,	ipiv,	info	)
call	zsytf2	(	uplo,	n,	a,	lda,	ipiv,	info	)

### Discussion

The routine **?sytf2** computes the factorization of a real/complex symmetric matrix *A* using the Bunch-Kaufman diagonal pivoting method:

A = U D U' or A = L D L'

where U (or L) is a product of permutation and unit upper (lower) triangular matrices, U' is the transpose of U, and D is symmetric and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

This is the unblocked version of the algorithm, calling Level 2 BLAS.

uplo	CHARACTER*1. Specifies whether the upper or lower triangular part of the symmetric matrix A is stored = 'U': Upper triangular = 'L': Lower triangular
n	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ .
a	REAL for ssytf2 DOUBLE PRECISION for dsytf2 COMPLEX for csytf2 COMPLEX*16 for zsytf2. Array, DIMENSION ( <i>lda</i> , <i>n</i> ).

On entry, the symmetric matrix *A*. If uplo = 'U', the leading *n*-by-*n* upper triangular part of a contains the upper triangular part of the matrix A, and the strictly lower triangular part of *a* is not referenced. If uplo = L', the leading *n*-by-*n* lower triangular part of a contains the lower triangular part of the matrix A, and the strictly upper triangular part of *a* is not referenced. lda INTEGER. The leading dimension of the array **a**.  $1 \text{da} \ge \max(1, n)$ . **Output Parameters** On exit, the block diagonal matrix D and the multipliers а used to obtain the factor U or L. ipiv INTEGER. Array, DIMENSION (n). Details of the interchanges and the block structure of DIf ipiv(k) > 0, then rows and columns k and ipiv(k)were interchanged and D(k,k) is a 1-by-1 diagonal block. If uplo = 'U' and ipiv(k) = ipiv(k-1) < 0, then rows and columns k-1 and -ipiv(k) were interchanged and D(k-1:k,k-1:k) is a 2-by-2 diagonal block. If uplo = L' and ipiv(k) = ipiv(k+1) < 0, then rows and columns k+1 and -ipiv(k) were interchanged and D(k:k+1,k:k+1) is a 2-by-2 diagonal block. info INTEGER. = 0: successful exit < 0: if *info* = -*k*, the *k*-th argument had an illegal value > 0: if info = k, D(k, k) is exactly zero. The factorization has been completed, but the block diagonal matrix D is exactly singular, and division by zero will occur if it is used to solve a system of equations.

## ?hetf2

Computes the factorization of a complex Hermitian matrix, using the diagonal pivoting method (unblocked algorithm).

> call chetf2 ( uplo, n, a, lda, ipiv, info ) call zhetf2 ( uplo, n, a, lda, ipiv, info )

### **Discussion**

The routine computes the factorization of a complex Hermitian matrix A using the Bunch-Kaufman diagonal pivoting method:

A = U D U' or A = L D L'

where U(or L) is a product of permutation and unit upper (lower) triangular matrices, U' is the conjugate transpose of U, and D is Hermitian and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

This is the unblocked version of the algorithm, calling Level 2 BLAS.

### **Input Parameters**

uplo	CHARACTER*1.
	Specifies whether the upper or lower triangular part of
	the Hermitian matrix A is stored:
	= ' <u>u</u> ': Upper triangular
	= 'L': Lower triangular
n	INTEGER.
	The order of the matrix A. $n \ge 0$ .
a	COMPLEX for chetf2
	COMPLEX*16 for zhetf2.
	Array, DIMENSION (lda, n).
	On entry, the Hermitian matrix A.
	If $uplo = 'U'$ , the leading <i>n</i> -by- <i>n</i> upper triangular part
	of a contains the upper triangular part of the matrix A,
	and the strictly lower triangular part of a is not
	referenced.

	If $uplo = L'$ , the leading <i>n</i> -by- <i>n</i> lower triangular part of a contains the lower triangular part of the matrix <i>A</i> , and the strictly upper triangular part of <i>a</i> is not referenced.
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $1 \text{da} \ge \max(1, n)$ .
Output Parame	eters
a	On exit, the block diagonal matrix $D$ and the multipliers used to obtain the factor $U$ or $L$ .
ipiv	INTEGER. Array, DIMENSION ( <i>n</i> ). Details of the interchanges and the block structure of <i>D</i> If $ipiv(k) > 0$ , then rows and columns <i>k</i> and $ipiv(k)$ were interchanged and $D(k,k)$ is a 1-by-1 diagonal block. If $uplo = 'U'$ and $ipiv(k) = ipiv(k-1) < 0$ , then rows and columns <i>k</i> -1 and $-ipiv(k)$ were interchanged and D(k-1:k,k-1:k) is a 2-by-2 diagonal block. If $uplo = 'L'$ and $ipiv(k) = ipiv(k+1) < 0$ , then rows and columns <i>k</i> +1 and $-ipiv(k)$ were interchanged and D(k:k+1,k:k+1) is a 2-by-2 diagonal block.
info	<pre>INTEGER. = 0: successful exit &lt; 0: if info = -k, the k-th argument had an illegal value &gt; 0: if info = k, D(k,k) is exactly zero. The factorization has been completed, but the block diagonal matrix D is exactly singular, and division by zero will occur if it is used to solve a system of equations.</pre>

## ?tgex2

Swaps adjacent diagonal blocks in an upper (quasi) triangular matrix pair by an orthogonal/unitary equivalence transformation.

### **Discussion**

The real routines stgex2/dtgex2 swap adjacent diagonal blocks (A11, B11) and (A22, B22) of size 1-by-1 or 2-by-2 in an upper (quasi) triangular matrix pair (A, B) by an orthogonal equivalence transformation. (A, B) must be in generalized real Schur canonical form (as returned by sgges/dgges), that is, A is block upper triangular with 1-by-1 and 2-by-2 diagonal blocks. B is upper triangular.

The complex routines ctgex2/ztgex2 swap adjacent diagonal 1-by-1 blocks (A11, B11) and (A22, B22) in an upper triangular matrix pair (A, B) by an unitary equivalence transformation. (A, B) must be in generalized Schur canonical form, that is, A and B are both upper triangular.

All routines optionally update the matrices Q and Z of generalized Schur vectors:

Q(in) *A(in)*Z(in)' = Q(out)*A(out)*Z(out)'Q(in)*B(in)*Z(in)' = Q(out)*B(out)*Z(out)'

### **Input Parameters**

wantq	LOGICAL. If wantq = .TRUE. : update the left transformation matrix Q; If wantq = .FALSE.: do not update Q.
wantz	LOGICAL. If wantz = .TRUE. : update the right transformation matrix Z; If wantz = .FALSE.: do not update Z.
п	<b>INTEGER.</b> The order of the matrices A and B. $n \ge 0$ .
a, b	REAL for stgex2 DOUBLE PRECISION for dtgex2 COMPLEX for ctgex2 COMPLEX*16 for ztgex2. Arrays, DIMENSION ( <i>1da</i> , <i>n</i> ) and ( <i>1db</i> , <i>n</i> ), respectively. On entry, the matrices <i>A</i> and <i>B</i> in the pair ( <i>A</i> , <i>B</i> ).
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $1 da \ge max(1,n)$ .
ldb	<b>INTEGER.</b> The leading dimension of the array <b>b</b> . $1db \ge max(1,n)$ .
q, z	REAL for stgex2 DOUBLE PRECISION for dtgex2 COMPLEX for ctgex2 COMPLEX*16 for ztgex2. Arrays, DIMENSION ( <i>ldq</i> , <i>n</i> ) and ( <i>ldz</i> , <i>n</i> ), respectively. On entry, if <i>wantq</i> = .TRUE., <i>q</i> contains the orthogonal/unitary matrix <i>Q</i> , and if <i>wantz</i> = .TRUE., <i>z</i> contains the orthogonal/unitary matrix <i>Z</i> .
ldq	INTEGER. The leading dimension of the array $q$ . $ldq \ge 1$ . If want $q = .$ TRUE., $ldq \ge n$ .

ldz	INTEGER. The leading dimension of the array $z$ . $ldz \ge 1$ . If want $z = .$ TRUE . , $ldz \ge n$ .
jl	<b>INTEGER.</b> The index to the first block (A11, B11). $1 \leq j_1 \leq n$ .
nl	<b>INTEGER.</b> Used with real flavors only. The order of the first block (A11, B11). $n1 = 0, 1 \text{ or } 2$ .
n2	<b>INTEGER.</b> Used with real flavors only. The order of the second block (A22, B22). $n2 = 0, 1 \text{ or } 2$ .
work	REAL for stgex2 DOUBLE PRECISION for dtgex2. Workspace array, DIMENSION ( <i>lwork</i> ). Used with real flavors only.
lwork	INTEGER. The dimension of the array work. $lwork \ge max(n*(n2+n1), 2*(n2+n1)^2)$

### **Output Parameters**

a	On exit, the updated matrix A.
b	On exit, the updated matrix <i>B</i> .
đ	On exit, the updated matrix $Q$ . Not referenced if want $q = .FALSE.$
Ζ	On exit, the updated matrix Z. Not referenced if $wantz = .FALSE$
info	INTEGER. =0: Successful exit For stgex2/dtgex2: if $info = 1$ , the transformed matrix (A, B) would be too far from generalized Schur form; the blocks are not swapped and (A, B) and (Q, Z) are unchanged. The problem of swapping is too ill-conditioned. If $info = -16$ : <i>lwork</i> is too small.

Appropriate value for *lwork* is returned in *work*(1).

For ctgex2/ztgex2: if info = 1, the transformed matrix pair (*A*, *B*) would be too far from generalized Schur form; the problem is ill-conditioned. (*A*, *B*) may have been partially reordered, and *ilst* points to the first row of the current position of the block being moved.

## ?tgsy2

Solves the generalized Sylvester equation (unblocked algorithm).

### **Discussion**

The routine 2 tgsy2 solves the generalized Sylvester equation: AR - LB = scale * C (1) DR - LE = scale * F,

using Level 1 and 2 BLAS, where R and L are unknown *m*-by-*n* matrices, (A, D), (B, E) and (C, F) are given matrix pairs of size *m*-by-*m*, *n*-by-*n* and *m*-by-*n*, respectively.

For stgsy2/dtgsy2, pairs (A, D) and (B, E) must be in generalized Schur

canonical form, that is, A, B are upper quasi triangular and D, E are upper triangular. For ctgsy2/ztgsy2, matrices A, B, D and E are upper triangular (that is, (A, D) and (B, E) in generalized Schur form).

The solution (R, L) overwrites (C, F).  $0 \leq cale \leq 1$  is an output scaling factor chosen to avoid overflow.

In matrix notation, solving equation (1) corresponds to solve

Zx = scale * b,

### where Z is defined as

$$Z = \begin{bmatrix} \operatorname{kron}(I_n, A) & -\operatorname{kron}(B', I_m) \\ \operatorname{kron}(I_n, D) & -\operatorname{kron}(E', I_m) \end{bmatrix}$$
(2)

Here  $I_k$  is the identity matrix of size k and X' is the transpose of X. kron(X, Y) denotes the Kronecker product between the matrices X and Y.

If trans = 'T', solve the transposed (conjugate transposed) system Z'y = scale * b

for y, which is equivalent to solve for R and L in

$$A' R + D' L = \text{scale} * C$$

$$R B' + L E' = \text{scale} * (-F)$$
(3)

This case is used to compute an estimate of  $Dif[(A, D), (B, E)] = sigma_min(Z)$  using reverse communication with ?lacon.

**?tgsy2** also (for  $ijob \ge 1$ ) contributes to the computation in **?tgsy1** of an upper bound on the separation between two matrix pairs. Then the input (A, D), (B, E) are sub-pencils of the matrix pair (two matrix pairs) in **?tgsy1**. See **?tgsy1** for details.

### **Input Parameters**

trans	CHARACTER If <i>trans</i> = 'N', solve the generalized Sylvester equation (1); If <i>trans</i> = 'T': solve the 'transposed' system (3).
ijob	<pre>INTEGER. Specifies what kind of functionality is to be performed. If ijob = 0: solve (1) only. If ijob = 1: a contribution from this subsystem to a</pre>

	Frobenius norm-based estimate of the separation between two matrix pairs is computed (look ahead strategy is used);
	If <i>ijob</i> = 2: a contribution from this subsystem to a Frobenius norm-based estimate of the separation between two matrix pairs is computed (?gecon on sub-systems is used). Not referenced if <i>trans</i> = 'T'.
m	<b>INTEGER.</b> On entry, $m$ specifies the order of $A$ and $D$ , and the row dimension of $C$ , $F$ , $R$ and $L$ .
n	<b>INTEGER.</b> On entry, <i>n</i> specifies the order of <i>B</i> and <i>E</i> , and the column dimension of <i>C</i> , <i>F</i> , <i>R</i> and <i>L</i> .
a, b	REAL for stgsy2 DOUBLE PRECISION for dtgsy2 COMPLEX for ctgsy2 COMPLEX*16 for ztgsy2. Arrays, DIMENSION ( <i>lda</i> , <i>m</i> ) and ( <i>ldb</i> , <i>n</i> ), respectively. On entry, <i>a</i> contains an upper (quasi) triangular matrix <i>A</i> and <i>b</i> contains an upper (quasi) triangular matrix <i>B</i> .
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $1 da \ge max(1, m)$ .
ldb	<b>INTEGER.</b> The leading dimension of the array <b>b.</b> $1db \ge max(1, n)$ .
c, f	REAL for stgsy2 DOUBLE PRECISION for dtgsy2 COMPLEX for ctgsy2 COMPLEX*16 for ztgsy2.
	Arrays, DIMENSION $(ldc, n)$ and $(ldf, n)$ , respectively. On entry, c contains the right-hand-side of the first matrix equation in (1) and f contains the right-hand-side of the second matrix equation in (1).

ldc	INTEGER. The leading dimension of the array $c$ . $ldc \ge max(1, m)$ .
d, e	REAL for stgsy2 DOUBLE PRECISION for dtgsy2 COMPLEX for ctgsy2 COMPLEX*16 for ztgsy2. Arrays, DIMENSION (1dd, m) and (1de, n), respectively. On entry, d contains an upper triangular matrix D and e contains an upper triangular matrix E.
ldd	INTEGER. The leading dimension of the array d. $1dd \ge \max(1, m)$ .
lde	<b>INTEGER.</b> The leading dimension of the array $e. \ lde \ge \max(1, n).$
ldf	INTEGER. The leading dimension of the array $f. \ ldf \ge \max(1, m)$ .
rdsum	REAL for stgsy2/ctgsy2 DOUBLE PRECISION for dtgsy2/ztgsy2. On entry, the sum of squares of computed contributions to the Dif-estimate under computation by ?tgsy1, where the scaling factor <i>rdscal</i> has been factored out.
rdscal	REAL for stgsy2/ctgsy2 DOUBLE PRECISION for dtgsy2/ztgsy2. On entry, scaling factor used to prevent overflow in <i>rdsum</i> .
iwork	<b>INTEGER</b> . Used with real flavors only. Workspace array, <b>DIMENSION</b> $(m+n+2)$ .
Output Parame	eters

С	On exit, if $i job = 0$ , <i>c</i> has been overwritten by the solution <i>R</i> .
f	On exit, if $i job = 0$ , $f$ has been overwritten by the solution $L$ .

scale	REAL for stgsy2/ctgsy2 DOUBLE PRECISION for dtgsy2/ztgsy2.
	On exit, $0 \leq scale \leq 1$ . If $0 < scale < 1$ , the solutions $R$ and $L$ ( $C$ and $F$ on entry) will hold the solutions to a slightly perturbed system, but the input matrices $A$ , $B$ , $D$ and $E$ have not been changed. If $scale = 0$ , $R$ and $L$ will hold the solutions to the homogeneous system with $C = F = 0$ . Normally $scale = 1$ .
rdsum	On exit, the corresponding sum of squares updated with the contributions from the current sub-system. If trans = 'T', rdsum is not touched. Note that rdsum only makes sense when ?tgsy2 is called by ?tgsy1.
rdscal	On exit, <i>rdscal</i> is updated with respect to the current contributions in <i>rdsum</i> . If <i>trans</i> = 'T', <i>rdscal</i> is not touched. Note that <i>rdscal</i> only makes sense when ?tgsy2 is called by ?tgsy1.
pđ	INTEGER. Used with real flavors only. On exit, the number of subsystems (of size 2-by-2, 4-by-4 and 8-by-8) solved by the routine stgsy2/dtgsy2.
info	<pre>INTEGER. On exit, if info is set to =0: Successful exit &lt;0: If info = -i, the i-th argument had an illegal value. &gt;0: The matrix pairs (A, D) and (B, E) have common or very close eigenvalues.</pre>

## ?trti2

Computes the inverse of a triangular matrix (unblocked algorithm).

call strti2 ( uplo, diag, n, a, lda, info )
call dtrti2 ( uplo, diag, n, a, lda, info )
call ctrti2 ( uplo, diag, n, a, lda, info )
call ztrti2 ( uplo, diag, n, a, lda, info )

### **Discussion**

The routine **?trti2** computes the inverse of a real/complex upper or lower triangular matrix.

This is the Level 2 BLAS version of the algorithm.

### **Input Parameters**

uplo	CHARACTER*1. Specifies whether the matrix <i>A</i> is upper or lower triangular. = ' <b>u</b> ': Upper triangular = ' <b>L</b> ': Lower triangular
diag	CHARACTER*1. Specifies whether or not the matrix <i>A</i> is unit triangular. = 'N': Non-unit triangular = 'U': Unit triangular
п	<b>INTEGER.</b> The order of the matrix A. $n \ge 0$ .
a	REAL for strti2 DOUBLE PRECISION for dtrti2 COMPLEX for ctrti2 COMPLEX*16 for ztrti2. Array, DIMENSION ( <i>lda</i> , <i>n</i> ). On entry, the triangular matrix <i>A</i> . If <i>uplo</i> = 'U', the leading <i>n</i> -by- <i>n</i> upper triangular part of the array <i>a</i>

	contains the upper triangular matrix, and the strictly	
	lower triangular part of $a$ is not referenced. If $uplo =$	
	'L', the leading <i>n</i> -by- <i>n</i> lower triangular part of the array a contains the lower triangular matrix, and the strictly upper triangular part of a is not referenced. If <i>diag</i> = 'U', the diagonal elements of a are also not referenced and are assumed to be 1.	
lda	<b>INTEGER.</b> The leading dimension of the array <b>a</b> . $1 da \ge max(1,n)$ .	
Output Parameters		
a	On exit, the (triangular) inverse of the original matrix, in the same storage format.	
info	<b>INTEGER.</b> = 0: successful exit	

< 0: if *info* = -*k*, the *k*-th argument had an illegal value

### xerbla

Error handling routine called by LAPACK routines.

```
call xerbla ( srname, info )
```

### **Discussion**

The routine xerbla is an error handler for the LAPACK routines. It is called by a LAPACK routine if an input parameter has an invalid value. A message is printed and execution stops.

Installers may consider modifying the stop statement in order to call system-specific exception-handling facilities.

### **Input Parameters**

srname	CHARACTER*6 The name of the routine which called xerbla.
info	<b>INTEGER</b> . The position of the invalid parameter in the parameter list of the calling routine.

# Vector Mathematical Functions



This chapter describes Vector Mathematical Functions Library (VML), which is designed to compute elementary functions on vector arguments. VML is an integral part of the Intel[®] MKL Kernel Library and the VML terminology is used here for simplicity in discussing this group of functions.

VML includes a set of highly optimized implementations of certain computationally expensive core mathematical functions (power, trigonometric, exponential, hyperbolic etc.) that operate on vectors.

Application programs that might significantly improve performance with VML include nonlinear programming software, integrals computation, and many others.

VML functions are divided into the following groups according to the operations they perform:

• <u>VML Mathematical Functions</u> compute values of elementary functions (such as sine, cosine, exponential, logarithm and so on) on vectors with unit increment indexing.

• <u>VML Pack/Unpack Functions</u> convert to and from vectors with positive increment indexing, vector indexing and mask indexing (see <u>Appendix A</u> for details on vector indexing methods).

• <u>VML Service Functions</u> allow the user to set /get the accuracy mode, and set/get the error code.

VML mathematical functions take an input vector as argument, compute values of the respective elementary function element-wise, and return the results in an output vector.

## **Data Types and Accuracy Modes**

Mathematical and pack/unpack vector functions in VML have been implemented for vector arguments of single and double precision real data. Both Fortran- and C-interfaces to all functions, including VML service functions, are provided in the library. The differences in naming and calling the functions for Fortran- and C-interfaces are detailed in the <u>Function</u> <u>Naming Conventions</u> section below.

Each vector function from VML (for each data format) can work in two modes: High Accuracy (HA) and Low Accuracy (LA). For many functions, using the LA version will improve performance at the cost of accuracy. For some cases, the advantage of relaxing the accuracy improves performance very little so the same function is employed for both versions. Error behavior depends not only on whether the HA or LA version is chosen, but also depends on the processor on which the software runs. In addition, special value behavior may differ between the HA and LA versions of the functions. Any information on accuracy behavior can be found in the *VML Release Notes*.

Switching between the two modes (HA and LA) is accomplished by using vmlSetMode(mode) (see Table 7-11). The function vmlGetMode() will return the currently used mode. The High Accuracy mode is used by default.

## **Function Naming Conventions**

Full names of all VML functions include only lowercase letters for Fortran-interface, whereas for C-interface names the lowercase letters are mixed with uppercase..



**NOTE.** This naming convention is followed in the function descriptions in the manual. Actual function names in the library may differ slightly (with respect to lower- and uppercase usage) and will be sufficient to meet the requirements of the supported compilers.

VML mathematical and pack/unpack function full names have the following structure:

v <name> <mod>

The initial letter v is a prefix indicating that a function belongs to VML. The  $\langle p \rangle$  field is a precision prefix that indicates the data type:

- **s REAL** for Fortran-interface, or **float** for C-interface
- d DOUBLE PRECISION for Fortran-interface, or double for C-interface.

The <name> field indicates the function short name, with some of its letters in uppercase for C-interface (see <u>Table 7-2</u>, <u>Table 7-9</u>).

The <mod> field (written in uppercase for C-interface) is present in pack/unpack functions only; it indicates the indexing method used:

- i indexing with positive increment
- v indexing with index vector
- m indexing with mask vector.

VML service function full names have the following structure:

vml <name>

where **vml** is a prefix indicating that a function belongs to VML, and **<name>** is the function short name, which includes some uppercase letters for C-interface (see <u>Table 7-10</u>).

To call VML functions from an application program, use conventional function calls. For example, the VML exponential function for single precision data can be called as

call vsexp ( n, a, y ) for Fortran–interface, or vsExp ( n, a, y ); for C–interface.

### **Functions Interface**

The interface to VML functions includes function full names and the arguments list.

The Fortran- and C-interface descriptions for different groups of VML functions are given below. Note that some functions (Div, Pow, and Atan2) have two input vectors a and b as their arguments, while SinCos function has two output vectors y and z.

### **VML Mathematical Functions:**

Fortran:

```
call v<name>( n, a, y )
call v<name>( n, a, b, y )
call v<name>( n, a, y, z )
C:
v<name>( n, a, y );
v<name>( n, a, b, y );
v<name>( n, a, y, z );
```

### **Pack Functions:**

Fortran:

```
call vpacki( n, a, inca, y )
call vpackv( n, a, ia, y )
call vpackm( n, a, ma, y )
C:
vPackI( n, a, inca, y );
vPackV( n, a, ia, y );
vPackM( n, a, ma, y );
```

### **Unpack Functions:**

#### Fortran:

C:

call vunpacki( n, a, y, incy )
call vunpackv( n, a, y, iy )
call vunpackm( n, a, y, my )

```
vUnpackI( n, a, y, incy );
vUnpackV( n, a, y, iy );
vUnpackM( n, a, y, my );
```

### **Service Functions:**

```
oldmode = vmlsetmode( mode )
mode = vmlgetmode( )
olderr = vmlseterrstatus ( err )
err = vmlgeterrstatus( )
olderr = vmlclearerrstatus( )
```

```
oldcallback = vmlseterrorcallback( callback )
callback = vmlgeterrorcallback()
oldcallback = vmlclearerrorcallback()

C:
    oldmode = vmlSetMode( mode );
    mode = vmlGetMode( void);
    olderr = vmlSetErrStatus ( err );
    err = vmlGetErrStatus(void);
    olderr = vmlClearErrStatus(void);
    oldcallback = vmlSetErrorCallBack(callback );
    callback = vmlClearErrorCallBack( void );
    oldcallback = vmlClearErrorCallBack(void );
```

### **Input Parameters:**

n	number of elements to be calculated
а	first input vector
b	second input vector
inca	vector increment for the input vector a
ia	index vector for the input vector a
ma	mask vector for the input vector a
incy	vector increment for the output vector $\mathbf{y}$
iy	index vector for the output vector $\mathbf{y}$
my	mask vector for the output vector $\mathbf{y}$
err	error code
mode	VML mode
callback	address of the callback function

### **Output Parameters:**

Y	first output vector
Z	second output vector
err	error code
mode	VML mode
olderr	former error code

oldmodeformer VML modeoldcallbackaddress of the former callback function

The data types of the parameters used in each function are specified in the respective function description section. All VML mathematical functions can perform in-place operations, which means that the same vector can be used as both input and output parameter. This holds true for functions with two input vectors as well, in which case one of them may be overwritten with the output vector. For functions with two output vectors, one of them may coincide with the input vector.

### **Vector Indexing Methods**

Current VML mathematical functions work only with unit increment. Arrays with other increments, or more complicated indexing, can be accommodated by gathering the elements into a contiguous vector and then scattering them after the computation is complete.

Three following indexing methods are used to gather/scatter the vector elements in VML:

- positive increment
- index vector
- mask vector.

The indexing method used in a particular function is indicated by the indexing modifier (see the description of the <mod> field in <u>Function Naming Conventions</u>). For more information on indexing methods see <u>Vector Arguments in VML</u> in Appendix A.

## **Error Diagnostics**

The VML library has its own error handler. The only difference for C- and Fortran- interfaces is that the Intel MKL error reporting routine XERBLA can be called after the Fortran- interface VML function encounters an error, and this routine gets information on VML_STATUS_BADSIZE and VML_STATUS_BADMEM input errors (see Table 7-13).

The VML error handler has the following properties:

- 1) The Error Status (vmlErrStatus) global variable is set after each VML function call. The possible values of this variable are shown in the <u>Table 7-13</u>.
- 2) Depending on the VML mode, the error handler function invokes:
  - errno variable setting. The possible values are shown in the Table 7-1
  - writing error text information to the stderr stream
  - raising the appropriate exception on error, if necessary
  - calling the additional error handler callback function.

#### Table 7-1Set Values of the errno Variable

Value of errno	Description
0	No errors are detected.
EINVAL	The array dimension is not positive.
EACCES	NULL pointer is passed.
EDOM	At least one of array values is out of a range of definition.
ERANGE	At least one of array values caused a singularity, overflow or underflow.

## **VML Mathematical Functions**

This section describes VML functions which compute values of elementary mathematical functions on real vector arguments with unit increment. Each function group is introduced by its short name, a brief description of its purpose, and the calling sequence for each type of data both for Fortranand C-interfaces, as well as a description of the input/output arguments.

For all VML mathematical functions, the input range of parameters is equal to the mathematical range of definition in the set of defined values for the respective data type. Several VML functions, specifically Div, Exp, Sinh, Cosh, and Pow, can result in an overflow. For these functions, the respective input threshold values that mark off the precision overflow are specified in the function description section. Note that in these specifications, FLT_MAX denotes the maximum number representable in single precision data type, while DBL_MAX denotes the maximum number representable in double precision data type.

<u>Table 7-2</u> lists available mathematical functions and data types associated with them.

### Table 7-2 VML Mathematical Functions

Function Short Name	Data Types	Description
Power and Roo	t Functions	
Inv	s, d	Inversion of the vector elements
Div	s, d	Divide elements of one vector by elements of second vector
<u>Sqrt</u>	s, d	Square root of vector elements
<u>InvSqrt</u>	s, d	Inverse square root of vector elements
<u>Cbrt</u>	s, d	Cube root of vector elements
<u>InvCbrt</u>	s, d	Inverse cube root of vector elements
Pow	s, d	Each vector element raised to the specified power
Powx	s, d	Each vector element raised to the constant power

Function Short Name	Data Types	Description		
Exponential and	Exponential and Logarithmic Functions			
<u>Exp</u>	s, d	Exponential of vector elements		
<u>Ln</u>	s, d	Natural logarithm of vector elements		
<u>Log10</u>	s, d	Denary logarithm of vector elements		
Trigonometric F	unctions			
Cos	s, d	Cosine of vector elements		
<u>Sin</u>	s, d	Sine of vector elements		
<u>SinCos</u>	s, d	Sine and cosine of vector elements		
<u>Tan</u>	s, d	Tangent of vector elements		
Acos	s, d	Inverse cosine of vector elements		
<u>Asin</u>	s, d	Inverse sine of vector elements		
Atan	s, d	Inverse tangent of vector elements		
Atan2	s, d	Four-quadrant inverse tangent of elements of two vectors		
Hyperbolic Functions				
<u>Cosh</u>	s, d	Hyperbolic cosine of vector elements		
<u>Sinh</u>	s, d	Hyperbolic sine of vector elements		
<u>Tanh</u>	s, d	Hyperbolic tangent of vector elements		
Acosh	s, d	Inverse hyperbolic cosine (nonnegative) of vector elements		
<u>Asinh</u>	s, d	Inverse hyperbolic sine of vector elements		
<u>Atanh</u>	s, d	Inverse hyperbolic tangent of vector elements		
Special Functio	ns			
Erf	s, d	Error function value of vector elements		
<u>Erfc</u>	s, d	Complementary error function value of vector elements		

### Table 6-2 VML Mathematical Functions (continued)

### Inv

Performs element by element inversion of the vector.

### Fortran:

```
call vsinv( n, a, y )
call vdinv( n, a, y )
C:
vsInv( n, a, y );
vdInv( n, a, y );
```

### **Input Parameters**

### Fortran:

п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vsinv DOUBLE PRECISION, INTENT(IN) for vdinv Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
a	const float*for vsInvconst double*for vdInvPointer to an array that contains the input vector a.

### **Output Parameters**

У	REAL	for vsinv	
	DOUBLE	PRECISION	for vdinv
	Array, sp	pecifies the out	tput vector <mark>y</mark> .

y float* for vsInv double* for vdInv Pointer to an array that contains the output vector y.

## Div

Performs element by element division of vector **a** by vector **b**.

C:

#### Fortran:

call vsdiv( n, a, b, y )
call vddiv( n, a, b, y )
C:
vsDiv( n, a, b, y );
vdDiv( n, a, b, y );

### **Input Parameters**

n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a, b	REAL, INTENT(IN) for vsdiv DOUBLE PRECISION, INTENT(IN) for vddiv Arrays, specify the input vectors a and b.
C:	
п	int. Specifies the number of elements to be calculated.
a, b	<pre>const float* for vsDiv const double* for vdDiv Pointers to arrays that contain the input vectors a and b.</pre>

### Table 7-3 Precision Overflow Thresholds for Div Function

Data Type	Threshold Limitations on Input Parameters		
single precision	<pre>abs(a[i]) &lt; abs(b[i]) * FLT_MAX</pre>		
double precision	<pre>abs(a[i]) &lt; abs(b[i]) * DBL_MAX</pre>		

### **Output Parameters**

Fortran:	
У	REAL for vsdiv DOUBLE PRECISION for vddiv Array, specifies the output vector y.
C:	
У	float* for vsDiv double* for vdDiv Pointer to an array that contains the output vector y.

## Sqrt

Computes a square root of vector elements.

```
call vssqrt( n, a, y )
call vdsqrt( n, a, y )
C:
vsSqrt( n, a, y );
vdSqrt( n, a, y );
```

### **Input Parameters**

### Fortran:

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lculated.
ora.

### **Output Parameters**

Fortran:

У	REAL for vssqrt DOUBLE PRECISION for vdsqrt Array, specifies the output vector y.
C:	
У	<pre>float* for vsSqrt double* for vdSqrt Pointer to an array that contains the output vector y.</pre>

## InvSqrt

Computes an inverse square root of vector elements.

### Fortran:

call vsinvsqrt( n, a, y )
call vdinvsqrt( n, a, y )

### **C**:

vsInvSqrt( n, a, y ); vdInvSqrt( n, a, y );

### **Input Parameters**

### Fortran:

n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vsinvsqrt DOUBLE PRECISION, INTENT(IN) for vdinvsqrt Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
a	<pre>const float* for vsInvSqrt const double* for vdInvSqrt Pointer to an array that contains the input vector a.</pre>

### **Output Parameters**

У	REAL for vsinvsqrt DOUBLE PRECISION for vdinvsqrt Array, specifies the output vector y.
C:	
У	<pre>float* for vsInvSqrt double* for vdInvSqrt Pointer to an array that contains the output vector y.</pre>

## Cbrt

Computes a cube root of vector elements.

### Fortran:

```
call vscbrt( n, a, y )
call vdcbrt( n, a, y )
C:
vsCbrt( n, a, y );
vdCbrt( n, a, y );
```

### **Input Parameters**

Fortran:

п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vscbrt DOUBLE PRECISION, INTENT(IN) for vdcbrt Array, specifies the input vector a.
C:	
п	int. Specifies the number of elements to be calculated.
a	const float*for vsCbrtconst double*for vdCbrtPointer to an array that contains the input vector a.

### **Output Parameters**

Y	REAL for vscbrt
	DOUBLE PRECISION for vdcbrt
	Array, specifies the output vector y.
C:	
У	float* for vsCbrt
	double* for vdCbrt
	Pointer to an array that contains the output vector <b>y</b> .

## InvCbrt

Computes an inverse cube root of vector elements.

### Fortran:

```
call vsinvcbrt( n, a, y )
call vdinvcbrt( n, a, y )
C:
vsInvCbrt( n, a, y );
vdInvCbrt( n, a, y );
```

### **Input Parameters**

### Fortran:

n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vsinvcbrt DOUBLE PRECISION, INTENT(IN) for vdinvcbrt Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
а	const float* for vsInvCbrt
	const double* for vdInvCbrt
	Pointer to an array that contains the input vector a.

### **Output Parameters**

У	REAL for vsinvcbrt DOUBLE PRECISION for vdinvcbrt Array, specifies the output vector y.
C:	
У	float* for vsInvCbrt double* for vdInvCbrt Pointer to an array that contains the output vector y.

### Pow

Computes a to the power b for elements of two vectors.

#### Fortran:

call vspow( n, a, b, y )
call vdpow( n, a, b, y )
C:
vsPow( n, a, b, y );
vdPow( n, a, b, y );

### **Input Parameters**

Fortran:

п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
	_
a, b	REAL, INTENT(IN) for vspow
	DOUBLE PRECISION, INTENT(IN) for vdpow
	Arrays, specify the input vectors a and b.
C:	
n	int. Specifies the number of elements to be calculated.
a, b	const float* for vsPow
	const double* for vdPow
	Pointers to arrays that contain the input vectors a and b.

### Table 7-4 Precision Overflow Thresholds for Pow Function

Data Type	Threshold Limitations on Input Parameters
single precision	abs(a[i]) < ( FLT_MAX ) ^{1/b[i]}
double precision	abs(a[i]) < ( <u>DBL_MAX</u> ) ^{1/b[i]}

### **Output Parameters**

Fortran:	
У	REAL for vspow DOUBLE PRECISION for vdpow Array, specifies the output vector y.
C:	
У	float* for vsPow double* for vdPow Pointer to an array that contains the output vector y.

### **Discussion**

The function Pow has certain limitations on the input range of a and b parameters. Specifically, if a[i] is positive, then b[i] may be arbitrary. For negative or zero a[i], the value of b[i] must be integer (either positive or negative).

### **Powx**

*Raises each element of a vector to the constant power.* 

### Fortran:

```
call vspowx( n, a, b, y )
call vdpowx( n, a, b, y )
C:
vsPowx( n, a, b, y );
vdPowx( n, a, b, y );
```

### **Input Parameters**

n	INTEGER,	INTENT(IN	). Specifies the number of elements
	to be calcul	lated.	
a, b	REAL, IN	TENT(IN)	for vspowx

DOUBLE PRECISION, INTENT(IN) for vdpowx Array a specifies the input vector; scalar value b is the constant power.

C.	
n	int. Specifies the number of elements to be calculated.
а	const float* for vsPowx
	const double* for vdPowx
	Pointer to an array that contains the input vector a.
b	const float for vsPowx
	const double for vdPowx
	Constant value for power b.

### Table 7-5 Precision Overflow Thresholds for Powx Function

Data Type	Threshold Limitations on Input Parameters
single precision	$abs(a[i]) < (FLT_MAX)^{1/b}$
double precision	$abs(a[i]) < (DBL_MAX)$ ^{1/b}

### **Output Parameters**

Fortran:

 $\mathbf{C}$ 

У	REAL for vspowx
	DOUBLE PRECISION for vdpowx
	Array, specifies the output vector y.
C:	
Y	float* for vsPowx
	double* for vdPowx
	Pointer to an array that contains the output vector <b>y</b> .

### **Discussion**

The function Powx has certain limitations on the input range of a and b parameters. Specifically, if a[i] is positive, then b may be arbitrary. For negative or zero a[i], the value of b must be integer (either positive or negative).

## Exp

*Computes an exponential of vector elements.* 

### Fortran:

```
call vsexp( n, a, y )
call vdexp( n, a, y )
C:
vsExp( n, a, y );
vdExp( n, a, y );
```

### **Input Parameters**

n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vsexp DOUBLE PRECISION, INTENT(IN) for vdexp Array, specifies the input vector a.
C:	
п	int. Specifies the number of elements to be calculated.
a	const float*for vsExpconst double*for vdExpPointer to an array that contains the input vector a.

### Table 7-6 Precision Overflow Thresholds for Exp Function

Data Type	Threshold Limitations on Input Parameters
single precision	a[i] < Ln( FLT_MAX )
double precision	<pre>a[i] &lt; Ln( DBL_MAX )</pre>

### **Output Parameters**

Fortran:

У	REAL for vsexp
	DOUBLE PRECISION for vdexp
	Array, specifies the output vector y.
C:	
У	float* for vsExp
	double* for vdExp
	Pointer to an array that contains the output vector <b>y</b> .

### Ln

Computes natural logarithm of vector elements.

#### Fortran:

```
call vsln( n, a, y )
call vdln( n, a, y )
C:
vsLn( n, a, y );
vdLn( n, a, y );
```

### **Input Parameters**

Fortran:

n

**INTEGER**, **INTENT(IN)**. Specifies the number of elements to be calculated.

а	REAL, INTENT(IN) for vsln	
	DOUBLE PRECISION, INTENT(IN) for vdln	
	Array, specifies the input vector a.	
C:		
п	int. Specifies the number of elements to be calculated.	
a	const float* for vsLn	
	const double* for vdLn	
	Pointer to an array that contains the input vector a.	
Output Parameters		
Fortran:		
i ortran.		
Y	REAL for vsln	
	DOUDLE DREGISION for adding	

### DOUBLE PRECISION for vdln Array, specifies the output vector y. C: float* for vsLn double* for vdLn Pointer to an array that contains the output vector $\mathbf{y}$ .

## Log10

Computes denary logarithm of vector elements.

 $\boldsymbol{Y}$ 

### Fortran:

```
call vslog10( n, a, y )
call vdlog10( n, a, y )
C:
vsLog10( n, a, y );
vdLog10( n, a, y );
```

### **Input Parameters**

n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vslog10 DOUBLE PRECISION, INTENT(IN) for vdlog10 Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
a	const float*for vsLog10const double*for vdLog10Pointer to an array that contains the input vector a.

# **Output Parameters**

Fortran:

У	REAL for vslog10 DOUBLE PRECISION for vdlog10 Array, specifies the output vector y.
C:	
У	<pre>float* for vsLog10 double* for vdLog10 Pointer to an array that contains the output vector y.</pre>

# Cos

Computes cosine of vector elements.

```
call vscos( n, a, y )
call vdcos( n, a, y )
C:
vsCos( n, a, y );
vdCos( n, a, y );
```

# **Input Parameters**

### Fortran:

п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vscos DOUBLE PRECISION, INTENT(IN) for vdcos Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
a	const float* for vsCos const double* for vdCos
	Pointer to an array that contains the input vector a.

# **Output Parameters**

### Fortran:

У	REAL for vscos
	DOUBLE PRECISION for vdcos
	Array, specifies the output vector y.
C:	
У	float* for vsCos
	double* for vdCos
	Pointer to an array that contains the output vector y.

# Sin

Computes sine of vector elements.

```
Fortran:
call vssin( n, a, y )
call vdsin( n, a, y )
C:
vsSin( n, a, y );
vdSin( n, a, y );
```

# **Input Parameters**

# Fortran:

п	<b>INTEGER</b> , <b>INTENT(IN)</b> . Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vssin DOUBLE PRECISION, INTENT(IN) for vdsin Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
a	const float* for vsSin const double* for vdSin
	Pointer to an array that contains the input vector a.

# **Output Parameters**

Fortran:

У	REAL for vssin
	DOUBLE PRECISION for vdsin
	Array, specifies the output vector y.
C:	
У	float* for vsSin
	double* for vdSin
	Pointer to an array that contains the output vector y.

# SinCos

Computes sine and cosine of vector elements.

# Fortran:

call vssincos( n, a, y, z )
call vdsincos( n, a, y, z )

# **C**:

vsSinCos( n, a, y, z ); vdSinCos( n, a, y, z );

# **Input Parameters**

# Fortran:

n	INTEGER, INTENT(IN). Specifies the number of elements
	to be calculated.
а	REAL, INTENT(IN) for vssincos
	DOUBLE PRECISION, INTENT(IN) for vdsincos
	Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
a	const float* for vsSinCos
	const double* for vdSinCos
	Pointer to an array that contains the input vector a.

# **Output Parameters**

y, z	<b>REAL</b> for vssincos DOUBLE PRECISION for vdsincos Arrays, specify the output vectors $y$ (for sine values) and $z$ (for cosine values).
C:	
y, z	float* for vsSinCos double* for vdSinCos Pointers to arrays that contain the output vectors $y$ (for sine values) and $z$ (for cosine values).

# Tan

Computes tangent of vector elements.

# Fortran:

```
call vstan( n, a, y )
call vdtan( n, a, y )
C:
vsTan( n, a, y );
vdTan( n, a, y );
```

# **Input Parameters**

# Fortran:

п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vstan DOUBLE PRECISION, INTENT(IN) for vdtan Array, specifies the input vector a.
C:	
п	int. Specifies the number of elements to be calculated.
a	const float*for vsTanconst double*for vdTanPointer to an array that contains the input vector a.

# **Output Parameters**

У	REAL for vstan DOUBLE PRECISION for vdtan Array, specifies the output vector y.
C:	
У	<pre>float* for vsTan double* for vdTan Pointer to an array that contains the output vector y.</pre>

# Acos

Computes inverse cosine of vector elements.

### Fortran:

```
call vsacos( n, a, y )
call vdacos( n, a, y )
C:
vsAcos( n, a, y );
vdAcos( n, a, y );
```

# **Input Parameters**

# Fortran:

п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vsacos DOUBLE PRECISION, INTENT(IN) for vdacos Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
a	const float* for vsAcos const double* for vdAcos Pointer to an array that contains the input vector a.

# **Output Parameters**

У	REAL for vsacos DOUBLE PRECISION for vdacos Array, specifies the output vector y.
C:	
У	float* for vsAcos double* for vdAcos Pointer to an array that contains the output vector y.

# Asin

Computes inverse sine of vector elements.

### Fortran:

```
call vsasin( n, a, y )
call vdasin( n, a, y )
C:
vsAsin( n, a, y );
vdAsin( n, a, y );
```

# **Input Parameters**

Fortran:

п	<b>INTEGER</b> , <b>INTENT(IN)</b> . Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vsasin DOUBLE PRECISION, INTENT(IN) for vdasin Array, specifies the input vector a.
C:	
п	int. Specifies the number of elements to be calculated.
a	const float* for vsAsin
	const double* for vdAsin
	Pointer to an array that contains the input vector a.

# **Output Parameters**

Fortran:

```
yREALfor vsasinDOUBLEPRECISIONfor vdasinArray, specifies the output vector y.
```

C:

float* for vsAsin
double* for vdAsin
Pointer to an array that contains the output vector y.

# Atan

*Computes inverse tangent of vector elements.* 

 $\boldsymbol{Y}$ 

# Fortran:

```
call vsatan( n, a, y )
call vdatan( n, a, y )
C:
vsAtan( n, a, y );
vdAtan( n, a, y );
```

# **Input Parameters**

### Fortran:

n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vsatan DOUBLE PRECISION, INTENT(IN) for vdatan Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
a	<pre>const float* for vsAtan const double* for vdAtan Pointer to an array that contains the input vector a.</pre>

# **Output Parameters**

У	REAL for vsatan
	DOUBLE PRECISION for vdatan
	Array, specifies the output vector y.
C:	
У	float* for vsAtan
	double* for vdAtan
	Pointer to an array that contains the output vector <b>y</b> .

# Atan2

Computes four-quadrant inverse tangent of elements of two vectors.

# Fortran:

call vsatan2( n, a, b, y )
call vdatan2( n, a, b, y )
C:
vsAtan2( n, a, b, y );
vdAtan2( n, a, b, y );

# **Input Parameters**

n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a, b	REAL, INTENT(IN) for vsatan2 DOUBLE PRECISION, INTENT(IN) for vdatan2 Arrays, specify the input vectors a and b.
C:	
n	int. Specifies the number of elements to be calculated.
a, b	<pre>const float* for vsAtan2 const double* for vdAtan2 Pointers to arrays that contain the input vectors a and b.</pre>

# **Output Parameters**

Fortran:	
У	REAL for vsatan2 DOUBLE PRECISION for vdatan2 Array, specifies the output vector y.
C:	
У	float* for vsAtan2 double* for vdAtan2 Pointer to an array that contains the output vector y.

The elements of the output vector  $\mathbf{y}$  are computed as the four-quadrant arctangent of  $\mathbf{a}[\mathbf{i}] / \mathbf{b}[\mathbf{i}]$ .

# Cosh

Computes hyperbolic cosine of vector elements.

### Fortran:

call vscosh( n, a, y )
call vdcosh( n, a, y )
C:
vsCosh( n, a, y );
vdCosh( n, a, y );

# **Input Parameters**

### Fortran:



**INTEGER**, **INTENT**(**IN**). Specifies the number of elements to be calculated.

a	REAL, INTENT(IN) for vscosh DOUBLE PRECISION, INTENT(IN) for vdcosh Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
a	const float* for vsCosh const double* for vdCosh
	Pointer to an array that contains the input vector a.

# Table 7-7 Precision Overflow Thresholds for Cosh Function

Data Type	Threshold Limitations on Input Parameters
single precision	-Ln(FLT_MAX)-Ln2 < a[i] < Ln(FLT_MAX)+Ln2
double precision	-Ln(DBL_MAX)-Ln2 < a[i] < Ln(DBL_MAX)+Ln2

# **Output Parameters**

У	REAL for vscosh
	DOUBLE PRECISION for vdcosh
	Array, specifies the output vector y.
C:	
У	float* for vsCosh
	double* for vdCosh
	Pointer to an array that contains the output vector y.

# Sinh

Computes hyperbolic sine of vector elements.

# Fortran:

```
call vssinh( n, a, y )
call vdsinh( n, a, y )
C:
vsSinh( n, a, y );
vdSinh( n, a, y );
```

# **Input Parameters**

п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vssinh DOUBLE PRECISION, INTENT(IN) for vdsinh Array, specifies the input vector a.
C:	
п	int. Specifies the number of elements to be calculated.
a	<pre>const float* for vsSinh const double* for vdSinh Pointer to an array that contains the input vector a.</pre>

# Table 7-8 Precision Overflow Thresholds for sinh Function

Data Type	Threshold Limitations on Input Parameters
single precision	-Ln(FLT_MAX)-Ln2 < a[i] < Ln(FLT_MAX)+Ln2
double precision	-Ln(DBL_MAX)-Ln2 < a[i] < Ln(DBL_MAX)+Ln2

# **Output Parameters**

Fortran:

У	REAL for vssinh DOUBLE PRECISION for vdsinh Array, specifies the output vector y.
C:	
У	<pre>float* for vsSinh double* for vdSinh Pointer to an array that contains the output vector y.</pre>

# Tanh

*Computes hyperbolic tangent of vector elements.* 

### Fortran:

```
call vstanh( n, a, y )
call vdtanh( n, a, y )
C:
vsTanh( n, a, y );
vdTanh( n, a, y );
```

# **Input Parameters**

Fortran:

*n* **INTEGER**, **INTENT**(**IN**). Specifies the number of elements to be calculated.

а	REAL, INTENT(IN) for vstanh
	DOUBLE PRECISION, INTENT(IN) for vdtanh
	Array, specifies the input vector a.
C:	
п	int. Specifies the number of elements to be calculated.
а	const float* for vsTanh
	const double* for vdTanh
	Pointer to an array that contains the input vector a.
Output Par	ameters
Fortran:	
У	REAL for vstanh
	DOUBLE PRECISION for vdtanh
	Array, specifies the output vector y.
C:	

float* for vsTanh
double* for vdTanh
Pointer to an array that contains the output vector y.

# Acosh

Computes inverse hyperbolic cosine (nonnegative) of vector elements.

 $\boldsymbol{Y}$ 

### Fortran:

```
call vsacosh( n, a, y )
call vdacosh( n, a, y )
C:
vsAcosh( n, a, y );
vdAcosh( n, a, y );
```

# **Input Parameters**

n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vsacosh DOUBLE PRECISION, INTENT(IN) for vdacosh Array, specifies the input vector a.
C:	
п	int. Specifies the number of elements to be calculated.
a	const float*for vsAcoshconst double*for vdAcoshPointer to an array that contains the input vector a.

# **Output Parameters**

Fortran:

У	REAL for vsacosh DOUBLE PRECISION for vdacosh Array, specifies the output vector y.
C:	
У	float* for vsAcosh double* for vdAcosh Pointer to an array that contains the output vector y.

# Asinh

Computes inverse hyperbolic sine of vector elements.

```
call vsasinh( n, a, y )
call vdasinh( n, a, y )
C:
vsAsinh( n, a, y );
vdAsinh( n, a, y );
```

# **Input Parameters**

### Fortran:

п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vsasinh DOUBLE PRECISION, INTENT(IN) for vdasinh Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
а	const float* for vsAsinh
	const double* for vdAsinh
	Pointer to an array that contains the input vector a.

# **Output Parameters**

### Fortran:

У	REAL for vsasinh
	DOUBLE PRECISION for vdasinh
	Array, specifies the output vector y.
C:	
У	float* for vsAsinh
	double* for vdAsinh
	Pointer to an array that contains the output vector y.

# Atanh

Computes inverse hyperbolic tangent of vector elements.

# Fortran:

call vsatanh( n, a, y )
call vdatanh( n, a, y )

# **C:** vsAtanh( *n*, *a*, *y* ); vdAtanh( *n*, *a*, *y* );

# **Input Parameters**

Fortran:

<ul> <li>REAL, INTENT(IN) for vsatanh DOUBLE PRECISION, INTENT(IN) for vdatanh Array, specifies the input vector a.</li> <li>int. Specifies the number of elements to be calculated.</li> <li>const float* for vsAtanh const double* for vdAtanh Pointer to an array that contains the input vector a.</li> </ul>	п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
<pre>n int. Specifies the number of elements to be calculated. a const float* for vsAtanh const double* for vdAtanh</pre>	a	DOUBLE PRECISION, INTENT(IN) for vdatanh
a const float* for vsAtanh const double* for vdAtanh	C:	
const double* for vdAtanh	п	int. Specifies the number of elements to be calculated.
	a	const double* for vdAtanh

# **Output Parameters**

# Fortran:

У	REAL for vsatanh DOUBLE PRECISION for vdatanh Array, specifies the output vector y.
C:	
У	float* for vsAtanh double* for vdAtanh Pointer to an array that contains the output vector y.

# Erf

Computes the error function value of vector elements.

# Fortran:

call vserf( n, a, y )
call vderf( n, a, y )

# **C**:

vsErf( n, a, y ); vdErf( n, a, y );

# **Input Parameters**

Fortran:

п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vserf DOUBLE PRECISION, INTENT(IN) for vderf Array, specifies the input vector a.
C:	
n	int. Specifies the number of elements to be calculated.
a	<pre>const float* for vsErf const double* for vdErf Pointer to an array that contains the input vector a.</pre>

# **Output Parameters**

# Fortran:

У	REAL for vserf
	DOUBLE PRECISION for vderf
	Array, specifies the output vector y.
C:	
У	float* for vsErf
	double* for vdErf
	Pointer to an array that contains the output vector y.

# **Discussion**

The function **Erf** computes the error function values for elements of the input vector *a* and writes them to the output vector *y*. The error function is defined as given by:

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^{2}} dt$$

# Erfc

Computes the complementary error function value of vector elements.

# Fortran:

```
call vserfc( n, a, y )
call vderfc( n, a, y )
C:
vsErfc( n, a, y );
vdErfc( n, a, y );
```

# **Input Parameters**

Fortran:

п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	REAL, INTENT(IN) for vserfc DOUBLE PRECISION, INTENT(IN) for vderfc Array, specifies the input vector a.
C:	
п	int. Specifies the number of elements to be calculated.
a	const float* for vsErfc
	const double* for vdErfc
	Pointer to an array that contains the input vector a.

# **Output Parameters**

Fortran:

```
yREALfor vserfcDOUBLEPRECISIONfor vderfcArray, specifies the output vector y.
```

C:

float* for vsErfc double* for vdErfc Pointer to an array that contains the output vector y.

# Discussion

 $\boldsymbol{Y}$ 

The function Erfc computes the complementary error function values for elements of the input vector  $\mathbf{a}$  and writes them to the output vector  $\mathbf{y}$ .

The complementary error function is defined as given by:

 $\operatorname{erfc}(x) = 1 - \operatorname{erf}(x)$ 

or, in other words,

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} e^{-t^{2}} dt$$

# **VML Pack/Unpack Functions**

This section describes VML functions which convert vectors with unit increment to and from vectors with positive increment indexing, vector indexing and mask indexing (see <u>Appendix A</u> for details on vector indexing methods).

<u>Table 7-9</u> lists available VML Pack/Unpack functions, together with data types and indexing methods associated with them.

Function Short Name	Data Types	Indexing Methods	Description
Pack	s, d	I,V,M	Gathers elements of arrays, indexed by different methods.
<u>Unpack</u>	s, d	I,V,M	Scatters vector elements to arrays with different indexing.

# Table 7-9 VML Pack/Unpack Functions

# Pack

Copies elements of an array with specified indexing to a vector with unit increment.

call	vspacki(	n,	a,	inca,	У	)
call	vspackv(	n,	a,	ia, j	Y	)
call	vspackm(	n,	a,	ma,	Y	)
call	vdpacki(	n,	a,	inca,	$\boldsymbol{Y}$	)
call	vdpackv(	n,	a,	ia,	$\boldsymbol{Y}$	)
call	vdpackm(	n,	a,	ma,	$\boldsymbol{Y}$	)

```
C:
vsPackI( n, a, inca, y );
vsPackV( n, a, ia, y );
vsPackM( n, a, ma, y );
vdPackI( n, a, inca, y );
vdPackV( n, a, ia, y );
```

# **Input Parameters**

п	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
а	<pre>REAL, INTENT(IN) for vspacki, vspackv, vspackm DOUBLE PRECISION, INTENT(IN) for vdpacki, vdpackv, vdpackm Array, DIMENSION at least (1 + (n-1)*inca) for vspacki, at least max( n,max(ia[j]) ), j=0,,n-1, for vspackv, at least n for vspackm, Specifies the input vector a.</pre>
inca	INTEGER, INTENT(IN) for vspacki, vdpacki. Specifies the increment for the elements of <i>a</i> .
ia	INTEGER, INTENT(IN) for vspackv, vdpackv. Array, DIMENSION at least $n$ Specifies the index vector for the elements of $a$ .
ma	INTEGER, INTENT(IN) for vspackm, vdpackm. Array, DIMENSION at least $n$ Specifies the mask vector for the elements of $a$ .
C:	
п	int. Specifies the number of elements to be calculated
a	const float* for vsPackI, vsPackV, vsPackM const double* for vdPackI, vdPackV, vdPackM Specifies the pointer to an array that contains the input vector a. Size of the array must be:

	<pre>at least (1 + (n-1)*inca) for vsPackI, at least max( n,max(ia[j]) ),j=0,,n-1, for vsPackV, at least n for vsPackM.</pre>
inca	int for vsPackI, vdPackI. Specifies the increment for the elements of <i>a</i> .
ia	<b>const int*</b> for <b>vsPackV</b> , <b>vdPackV</b> . Specifies the pointer to an array of size at least <i>n</i> that contains the index vector for the elements of <i>a</i> .
ma	<b>const int*</b> for <b>vsPackM</b> , <b>vdPackM</b> . Specifies the pointer to an array of size at least <i>n</i> that contains the mask vector for the elements of <b>a</b> .

# **Output Parameters**

## Fortran:

У	REAL for vspacki, vspackv, vspackm DOUBLE PRECISION for vdpacki, vdpackv, vdpackm Array, DIMENSION at least <i>n</i> , specifies the output vector <i>y</i> .
C:	
У	<pre>float* for vsPackI, vsPackV, vsPackM double* for vdPackI, vdPackV, vdPackM Specifies the pointer to an array of size at least n that contains the output vector y.</pre>

# Unpack

Copies elements of a vector with unit increment to an array with specified indexing.

```
call vsunpacki( n, a, y, incy )
call vsunpackv( n, a, y, iy )
call vsunpackm( n, a, y, my )
```

```
call vdunpacki( n, a, y, incy )
call vdunpackv( n, a, y, iy )
call vdunpackm( n, a, y, my )
C:
vsUnpackI( n, a, y, incy );
vsUnpackV( n, a, y, iy );
vsUnpackI( n, a, y, incy );
vdUnpackI( n, a, y, iy );
vdUnpackV( n, a, y, iy );
```

# **Input Parameters**

n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the number of elements to be calculated.
a	<pre>REAL, INTENT(IN) for vsunpacki, vsunpackv, vsunpackm DOUBLE PRECISION, INTENT(IN) for vdunpacki, vdunpackv, vdunpackm. Array, DIMENSION at least n, specifies the input vector a.</pre>
incy	INTEGER, INTENT(IN) for vsunpacki, vdunpacki. Specifies the increment for the elements of $y$ .
iy	INTEGER, INTENT(IN) for vsunpackv, vdunpackv. Array, DIMENSION at least $n$ , specifies the index vector for the elements of $y$ .
my	INTEGER, INTENT(IN) for vsunpackm, vdunpackm. Array, DIMENSION at least $n$ , specifies the mask vector for the elements of $y$ .
C:	
n	int. Specifies the number of elements to be calculated.
a	<pre>const float* for vsUnpackI, vsUnpackV, vsUnpackM const double* for vdUnpackI, vdUnpackV, vdUnpackM Specifies the pointer to an array of size at least n that contains the input vector a.</pre>

incy	int for vsUnpackI, vdUnpackI. Specifies the increment for the elements of y.
iy	const int* for vsUnpackV, vdUnpackV. Specifies the pointer to an array of size at least $n$ that contains the index vector for the elements of $a$ .
my	const int* for vsUnpackM, vdUnpackM. Specifies the pointer to an array of size at least $n$ that contains the mask vector for the elements of $a$ .

# **Output Parameters**

### Fortran:

 $\boldsymbol{Y}$ 

REAL for vsunpacki, vsunpackv, vsunpackm
DOUBLE PRECISION for vdunpacki, vdunpackv,
vdunpackm.
Array, DIMENSION
at least $(1 + (n-1)*incy)$ for vsunpacki,
at least max( n, max(iy[j]) ), j=0,, n-1, for vsunpackv,
at least <i>n</i> for vsunpackm
Specifies the output vector y.

# C: *Y*

float* for vsUnpackI, vsUnpackV, vsUnpackM
double* for vdUnpackI, vdUnpackV, vdUnpackM
Specifies the pointer to an array that contains the output vector y.
Size of the array must be:
 at least (1 + (n-1)*incy) for vsUnPackI,
 at least max( n,max(ia[j]) ), j=0,...,n-1, for vsUnPackV,

at least *n* for vsUnPackM.

# **VML Service Functions**

This section describes VML functions which allow the user to set /get the accuracy mode, and set/get the error code. All these functions are available both in Fortran- and C- interfaces.

<u>Table 7-10</u> lists available VML Service functions and their short description.

# Table 7-10VML Service Functions

Function Short Name	Description
SetMode	Sets the VML mode
<u>GetMode</u>	Gets the VML mode
<u>SetErrStatus</u>	Sets the VML error status
<u>GetErrStatus</u>	Gets the VML error status
<u>ClearErrStatus</u>	Clears the VML error status
SetErrorCallBack	Sets the additional error handler callback function
GetErrorCallBack	Gets the additional error handler callback function
ClearErrorCallBack	Deletes the additional error handler callback function

# **SetMode**

Sets the new mode for VML functions according to mode parameter and stores the previous VML mode to oldmode.

# Fortran: oldmode = vmlsetmode( mode ) C: oldmode = vmlSetMode( mode );

# **Input Parameters**

Fortran:	
mode	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the VML mode to be set.
C:	
mode	int. Specifies the VML mode to be set.

# **Output Parameters**

Fortran:	
oldmode	<b>INTEGER</b> . Specifies the former VML mode.
C:	
oldmode	int. Specifies the former VML mode.

# **Discussion**

The *mode* parameter is designed to control accuracy, FPU and error handling options. <u>Table 7-11</u> lists values of the *mode* parameter. All other possible values of the *mode* parameter may be obtained from these values by using bitwise OR (|) operation to combine one value for accuracy, one for FPU, and one for error control options. The default value of the *mode* parameter is VML_HA | VML_ERRMODE_DEFAULT. Thus, the current FPU control word (FPU precision and the rounding method) is used by default.

If any VML mathematical function requires different FPU precision, or rounding method, it changes these options automatically and then restores the former values. The *mode* parameter enables you to minimize switching the internal FPU mode inside each VML mathematical function that works with similar precision and accuracy settings. To accomplish this, set the *mode* parameter to VML_FLOAT_CONSISTENT for single precision functions, or to VML_DOUBLE_CONSISTENT for double precision functions. These values of the *mode* parameter are the optimal choice for the respective function groups, as they are required for most of the VML mathematical functions. After the execution is over, set the *mode* to VML_RESTORE if you need to restore the previous FPU mode.

# Table 7-11Values of the mode Parameter

Value of mode	Description		
Accuracy Control			
VML_HA	High accuracy versions of VML functions will be used		
VML_LA	Low accuracy versions of VML functions will be used		
Additional FPU Mode Control			
VML_FLOAT_CONSISTENT	The optimal FPU mode (control word) for single precision functions is set, and the previous FPU mode is saved		
VML_DOUBLE_CONSISTENT	The optimal FPU mode (control word) for double precision functions is set, and the previous FPU mode is saved		
VML_RESTORE	The previously saved FPU mode is restored		
Error Mode Control			
VML_ERRMODE_IGNORE	No action is set for computation errors		
VML_ERRMODE_ERRNO	On error, the errno variable is set		
VML_ERRMODE_STDERR	On error, the error text information is written to stderr		
VML_ERRMODE_EXCEPT	On error, an exception is raised		
VML_ERRMODE_CALLBACK	On error, an additional error handler function is called		
VML_ERRMODE_DEFAULT	On error, the errno variable is set, an exception is raised, and an additional error handler function is called		

# **Examples**

Several examples of calling the function **vmlSetMode()** with different values of the *mode* parameter are given below:

C: vmlSetMode( VML_LA ); vmlSetMode( VML_LA | VML_FLOAT_CONSISTENT | VML_ERRMODE_IGNORE ); vmlSetMode( VML_RESTORE);

# **GetMode**

Gets the VML mode.

### Fortran:

```
mod = vmlgetmode()
C:
mod = vmlGetMode( void );
```

# **Output Parameters**

Fortran:

mod	<b>INTEGER.</b> Specifies the packed <i>mode</i> parameter.
C:	
mod	int. Specifies the packed mode parameter.

# **Discussion**

The function vmlGetMode() returns the VML mode parameter which controls accuracy, FPU and error handling options. The mod variable value is some combination of the values listed in the <u>Table 7-11</u>. You can obtain some of these values using the respective mask from the <u>Table 7-12</u>, for example:

```
mod = vmlgetmode()
accm = IAND(mod, VML_ACCURACY_MASK)
fpum = IAND(mod, VML_FPUMODE_MASK)
errm = IAND(mod, VML_ERRMODE_MASK)
C:
```

accm = vmlGetMode(void )& VML_ACCURACY_MASK; fpum = vmlGetMode(void )& VML_FPUMODE _MASK; errm = vmlGetMode(void )& VML_ERRMODE _MASK;

### Table 7-12 Values of Mask for the mode Parameter

Value of mask	Description
VML_ACCURACY_MASK	Specifies mask for accuracy mode selection.
VML_FPUMODE_MASK	Specifies mask for FPU mode selection.
VML_ERRMODE_MASK	Specifies mask for error <i>mode</i> selection.

# **SetErrStatus**

Sets the new VML error status according to err and stores the previous VML error status to olderr.

### Fortran:

olderr = vmlseterrstatus( err )
C:
olderr = vmlSetErrStatus( err );

# **Input Parameters**

Fortran:

err	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Specifies the VML error status to be set.
C:	
err	int. Specifies the VML error status to be set.

# **Output Parameters**

olderrINTEGER. Specifies the former VML error status.C:olderrint. Specifies the former VML error status.Table 7-13 lists possible values of the err parameter.

# Table 7-13 Values of the VML Error Status

Error Status	Description
VML_STATUS_OK	The execution was completed successfully.
VML_STATUS_BADSIZE	The array dimension is not positive.
VML_STATUS_BADMEM	NULL pointer is passed.
VML_STATUS_ERRDOM	At least one of array values is out of a range of definition.
VML_STATUS_SING	At least one of array values caused a singularity.
VML_STATUS_OVERFLOW	An overflow has happened during the calculation process.
VML_STATUS_UNDERFLOW	An underflow has happened during the calculation process.

# **Examples:**

```
vmlSetErrStatus( VML_STATUS_OK );
vmlSetErrStatus( VML_STATUS_ERRDOM );
vmlSetErrStatus( VML_STATUS_UNDERFLOW );
```

# **GetErrStatus**

Gets the VML error status.

# Fortran: err = vmlgeterrstatus() C: err = vmlGetErrStatus( void ); Output Parameters Fortran: err INTEGER. Specifies the VML error status. C: err int. Specifies the VML error status.

# **ClearErrStatus**

Sets the VML error status to VML_STATUS_OK and stores the previous VML error status to olderr.

# Fortran:

```
olderr = vmlclearerrstatus( )
C:
olderr = vmlClearErrStatus( void );
```

# **Output Parameters**

Fortran:

*olderr* **INTEGER**. Specifies the former VML error status.

C: olderr int. Specifies the former VML error status.

# **SetErrorCallBack**

Sets the additional error handler callback function and gets the old callback function.

# Fortran:

```
oldcallback = vmlseterrorcallback( callback )
C:
oldcallback = vmlSetErrorCallBack( callback );
```

# **Input Parameters**

```
Address of the callback function.
callback
            The callback function has the following format:
            INTEGER FUNCTION ERRFUNC(par)
             TYPE (ERROR_STRUCTURE) par
             1 ....
             ! user error processing
             1 ...
             ERRFUNC = 0
             ! if ERRFUNC = 0 - standard VML error
            handler
             ! is called after the callback
             ! if ERRFUNC != 0 - standard VML error
            handler
             ! is not called
            END
            The passed error structure is defined as follows:
```

C:

```
TYPE ERROR_STRUCTURE
                 SEQUENCE
                 INTEGER*4 ICODE
                 INTEGER*4 IINDEX
                 REAL*8 DBA1
                 REAL*8 DBA2
                 REAL*8 DBR1
                 REAL*8 DBR2
                 CHARACTER(64) CFUNCNAME
                 INTEGER*4 IFUNCNAMELEN
            END TYPE ERROR STRUCTURE
callback
            Pointer to the callback function.
           The callback function has the following format:
           static int __stdcall
           MyHandler(DefVmlErrorContext*
           pContext)
            {
                /* Handler body */
           };
           The passed error structure is defined as follows:
           typedef struct _DefVmlErrorContext
            {
                                  /* Error status value */
               int iCode;
                int iIndex;
                                 /* Index for bad array
                                   element, or bad array
                                   dimension, or bad
                                   array pointer */
                double dbA1;
                                  * Error argument 1 */
                double dbA2;
                                  /* Error argument 2 */
                double dbR1;
                                  /* Error result 1 */
                double dbR2;
                                  /* Error result 2 */
                char cFuncName[64]; /* Function name */
                int iFuncNameLen; /* Length of function
                name*/
            } DefVmlErrorContext;
```

# **Output Parameters**

Fortran:	
oldcallback	Address of the former callback function.
C:	
oldcallback	Pointer to the former callback function.

# **Discussion**

The callback function is called on each VML mathematical function error if VML_ERRMODE_CALLBACK error mode is set (see <u>Table 7-11</u>).

Use the **vmlSetErrorCallBack()** function if you need to define your own callback function instead of default empty callback function.

The input structure for a callback function contains the following information

about the encountered error:

- the input value which caused an error
- location (array index) of this value
- the computed result value
- error code
- name of the function in which the error occurred.

You can insert your own error processing into the callback function. This may include correcting the passed result values in order to pass them back and resume computation. The standard error handler is called after the callback function only if it returns 0.

# GetErrorCallBack

*Gets the additional error handler callback function.* 

# Fortran:

fun = vmlgeterrorcallback( )

<b>C:</b> fun = vi	nlGetErrorCallBack( void );
Output Parameters	
Fortran:	
fun	Address of the callback function.
C:	
fun	Pointer to the callback function.

# ClearErrorCallBack

Deletes the additional error handler callback function and retrieves the former callback function.

### Fortran:

oldcallback = vmlclearerrorcallback( )
C:
oldcallback = vmlClearErrorCallBack( void );

# **Output Parameters**

Fortran:	
oldcallback	<b>INTEGER</b> . Address of the former callback function.
C:	
oldcallback	int. Pointer to the former callback function.

# Vector Generators of Statistical Distributions



This chapter describes the part of Intel[®] MKL which is known as Vector Statistical Library (VSL) and is designed for the purpose of generating vectors of pseudorandom numbers.

VSL provides a set of pseudorandom number generator subroutines implementing basic continuous and discrete distributions. To speed up performance, all these subroutines were developed using the calls to the highly optimized *Basic Random Number Generators* (BRNGs) and the library of vector mathematical functions (VML, see <u>chapter 7</u>).

All VSL subroutines can be classified into three major categories:

- Pseudorandom number generators for different types of statistical distributions, for example, uniform, normal (Gaussian), binomial, etc. Detailed description of the generators can be found in <u>Pseudorandom Generators</u> section.
- Basic subroutines to handle random number streams: create, initialize, delete, copy, get the index of a basic generator. The description of these subroutines can be found in <u>Service Subroutines</u> section.
- Registration subroutines for basic pseudorandom generators and subroutines that obtain properties of the registered generators (see <u>Advanced Service Subroutines</u> section).

The last two categories will be referred to as service subroutines.

### Conventions

In this discussion, a Random Number Generator (RNG) means a number-theoretic deterministic algorithm that generates number sequences, which can be interpreted as random samplings from a universal set with a given probability distribution function. Since random numbers are generated by a deterministic algorithm, they cannot be truly random and should be referred to as pseudorandom. The respective generators should be also called pseudorandom. However, in this chapter no specific differentiation is made between random and pseudorandom numbers, as well as between random and pseudorandom generators unless the context requires otherwise. Likewise, the terms *random number* and *variate*, *statistical distribution* and *probability distribution*, are not distinguished here either.

The choice of a number-theoretic algorithm A and initial conditions I identifies a unique sequence of random numbers, which is called a random stream. The pair  $\langle A, I \rangle$  is referred to as the random stream state. In VSL a stream is identified by a *stream descriptor* represented as TYPE (VSL_STREAM_STATE) structure in FORTRAN interface, and VSLStreamStatePtr pointer in C interface.

All generators of nonuniform distributions, both discrete and continuous, are built on the basis of the uniform distribution generators, called Basic Random Number Generators (BRNGs). The pseudorandom numbers with nonuniform distribution are obtained through an appropriate transformation of the uniformly distributed pseudorandom numbers. The most common transformation techniques include the inverse Cumulative Distribution Function (CDF), acceptance/rejection method, and mixtures. For certain types of distribution, several generation methods are implemented.

VSL subroutines for pseudorandom number generation accept the stream descriptor and the distribution parameters as input and write the result in a vector of pseudorandom numbers with a given distribution. For a given statistical distribution, several generation methods can be used, which may differ in efficiency for particular ranges of input parameters. Consequently, the most efficient generators often use different methods for different ranges. To establish the generation method to be used in the subroutine, you

should specify the input parameter called the method number. Description of methods available for each generator can be found in Pseudorandom Generators section.

In the discussion that follow, the terms *multiprocessor system*, computational node, and processor refer to any configuration of the system with shared or distributed memory, or combination of the two. Specifically, a computational node, or a processor, refers to a computational unit capable of performing independent parallel computations (this may be either a physical processor, a cluster node, or a logical parallel process).

### **Mathematical Notation**

The following notation is used throughout the text:

Ν	The set of natural numbers $N = \{1, 2, 3\}$ .
Ζ	The set of integers $Z = \{ \dots -3, -2, -1, 0, 1, 2, 3 \dots \}$ .
R	The set of real numbers.
a	The floor of <b>a</b> (the largest integer less than or equal to <b>a</b> ).
$\oplus$ or <b>xor</b>	Bitwise exclusive OR.
$C^k_{\alpha}$ or $\begin{pmatrix} \alpha \\ k \end{pmatrix}$	Binomial coefficient or combination ( $\alpha \in R$ , $\alpha \ge 0$ ; $k \in N \cup \{0\}$ ). $C_{\alpha}^{0} = 1$ . For $\alpha \ge k$ binomial coefficient is defined as
	$C_{\alpha}^{k} = \frac{\alpha(\alpha-1) \dots (\alpha-k+1)}{1}$ . If $\alpha < k$ , then $C_{\alpha}^{k} = 0$ .

$$C_{\alpha}^{k} = \frac{\alpha(\alpha - 1) \dots (\alpha - k + 1)}{k!} \text{ If } \alpha < k \text{, then } C_{\alpha}^{k} = 0.$$

 $\Phi(x)$ 

Cumulative Gaussian distribution function

$$\Phi(x) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} exp\left(-\frac{y^2}{2}\right) dy \text{ , defined over } -\infty < x < +\infty.$$

 $\Phi(-\infty) = 0$ ,  $\Phi(+\infty) = 1$ .

Linear Congruential Generator  $x_{n+1} = (ax_n + c) \mod m$ , where LCG(a, c, m)a is called the *multiplier*, c is called the *increment* and m is called the modulus of the generator.

MCG(a,m)	Multiplicative Congruential Generator $x_{n+1} = (ax_n) \mod m$ is a special case of Linear Congruential Generator, where the increment <i>c</i> is taken to be 0.
GFSR(p,q)	Generalized Feedback Shift Register Generator $x_n = x_{n-p} \oplus x_{n-q}$ .

### **Naming Conventions**

The names of all VSL functions in FORTRAN are lowercase; names in C may contain both lowercase and uppercase letters.



**NOTE.** This naming convention is followed in the function descriptions in the manual. Actual function names in the library may differ slightly (with respect to lower- and uppercase usage) and will be sufficient to meet the requirements of the supported compilers.

The names of generator subroutines have the following structure:

v <type of<="" th=""><th>result&gt;rng<distribution></distribution></th><th>for FORTRAN-interface</th></type>	result>rng <distribution></distribution>	for FORTRAN-interface
v <type of<="" td=""><td>result&gt;Rng<distribution></distribution></td><td>for C-interface</td></type>	result>Rng <distribution></distribution>	for C-interface

where v is the prefix of a VSL vector function, and the field *<type of result>* is either s, d, or i and specifies one of the following types:

S	<b>REAL</b> for FORTRAN-interface <b>float</b> for C-interface
d	DOUBLE PRECISION for FORTRAN-interface double for C-interface
i	INTEGER for FORTRAN-interface int for C-interface

Prefixes s and d apply to continuous distributions only, prefix i applies only to discrete case. The prefix rng indicates that the subroutine is a pseudorandom generator, and the *<distribution>* field specifies the type of statistical distribution. Names of service subroutines follow the template below:

vsl<name>,

where vsl is the prefix of a VSL service function. The field <*name*> contains a short function name. For a more detailed description of service subroutines refer to <u>Service Subroutines</u> and <u>Advanced Service Subroutines</u> sections.

Prototype of each generator subroutine implementing a given type of random number distribution fits the following structure:

```
<function name>( method, stream, n, r, [<distribution parameters>] ),
```

where

- *method* is the number specifying the method of generation. A detailed description of this parameter can be found in <u>Pseudorandom</u> <u>Generators</u> section.
- *stream* defines the random stream descriptor and must have a nonzero value. Random streams and their usage are discussed further in <u>Random Streams</u> and <u>Service Subroutines</u>.
- *n* defines the number of pseudorandom values to be generated. If *n* is less than or equal to zero, no values are generated. Furthermore, if *n* is negative, an error condition is set.
- *r* defines the destination array for the generated numbers. The dimension of the array must be large enough to store at least *n* pseudorandom numbers.

Additional parameters included into *<distribution parameters>* field are individual for each generator subroutine and are described in detail in <u>Pseudorandom Generators</u> section.

To invoke a pseudorandom generator, use a call to the respective VSL subroutine. For example, to obtain a vector **r**, composed of **n** independent and identically distributed pseudorandom numbers with normal (Gaussian) distribution, that have the mean value **a** and standard deviation *sigma*, write the following:

for FORTRAN-interface

```
call vsrnggaussian( method, stream, n, r, a, sigma )
for C-interface
vsRngGaussian( method, stream, n, r, a, sigma )
```

## **Basic Pseudorandom Generators**

Basic Random Number Generators (BRNGs) are the major and widely spread tool to obtain uniformly distributed pseudorandom numbers.

VSL provides a number of basic generators that differ in speed and quality: the 32-bit multiplicative congruential generator  $MCG(1132489760, 2^{31} - 1)$  [L'Ecuyer99], the 32-bit generalized feedback shift register generator GFSR(250,103) [Kirkpatrick81], and the combined multiple recursive generator MRG-32k3a [L'Ecuyer99a], as well as the 59-bit multiplicative congruential generator  $MCG(13^{13}, 2^{59})$  and Wichmann-Hill generator (in fact, this is a set of 273 basic generators) from NAG Numerical Libraries [NAG]. Essentially, applicability of a basic generator to a given computational task is very difficult to estimate. To ensure more reliable results, basic generators are usually tested in a series of statistical tests prior to actual computation. Comparative performance analysis of the generators and testing results can be found in <u>VSLNotes</u>.

Users may want to design and use their own basic generators. VSL provides means of registration of such user-designed generators through the steps described in <u>Advanced Service Subroutines</u> section.

For some basic generators, VSL provides two methods of creating independent random streams in multiprocessor computations, which are the leapfrog method and the block-splitting method. The properties of the generators designed for parallel computations are discussed in detail in [Coddington94].

For a more detailed description of the generator properties and testing results refer to <u>VSLNotes</u>.

### **Random Streams**

Several random streams may be used in one application for a number of reasons.

First, it may be necessary to supply random data to different computational nodes of a multiprocessor system. In this case, the following options are available:

• use an individual basic generator for each computational node, so that each random stream is filled from a different basic generator;

- use one basic generator for all computational nodes and generate several independent random streams using the leapfrog method or the block-splitting method;
- use combination of the two approaches, when one basic generator is used to generate independent streams for all nodes and each of the nodes in turn uses its own generator.

Another reason is related to the fact that many Monte Carlo simulations require additional randomization. A simple illustration is the necessity to assign random streams to different elements of the model or to run variance reduction methods [Bratley87].

In either case, the correlation between different random streams can affect reliability of the final result.

### **Data Types**

**Stream State.** Random numbers can be generated by portions using the notion of a *stream state*, which is a structure created after a call to the stream creating subroutine. A stream state descriptor is used to access the structure:

#### FORTRAN

```
TYPE VSL_STREAM_STATE

INTEGER*4 descriptor1

INTEGER*4 descriptor2

END TYPE VSL_STREAM_STATE

C

typedef (void*) VSLStreamStatePtr;
```

See <u>Advanced Service Subroutines</u> for the format of the stream state structure for user-designed generators.

### **Service Subroutines**

Stream handling comprises subroutines for creating, deleting, or copying the streams and getting the index of a basic generator.

Table 8-1	Service Subroutines	
	Subroutine	Short Description
	NewStream	Creates and initializes a random stream.
	NewStreamEx	Creates and initializes a random stream for the generators with multiple initial conditions.
	DeleteStream	Deletes previously created stream.
	CopyStream	Copies a stream to another stream.
	CopyStreamState	Creates a copy of a random stream state.
	LeapfrogStream	Initializes the stream of <i>k</i> -th computational node in a <i>nstreams</i> -node cluster by the leapfrog method.
	SkipAheadStream	Initializes the stream by the block-splitting method.
	<u>GetStreamStateBrng</u>	Obtains the index of the basic generator responsible for the generation of a given random stream.
	GetNumRegBrng	Obtains the number of currently registered basic generators.

Table 8-1 lists all available service subroutines



**NOTE.** In the above table, the vsl prefix in the function names is omitted. In the function reference this prefix is always used in function prototypes and code examples.

Most of the generator-based work comprises three basic steps:

- Creating and initializing a stream (NewStream, NewStreamEx, CopyStream, CopyStreamState, LeapfrogStream, SkipAheadStream).
- 2. Generating pseudorandom numbers with given distribution, see <u>Pseudorandom Generators</u>.
- 3. Deleting the stream (DeleteStream).

Note that you can concurrently create multiple streams and obtain pseudorandom data from one or several generators by using the stream state. You must use the DeleteStream function to delete all the streams afterwards.

### **NewStream**

Creates and initializes a random stream.

#### Fortran:

call vslnewstream( stream, brng, seed )

#### **C**:

vslNewStream( stream, brng, seed )

#### **Discussion**

For a basic generator with number *brng*, this function creates a new stream and initializes it with a 32-bit seed. The function is also applicable for generators with multiple initial conditions. See <u>VSLNotes</u> for a more detailed description of stream initialization for different basic generators.

#### **Input Parameters**

brng	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Index of the basic generator to initialize the stream.
seed	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Initial condition of the stream.
C:	
brng	int. Index of the basic generator to initialize the stream.
seed	unsigned int. Initial condition of the stream.

Output Parameters FORTRAN:	
stream	TYPE(VSL_STREAM_STATE), INTENT(OUT). Stream state descriptor.
C:	
stream	VSLStreamStatePtr*. Pointer to the stream state structure.

# **NewStreamEx**

*Creates and initializes a random stream for generators with multiple initial conditions.* 

#### Fortran:

call vslnewstreamex( stream, brng, n, params )

#### **C**:

vslNewStreamEx( stream, brng, n, params )

#### **Discussion**

This function provides an advanced tool to set the initial conditions for a basic generator if its input arguments imply several initialization parameters. This subroutine should not be used unless it is specially necessary. Whenever possible, use vslNewStream, which is analogous to vslNewStreamEx except that it takes only one 32-bit initial condition. In particular, vslNewStreamEx may be used to initialize the seed tables in Generalized Feedback Shift Register Generators (GFSRs). A more detailed description of this issue can be found in <u>VSLNotes</u>.

### **Input Parameters**

TORTRAIN.	
brng	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Index of the basic generator to initialize the stream.
n	<b>INTEGER</b> , <b>INTENT</b> (IN). Number of initial conditions contained in <i>params</i> .
params	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Array of initial conditions necessary for the basic generator <i>brng</i> to initialize the stream.
C:	
brng	int. Index of the basic generator to initialize the stream.
n	int. Number of initial conditions contained in <i>params</i> .
params	<pre>const unsigned int[]. Array of initial conditions necessary for the basic generator brng to initialize the stream.</pre>
Output Parameters	
FORTRAN:	
stream	TYPE(VSL_STREAM_STATE), INTENT(OUT). Stream state descriptor.
C:	
stream	VSLStreamStatePtr*. Pointer to the stream state structure.

### **DeleteStream**

Deletes a random stream.

#### Fortran:

call vsldeletestream( stream )

**C**:

vslDeleteStream( stream )

#### **Discussion**

This function deletes the random stream created by one of the initialization functions.

#### **Input/Output Parameters**

FORTRAN:

stream	TYPE (VSL_STREAM_STATE), INTENT(INOUT). Descriptor of the stream to be deleted; must have non-zero value.
C:	
stream	VSLStreamStatePtr*. Pointer to the stream state structure; must have non-zero value. After the stream is successfully deleted, the <i>stream</i> pointer is set to NULL.

# CopyStream

Creates a copy of a random stream.

#### Fortran:

call vslcopystream( newstream, srcstream )

#### **C**:

vslCopyStream( newstream, srcstream )

### **Discussion**

The function creates an exact copy of *srcstream* and stores its descriptor to *newstream*.

Input Parameters FORTRAN:	
scrstream	TYPE(VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream to be copied.
C:	
srcstream	VSLStreamStatePtr. Pointer to the stream state structure to be copied.
Output Parameters FORTRAN:	
newstream	TYPE(VSL_STREAM_STATE), INTENT(OUT). Descriptor of the stream copy.
C:	
newstream	VSLStreamStatePtr*. Pointer to the copy of the stream state structure.

# CopyStreamState

*Creates a copy of a random stream state.* 

#### Fortran:

call vslcopystreamstate( deststream, srcstream )

#### **C**:

vslCopyStreamState( deststream, srcstream )

#### **Discussion**

The function copies a stream state from *srcstream* to the existing *deststream* stream. Both streams should be generated by the same basic generator. En error message is generated when the index of the BRNG that produced *deststream* stream differs from the index of the BRNG that generated *srcstream* stream.

Unlike <u>CopyStream</u> function, which creates a new stream and copies both the stream state and other data from *srcstream*, the function CopyStreamState copies only *srcstream* stream state data to the generated *deststream* stream.

#### **Input Parameters**

FORTRAN:	
scrstream	TYPE(VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream with the state to be copied.
C:	
srcstream	VSLStreamStatePtr. Pointer to the stream state structure from which the stream state is copied.
Output Parameters	
FORTRAN:	
deststream	TYPE(VSL_STREAM_STATE), INTENT(IN). Descriptor of the destination

stream is copied.

stream where the state of *scrstream* 

C:

deststream

VSLStreamStatePtr. Pointer to the stream state structure where the stream state is copied.

# LeapfrogStream

Initializes stream of k-th computational node in nstreams-node cluster using the leapfrog method.

#### Fortran:

call vslleapfrogstream( stream, k, nstreams )

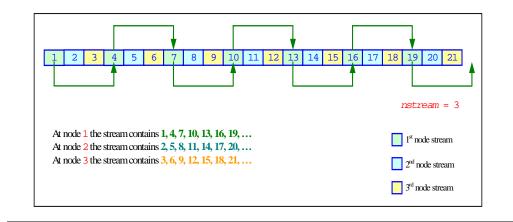
#### **C**:

vslLeapfrogtream( stream, k, nstreams )

#### **Discussion**

The function uses the leapfrog method (see <u>Figure 8-1</u>) to generate an independent random stream for the computational node k,  $0 \le < nstreams$ , where *nstreams* is the largest number of computational nodes used.

#### Figure 8-1 Leapfrog Method



The following code examples illustrate the initialization of three independent streams using the leapfrog method:

#### Example 8-1 FORTRAN Code for Leapfrog Method

```
type(VSL STREAM STATE)stream1
type(VSL_STREAM_STATE)stream2
type(VSL_STREAM_STATE)stream3
! Creating 3 identical streams
call vslnewstream(stream1, VSL_BRNG_MCG31, 174)
call vslcopystream(stream2, stream1)
call vslcopystream(stream3, stream1)
! Leapfrogging the streams
call vslleapfrogstream(stream1, 0, 3)
call vslleapfrogstream(stream2, 1, 3)
call vslleapfrogstream(stream3, 2, 3)
! Generating random numbers
! Deleting the streams
call vsldeletestream(stream1)
call vsldeletestream(stream2)
call vsldeletestream(stream3)
....
```

#### Example 8-2 C Code for Leapfrog Method

```
VSLStreamStatePtr stream1;
VSLStreamStatePtr stream2;
VSLStreamStatePtr stream3;
/* Creating 3 identical streams */
vslNewStream(&stream1, VSL_BRNG_MCG31, 174);
vslCopyStream(&stream2, stream1);
vslCopyStream(&stream3, stream1);
/* Leapfrogging the streams */
vslLeapfrogStream(stream1, 0, 3);
vslLeapfrogStream(stream2, 1, 3);
vslLeapfrogStream(stream3, 2, 3);
/* Generating random numbers */
/* Deleting the streams */
vslDeleteStream(&stream1);
vslDeleteStream(&stream2);
vslDeleteStream(&stream3);
....
```

#### **Input Parameters**

stream	TYPE(VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream to which the leapfrog method is applied.
k	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Index of the computational node, or stream number.
nstreams	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Largest number of computational nodes, or number of independent streams.

C:	
stream	VSLStreamStatePtr. Pointer to the stream state structure to which the leapfrog method is applied.
k	<b>int</b> . Index of the computational node, or stream number.
nstreams	int. Largest number of computational nodes, or number of independent steams.

# SkipAheadStream

Initializes a stream using the block-splitting method.

#### Fortran:

call vslskipaheadstream( stream, nskip )

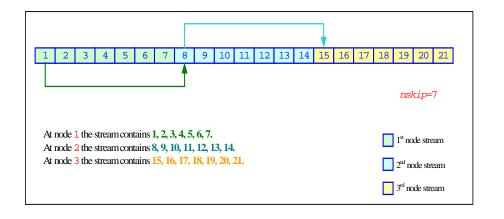
C:

vslSkipAheadStream( stream, nskip )

#### **Discussion**

This function initializes an independent random stream of a given computational node through the block-splitting method (see <u>Figure 8-2</u>). The maximum number of computational nodes is unlimited. The largest number of elements skipped in a given stream is *nskip*.

#### Figure 8-2 Block-Splitting Method



The following code examples illustrate how to initialize three independent streams using the SkipAheadStream function:

#### Example 8-3 FORTRAN Code for Block-Splitting Method

```
TYPE(VSL STREAM STATE)stream1
TYPE(VSL_STREAM_STATE)stream2
TYPE(VSL_STREAM_STATE)stream3
! Creating the 1st stream
call vslnewstream(stream1, VSL_BRNG_MCG31, 174)
! Skipping ahead by 7 elements the 2nd stream
call vslcopystream(stream2, stream1);
call vslskipaheadstream(stream2, 7);
! Skipping ahead by 7 elements the 3rd stream
call vslcopystream(stream3, stream2);
call vslskipaheadstream(stream3, 7);
! Generating random numbers
! Deleting the streams
call vsldeletestream(stream1)
call vsldeletestream(stream2)
call vsldeletestream(stream3)
```

#### Example 8-4 C Code for Block-Splitting Method

```
VSLStreamStatePtr stream1;
VSLStreamStatePtr stream2;
VSLStreamStatePtr stream3;
/* Creating the 1st stream */
vslNewStream(&stream1, VSL_BRNG_MCG31, 174);
/* Skipping ahead by 7 elements the 2nd stream */
vslCopyStream(&stream2, stream1);
vslSkipAheadStream(stream2, 7);
/* Skipping ahead by 7 elements the 3rd stream */
vslCopyStream(&stream3, stream2);
vslSkipAheadStream(stream3, 7);
/* Generating random numbers */
••••
/* Deleting the streams */
vslDeleteStream(&stream1);
vslDeleteStream(&stream2);
vslDeleteStream(&stream3);
....
```

#### **Input Parameters**

stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream to which the block-splitting method is applied.
nskip	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of skipped elements.
C:	
stream	VSLStreamStatePtr. Pointer to the stream state structure to which the block-splitting method is applied.
nskip	int. Number of skipped elements.

# GetStreamStateBrng

Returns index of a basic generator used for generation of a given random stream.

#### Fortran:

brng = vslgetstreamstatebrng( stream )

#### **C**:

brng = vslGetStreamStateBrng( stream )

#### **Discussion**

This function retrieves the index of a basic generator used for generation of a given random stream.

#### **Input Parameters**

stream	TYPE(VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state.
C:	
stream	VSLStreamStatePtr. Pointer to the stream state structure.
Output Parameters FORTRAN:	
brng	<b>INTEGER.</b> Index of the basic generator assigned for the generation of <i>stream</i> ; negative in case of an error.

C:

brng

int. Index of the basic generator assigned for the generation of *stream*; negative in case of an error.

# GetNumRegBrng

*Obtains the number of currently registered basic generators.* 

#### Fortran:

nregbrng = vslgetnumregbrngs( )

#### **C**:

nregbrng = vslGetNumRegBrngs( void )

#### **Discussion**

This function obtains the number of currently registered basic generators. Whenever the user registers a user-defined basic generator, the number of registered basic generators is incremented. The maximum number of basic generators that can be registered is determined by VSL_MAX_REG_BRNGS parameter.

#### **Output Parameters**

nregbrngs	<b>INTEGER</b> . The number of basic generators registered at the moment of the function call.
C:	
nregbrngs	int. The number of basic generators registered at the moment of the function call.

### **Pseudorandom Generators**

This section contains description of VSL subroutines for generating random numbers with different types of distribution. Each function group is introduced by the type of underlying distribution and contains a short description of its functionality, as well as specifications of the call sequence for both FORTRAN and C-interface and the explanation of input and output parameters.

<u>Table 8-2</u> and <u>Table 8-3</u> list the pseudorandom number generator subroutines, together with used data types and output distributions.

Table 0-2 Continuous Distribution Generators		
Type of Distribution	Data Types	Description
Uniform	s, d	Uniform continuous distribution on the interval ( <i>a,b</i> ).
Gaussian	s, d	Normal (Gaussian) distribution.
Exponentia	<u>l</u> s, d	Exponential distribution.
Laplace	s, d	Laplace distribution (double exponential distribution).
Weibull	s, d	Weibull distribution.
Cauchy	s, d	Cauchy distribution.
Rayleigh	s, d	Rayleigh distribution.
Lognormal	s, d	Lognormal distribution.
Gumbel	s, d	Gumbel (extreme value) distribution.

#### Table 8-2 Continuous Distribution Generators

#### Table 8-3 Discrete Distribution Generators

Type of Distribution	Data Types	Description
Uniform	i	Uniform discrete distribution on the interval [a,b).
UniformBits	i	Generator of integer random values with uniform bit distribution.
Bernoulli	i	Bernoulli distribution.
Geometric	i	Geometric distribution.
Binomial	i	Binomial distribution.
Hypergeometric	i	Hypergeometric distribution.

Table 0.2

Table 6-3 Discrete Distribution Generators (continued)		
Type of Distribution	Data Types	Description
Poisson	i	Poisson distribution.
NegBinomial	i	Negative binomial distribution, or Pascal distribution.

Distribution Constants (continued)

# Continuous Distributions

This section describes routines for generating pseudorandom numbers with continuous distribution.

# Uniform

Generates pseudorandom numbers with uniform distribution.

#### Fortran:

call vsrnguniform( method, stream, n, r, a, b )
call vdrnguniform( method, stream, n, r, a, b )

#### **C**:

```
vsRngUniform( method, stream, n, r, a, b )
vdRngUniform( method, stream, n, r, a, b )
```

#### **Discussion**

This function generates pseudorandom numbers uniformly distributed over the interval (a, b), where a, b are the left and right bounds of the interval, respectively, and  $a, b \in R$ ; a < b.

The probability density function is given by:

$$f_{a, b}(x) = \begin{cases} \frac{1}{b-a}, & x \in (a, b) \\ 0, & x \notin (a, b) \end{cases}, \quad -\infty < x < +\infty.$$

The cumulative distribution function is as follows:

$$F_{a, b}(x) = \begin{cases} 0, & x < a \\ \frac{x-a}{b-a}, & a \le x < b \\ 1, & x \ge b \end{cases}$$

### **Input Parameters**

method	<b>INTEGER</b> , <b>INTENT(IN)</b> . Generation method; dummy and set to 0 in case of uniform distribution.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
a	REAL, INTENT(IN) for vsrnguniform.
	DOUBLE PRECISION, INTENT(IN) for vdrnguniform.
	Left bound a.
b	REAL, INTENT(IN) for vsrnguniform.
b	REAL, INTENT(IN) <b>for</b> vsrnguniform. DOUBLE PRECISION, INTENT(IN) <b>for</b> vdrnguniform.
b	DOUBLE PRECISION, INTENT(IN) for
b C:	DOUBLE PRECISION, INTENT(IN) for vdrnguniform.
	DOUBLE PRECISION, INTENT(IN) for vdrnguniform.

п	int. Number of random values to be generated.
a	float for vsRngUniform.
	double for vdRngUniform.
	Left bound a.
b	float for vsRngUniform.
	double for vdRngUniform.
	Right bound b.
Output Parameters FORTRAN:	
r	REAL, INTENT(OUT) for vsrnguniform.
	DOUBLE PRECISION, INTENT(OUT) for vdrnguniform.
	Vector of $n$ pseudorandom numbers uniformly distributed over the interval $(a,b)$ .
C:	
r	float* for vsRngUniform.
	double* for vdRngUniform.
	Vector of $n$ pseudorandom numbers uniformly distributed over the interval $(a,b)$ .

# Gaussian

*Generates normally distributed pseudorandom numbers.* 

#### Fortran:

call vsrnggaussian( method, stream, n, r, a, sigma )

```
call vdrnggaussian( method, stream, n, r, a, sigma )
C:
```

```
vsRngGaussian( method, stream, n, r, a, sigma )
vdRngGaussian( method, stream, n, r, a, sigma )
```

#### **Discussion**

This function generates pseudorandom numbers with normal (Gaussian) distribution with mean value a and standard deviation  $\sigma$ , where

a,  $\sigma \in R$ ;  $\sigma > 0$ .

The probability density function is given by:

$$f_{a,\sigma}(x) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(x-a)^2}{2\sigma^2}\right), \quad -\infty < x < +\infty.$$

The cumulative distribution function is as follows:

$$F_{a,\sigma}(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(y-a)^2}{2\sigma^2}\right) dy , \quad -\infty < x < +\infty.$$

The cumulative distribution function  $F_{a,\sigma}(x)$  can be expressed in terms of standard normal distribution  $\Phi(x)$  as

$$F_{a, \sigma}(x) = \Phi((x-a)/\sigma).$$

### **Input Parameters**

method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.

a	REAL, INTENT(IN) for vsrnggaussian.
	DOUBLE PRECISION, INTENT(IN) for vdrnggaussian.
	Mean value a.
sigma	REAL, INTENT(IN) for vsrnggaussian.
	DOUBLE PRECISION, INTENT(IN) for vdrnggaussian.
	Standard deviation $\sigma$ .
C:	
method	int. Generation method.
stream	<b>VSLStreamStatePtr</b> . Pointer to the stream state structure.
n	int. Number of random values to be generated.
а	float for vsRngGaussian.
	double for vdRngGaussian.
	Mean value a.
sigma	float for vsRngGaussian.
	double for vdRngGaussian.
	Standard deviation $\sigma$ .
Output Parameters	
FORTRAN:	
r	REAL, INTENT(OUT) for vsrnggaussian.

REAL, INTENT(OUT) for vsrnggaussian DOUBLE PRECISION, INTENT(OUT) for vdrnggaussian.

Vector of *n* normally distributed pseudorandom numbers.

float* for vsRngGaussian. double* for vdRngGaussian. Vector of *n* normally distributed pseudorandom numbers.

# **Exponential**

*Generates exponentially distributed pseudorandom numbers.* 

C:

r

#### Fortran:

```
call vsrngexponential( method, stream, n, r, a, beta )
call vdrngexponential( method, stream, n, r, a, beta )
```

#### C:

vsRngExponential( method, stream, n, r, a, beta )
vdRngExponential( method, stream, n, r, a, beta )

#### **Discussion**

This function generates pseudorandom numbers with exponential distribution that has the displacement a and scalefactor  $\beta$ , where a,  $\beta \in R$ ;  $\beta > 0$ .

The probability density function is given by:

$$f_{a,\beta}(x) = \begin{cases} \frac{1}{\beta} \exp((-(x-a))/\beta), & x \ge a \\ 0, & x < a \end{cases}, -\infty < x < +\infty.$$

The cumulative distribution function is as follows:

$$F_{a, \beta}(x) = \begin{cases} 1 - \exp((-(x-a))/\beta), & x \ge a \\ 0, & x < a \end{cases}, -\infty < x < +\infty$$

### Input Parameters

method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
a	REAL, INTENT(IN) for vsrngexponential.
	DOUBLE PRECISION, INTENT(IN) for vdrngexponential.
	Displacement a.
beta	REAL, INTENT(IN) for vsrngexponential.
	DOUBLE PRECISION, INTENT(IN) for vdrngexponential.
	Scalefactor $\beta$ .
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
п	int. Number of random values to be generated.
а	float for vsRngExponential.
	double for vdRngExponential.
	Displacement a.

beta	float for vsRngExponential.
	double for vdRngExponential.
	Scalefactor $\beta$ .

#### **Output Parameters**

FORTRAN:

r	REAL, INTENT(OUT) for vsrngexponential.
	DOUBLE PRECISION, INTENT(OUT) for vdrngexponential.
	Vector of <b>n</b> exponentially distributed pseudorandom numbers.
C:	
r	<pre>float* for vsRngExponential.</pre>
	double* for vdRngExponential.
	Vector of <b>n</b> exponentially distributed pseudorandom numbers.

# Laplace

Generates pseudorandom numbers with Laplace distribution.

#### Fortran:

```
call vsrnglaplace( method, stream, n, r, a, beta )
call vdrnglaplace( method, stream, n, r, a, beta )
C:
vsRngLaplace( method, stream, n, r, a, beta )
vdRngLaplace( method, stream, n, r, a, beta )
```

### Discussion

This function generates pseudorandom numbers with Laplace distribution with mean value (or average) a and scalefactor  $\beta$  , where

**a**,  $\beta \in R$ ;  $\beta > 0$ . The scale factor value determines the standard deviation as

$$\sigma = \beta \sqrt{2}$$

The probability density function is given by:

$$f_{a,\beta}(x) = \frac{1}{\sqrt{2\beta}} \exp\left(-\frac{|x-a|}{\beta}\right), -\infty < x < +\infty.$$

The cumulative distribution function is as follows:

$$F_{a,\beta}(x) = \begin{cases} \frac{1}{2} \exp\left(-\frac{|x-a|}{\beta}\right), & x < a\\ 1 - \frac{1}{2} \exp\left(-\frac{|x-a|}{\beta}\right), & x \ge a \end{cases}, \quad -\infty < x < +\infty.$$

### **Input Parameters**

method	<b>INTEGER</b> , <b>INTENT</b> (IN). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
a	REAL, INTENT(IN) for vsrnglaplace.
	DOUBLE PRECISION, INTENT(IN) for vdrnglaplace.
	Mean value a.

beta	REAL, INTENT(IN) for vsrnglaplace.
	DOUBLE PRECISION, INTENT(IN) for vdrnglaplace.
	Scalefactor $\beta$ .
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state descriptor.
n	int. Number of random values to be generated.
a	float for vsRngLaplace.
	double for vdRngLaplace.
	Mean value a.
beta	float for vsRngLaplace.
	double for vdRngLaplace.
	Scalefactor $\beta$ .

### **Output Parameters**

r	REAL, INTENT(OUT) for vsrnglaplace.
	DOUBLE PRECISION, INTENT(OUT) for vdrnglaplace.
	Vector of <i>n</i> Laplace distributed pseudorandom numbers.
C:	
r	float* for vsRngLaplace.
	double* for vdRngLaplace.
	Vector of <i>n</i> Laplace distributed pseudorandom numbers.

### **Weibull**

*Generates Weibull distributed pseudorandom numbers.* 

#### Fortran:

call vsrngweibull( method, stream, n, r, alpha, a, beta )
call vdrngweibull( method, stream, n, r, alpha, a, beta )

#### **C**:

vsRngWeibull( method, stream, n, r, alpha, a, beta )
vdRngWeibull( method, stream, n, r, alpha, a, beta )

#### **Discussion**

This function generates Weibull distributed pseudorandom numbers with displacement a, scalefactor  $\beta$ , and shape  $\alpha$ , where  $\alpha$ ,  $\beta$ ,  $a \in R$ ;  $\alpha > 0$ ;  $\beta > 0$ .

The probability density function is given by:

$$f_{a, \alpha, \beta}(x) = \begin{cases} \frac{\alpha}{\beta^{\alpha}} (x-a)^{\alpha-1} \exp\left(-\left(\frac{x-a}{\beta}\right)^{\alpha}\right), & x \ge a\\ 0, & x < a \end{cases}$$

The cumulative distribution function is as follows:

~

$$F_{a, \alpha, \beta}(x) = \begin{cases} 1 - \exp\left(-\left(\frac{x-a}{\beta}\right)^{\alpha}\right), & x \ge a \\ 0, & x < a \end{cases}, -\infty < x < +\infty.$$

### **Input Parameters**

method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
alpha	REAL, INTENT(IN) for vsrngweibull.
	DOUBLE PRECISION, INTENT(IN) for vdrngweibull.
	Shape $\alpha$ .
a	REAL, INTENT(IN) for vsrngweibull.
	DOUBLE PRECISION, INTENT(IN) for vdrngweibull.
	Displacement a.
beta	REAL, INTENT(IN) for vsrngweibull.
	DOUBLE PRECISION, INTENT(IN) for vdrngweibull.
	Scalefactor $\beta$ .
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	<b>int</b> . Number of random values to be generated.
alpha	float for vsRngWeibull.
	double for vdRngWeibull.
	Shape $\alpha$ .

a	float for vsRngWeibull.
	double for vdRngWeibull.
	Displacement a.
beta	float for vsRngWeibull.
	double for vdRngWeibull.
	Scalefactor $\beta$ .
Output Parameters FORTRAN:	
r	REAL, INTENT(OUT) for vsrngweibull.
	DOUBLE PRECISION, INTENT(OUT) for vdrngweibull.
	Vector of <b>n</b> Weibull distributed pseudorandom numbers.
C:	
r	float* for vsRngWeibull.
	double* for vdRngWeibull.
	Vector of <i>n</i> Weibull distributed pseudorandom numbers.

# Cauchy

*Generates Cauchy distributed pseudorandom values.* 

#### Fortran:

call vsrngcauchy( method, stream, n, r, a, beta )
call vdrngcauchy( method, stream, n, r, a, beta )

**C**:

```
vsRngCauchy( method, stream, n, r, a, beta )
vdRngCauchy( method, stream, n, r, a, beta )
```

### **Discussion**

This function generates Cauchy distributed pseudorandom numbers with displacement *a* and scalefactor  $\beta$ , where *a*,  $\beta \in R$ ;  $\beta > 0$ .

The probability density function is given by:

$$f_{a,\beta}(x) = \frac{1}{\pi\beta\left(1 + \left(\frac{x-a}{\beta}\right)^2\right)}, \quad -\infty < x < +\infty.$$

The cumulative distribution function is as follows:

$$F_{a, \beta}(x) = \frac{1}{2} + \frac{1}{\pi} \arctan\left(\frac{x-a}{\beta}\right), \ -\infty < x < +\infty.$$

### **Input Parameters**

method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
a	REAL, INTENT(IN) for vsrngcauchy.
	DOUBLE PRECISION, INTENT(IN) for vdrngcauchy.
	Displacement a.

$\begin{array}{llllllllllllllllllllllllllllllllllll$	beta	REAL, INTENT(IN) for vsrngcauchy.
Scalefactor β.         C:         method       int. Generation method.         stream       VSLStreamStatePtr. Pointer to the stream state structure.         n       int. Number of random values to be generated.         a       float for vsRngCauchy.         double for vdRngCauchy.         beta       float for vsRngCauchy.         double for vdRngCauchy.		DOUBLE PRECISION, INTENT(IN) for
C: method int. Generation method. stream VSLStreamStatePtr. Pointer to the stream state structure. n int. Number of random values to be generated. a float for vsRngCauchy. double for vdRngCauchy. beta float for vsRngCauchy. ouble for vdRngCauchy.		vdrngcauchy.
method       int. Generation method.         stream       VSLStreamStatePtr. Pointer to the stream state structure.         n       int. Number of random values to be generated.         a       float for vsRngCauchy.         double for vdRngCauchy.       Displacement a.         beta       float for vsRngCauchy.         double for vdRngCauchy.       Displacement a.		Scalefactor $\beta$ .
stream       VSLStreamStatePtr. Pointer to the stream state structure.         n       int. Number of random values to be generated.         a       float for vsRngCauchy.         double for vdRngCauchy.       Displacement a.         beta       float for vsRngCauchy.         double for vdRngCauchy.       Displacement a.	C:	
n       int. Number of random values to be generated.         a       float for vsRngCauchy.         double for vdRngCauchy.         beta       float for vsRngCauchy.         double for vdRngCauchy.	method	int. Generation method.
a float for vsRngCauchy. double for vdRngCauchy. Displacement a. beta float for vsRngCauchy. double for vdRngCauchy.	stream	
double for vdRngCauchy.         Displacement a.         beta       float for vsRngCauchy.         double for vdRngCauchy.	n	
beta float for vsRngCauchy. double for vdRngCauchy.	а	float for vsRngCauchy.
beta float for vsRngCauchy. double for vdRngCauchy.		double for vdRngCauchy.
double for vdRngCauchy.		Displacement a.
	beta	float for vsRngCauchy.
Scalefactor $\beta$ .		double for vdRngCauchy.
		Scalefactor $\beta$ .

# **Output Parameters**

r	REAL, INTENT(OUT) for vsrngcauchy.
	DOUBLE PRECISION, INTENT(OUT) for vdrngcauchy.
	Vector of <i>n</i> Cauchy distributed pseudorandom numbers.
C:	
r	float* for vsRngCauchy.
	double* for vdRngCauchy.
	Vector of <i>n</i> Cauchy distributed pseudorandom numbers.

# Rayleigh

Generates Rayleigh distributed pseudorandom values.

### Fortran:

```
call vsrngrayleigh( method, stream, n, r, a, beta )
call vdrngrayleigh( method, stream, n, r, a, beta )
```

### C:

```
vsRngRayleigh( method, stream, n, r, a, beta )
vdRngRayleigh( method, stream, n, r, a, beta )
```

## **Discussion**

This function generates Rayleigh distributed pseudorandom numbers with displacement *a* and scalefactor  $\beta$ , where *a*,  $\beta \in R$ ;  $\beta > 0$ .

Rayleigh distribution is a special case of Weibull distribution, where the shape parameter  $\alpha = 2$ .

The probability density function is given by:

$$f_{a,\beta}(x) = \begin{cases} \frac{2(x-a)}{\beta^2} \exp\left(-\frac{(x-a)^2}{\beta^2}\right), & x \ge a\\ 0, & x < a \end{cases}, \quad -\infty < x < +\infty.$$

The cumulative distribution function is as follows:

$$F_{a,\beta}(x) = \begin{cases} 1 - \exp\left(-\frac{(x-a)^2}{\beta^2}\right), & x \ge a\\ 0, & x < a \end{cases}, \quad -\infty < x < +\infty. \end{cases}$$

# **Input Parameters**

FORTRAN:	
method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
a	REAL, INTENT(IN) for vsrngrayleigh.
	DOUBLE PRECISION, INTENT(IN) for vdrngrayleigh.
	Displacement a.
beta	REAL, $INTENT(IN)$ for vsrngrayleigh.
	DOUBLE PRECISION, INTENT(IN) for vdrngrayleigh.
	Scalefactor $\beta$ .
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	int. Number of random values to be generated.
a	float for vsRngRayleigh.
	double for vdRngRayleigh.
	Displacement a.
beta	float for vsRngRayleigh.
	double for vdRngRayleigh.
	Scalefactor $\beta$ .

Output Parameters FORTRAN:	
r	REAL, INTENT(OUT) for vsrngrayleigh.
	DOUBLE PRECISION, INTENT(OUT) for vdrngrayleigh.
	Vector of <b>n</b> Rayleigh distributed pseudorandom numbers.
C:	
r	float* for vsRngRayleigh.
	double* for vdRngRayleigh.
	Vector of n Rayleigh distributed pseudorandom numbers.

# Lognormal

*Generates lognormally distributed pseudorandom numbers.* 

### Fortran:

```
call vsrnglognormal( method, stream, n, r, a, sigma, b,
beta )
call vdrnglognormal( method, stream, n, r, a, sigma, b,
beta )
```

### **C**:

```
vsRngLognormal( method, stream, n, r, a, sigma, b, beta )
vdRngLognormal( method, stream, n, r, a, sigma, b, beta )
```

### **Discussion**

This function generates lognormally distributed pseudorandom numbers with average of distribution a and standard deviation  $\sigma$  of subject normal distribution, displacement b, and scalefactor  $\beta$ , where

a,  $\sigma$ , b,  $\beta \in R$ ;  $\sigma > 0$ ;  $\beta > 0$ .

The probability density function is given by:

$$f_{a, \sigma, b, \beta}(x) = \begin{cases} \frac{1}{\sigma(x-b)\sqrt{2\pi}} \exp\left(-\frac{\left[\ln\left((x-b)/\beta\right) - a\right]^2}{2\sigma^2}\right), & x > b\\ 0, & x \le b \end{cases}$$

The cumulative distribution function is as follows:

$$F_{a, \sigma, b, \beta}(x) = \begin{cases} \Phi((\ln((x-b)/\beta) - a)/\sigma), & x > b \\ 0, & x \le b \end{cases}$$

### **Input Parameters**

method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
a	REAL, INTENT(IN) for vsrnglognormal.
	DOUBLE PRECISION, INTENT(IN) for vdrnglognormal.
	Average a of the subject normal distribution.

sigma	REAL, INTENT(IN) for vsrnglognormal.
	DOUBLE PRECISION, INTENT(IN) for vdrnglognormal.
	Standard deviation $\sigma$ of the subject normal distribution.
b	REAL, INTENT(IN) for vsrnglognormal.
	DOUBLE PRECISION, INTENT(IN) for vdrnglognormal.
	Displacement b.
beta	REAL, INTENT(IN) for vsrnglognormal.
	DOUBLE PRECISION, INTENT(IN) for vdrnglognormal.
	Scalefactor value $\beta$ .
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	<b>int</b> . Number of random values to be generated.
a	float for vsRngLognormal.
	double for vdRngLognormal.
	Average a of the subject normal distribution.
sigma	float for vsRngLognormal.
	double for vdRngLognormal.
	Standard deviation $\sigma$ of the subject normal distribution.
b	float for vsRngLognormal.
	double for vdRngLognormal.
	Displacement b.

beta	float for vsRngLognormal.
	double for vdRngLognormal.
	Scalefactor value $\beta$ .
Output Parameters FORTRAN:	
r	REAL, INTENT(OUT) for vsrnglognormal.
	DOUBLE PRECISION, INTENT(OUT) for vdrnglognormal.
	Vector of <b>n</b> lognormally distributed pseudorandom numbers.
C:	
r	float* for vsRngLognormal.
	double* for vdRngLognormal.
	Vector of <i>n</i> lognormally distributed pseudorandom numbers.

# Gumbel

*Generates Gumbel distributed pseudorandom values.* 

#### Fortran:

```
call vsrnggumbel( method, stream, n, r, a, beta )
call vdrnggumbel( method, stream, n, r, a, beta )
C:
vsRngGumbel( method, stream, n, r, a, beta )
vdRngGumbel( method, stream, n, r, a, beta )
```

# Discussion

This function generates Gumbel distributed pseudorandom numbers with displacement *a* and scalefactor  $\beta$ , where *a*,  $\beta \in R$ ;  $\beta > 0$ .

The probability density function is given by:

$$f_{a, \beta}(x) = \frac{1}{\beta} \exp\left(\frac{x-a}{\beta}\right) \exp\left(-\exp\left(\frac{x-a}{\beta}\right) \beta\right), -\infty < x < +\infty$$

The cumulative distribution function is as follows:

$$F_{a,\beta}(x) = 1 - \exp(-\exp((x-a)/\beta)), -\infty < x < +\infty$$

### **Input Parameters**

method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
a	REAL, INTENT(IN) for vsrnggumbel.
	DOUBLE PRECISION, INTENT(IN) for vdrnggumbel.
	Displacement a.
beta	REAL, INTENT(IN) for vsrnggumbel.
	DOUBLE PRECISION, INTENT(IN) for vdrnggumbel.
	Scalefactor $\beta$ .
C:	
method	int. Generation method.

stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	<b>int</b> . Number of random values to be generated.
a	float for vsRngGumbel.
	double for vdRngGumbel.
	Displacement a.
beta	float for vsRngGumbel.
	double for vdRngGumbel.
	Scalefactor $\beta$ .
Output Parameters FORTRAN:	
r	REAL, INTENT(OUT) for vsrnggumbel.
	DOUBLE PRECISION, INTENT(OUT) for vdrnggumbel.
	Vector of <i>n</i> pseudorandom values with Gumbel distribution.
C:	
r	float* for vsRngGumbel.
	double* for vdRngGumbel.
	Vector of <b>n</b> pseudorandom values with Gumbel distribution.

# **Discrete Distributions**

This section describes routines for generating pseudorandom numbers with discrete distribution.

# Uniform

Generates pseudorandom numbers uniformly distributed over the interval [a, b].

### Fortran:

call virnguniform( method, stream, n, r, a, b )

### **C**:

viRngUniform( method, stream, n, r, a, b )

## **Discussion**

This function generates pseudorandom numbers uniformly distributed over the interval [a, b], where a, b are the left and right bounds of the interval, respectively, and  $a, b \in Z$ ; a < b.

The probability distribution is given by:

$$P(X = k) = \frac{1}{b-a}, k \in \{a, a+1, .., b-1\}.$$

The cumulative distribution function is as follows:

$$F_{a, b}(x) = \begin{cases} 0, & x < a \\ \frac{\lfloor x - a + 1 \rfloor}{b - a}, & a \le x < b, x \in R. \\ 1, & x \ge b \end{cases}$$

**Input Parameters** 

FORTRAN:

method

**INTEGER**, **INTENT**(**IN**). Generation method.

stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
a	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Left interval bound <i>a</i> .
b	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Right interval bound <i>b</i> .
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	int. Number of random values to be generated.
а	int. Left interval bound a.
b	int. Right interval bound <i>b</i> .

# **Output Parameters**

r	<b>INTEGER</b> , <b>INTENT</b> (OUT). Vector of $n$ pseudorandom values uniformly distributed over the interval [ $a,b$ ).
C:	
r	<b>int</b> *. Vector of <i>n</i> pseudorandom values uniformly distributed over the interval [ <i>a</i> , <i>b</i> ).

# **UniformBits**

*Generates integer random values with uniform bit distribution.* 

### Fortran:

call virnguniformbits( method, stream, n, r )

### **C**:

viRngUniformBits( method, stream, n, r )

## **Discussion**

This function generates integer random values with uniform bit distribution. The generators of uniformly distributed numbers can be represented as recurrence relations over integer values in modular arithmetic. Apparently, each integer can be treated as a vector of several bits. In a truly random generator, these bits are random, while in pseudorandom generators this randomness can be violated. For example, a well known drawback of linear congruential generators is that lower bits are less random than higher bits (for example, see [Knuth81]). For this reason, care should be taken when using this function. Typically, in a 32-bit *LCG* only 24 higher bits of an integer value can be considered truly random. See <u>VSLNotes</u> for details.

### **Input Parameters**

method	INTEGER, INTENT(IN). Generation
	method. A dummy argument in
	virnguniformbits. Should be zero.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.

C:	
method	int. Generation method. A dummy argument in viRngUniformBits. Should be zero.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	int. Number of random values to be generated.

### **Output Parameters**

FORTRAN:

r

INTEGER, INTENT(OUT). Vector of *n* pseudorandom integer numbers. If the *stream* was generated by a 64 or a 128-bit generator, each integer value is represented by two or four elements of *r* respectively. The number of bytes occupied by each integer is contained in the field *wordsize* of the structure VSL_BRNG_PROPERTIES. The total number of bits that are actually used to store the value are contained in the field *nbits* of the same structure. See <u>Advanced Service</u> <u>Subroutines</u> for a more detailed discussion of VSL_BRNG_PROPERTIES. unsigned int*. Vector of n pseudorandom integer numbers. If the stream was generated by a 64 or a 128-bit generator, each integer value is represented by two or four elements of r respectively. The number of bytes occupied by each integer is contained in the field WordSize of the structure VSLBrngProperties. The total number of bits that are actually used to store the value are contained in the field NBits of the same structure. See Advanced Service Subroutines for a more detailed discussion of VSLBrngProperties.

# **Bernoulli**

*Generates Bernoulli distributed pseudorandom values.* 

C:

r

#### Fortran:

call virngbernoulli( method, stream, n, r, p )

#### **C**:

viRngBernoulli( method, stream, n, r, p )

### **Discussion**

This function generates Bernoulli distributed pseudorandom numbers with probability p of a single trial success, where

 $p \in \mathbf{R}; 0 \le p \le 1$ .

A variate is called Bernoulli distributed, if after a trial it is equal to 1 with probability of success p, and to 0 with probability 1-p.

The probability distribution is given by:

$$P(X = 1) = p,$$
  
 $P(X = 0) = 1 - p$ 

The cumulative distribution function is as follows:

$$F_p(x) = \begin{cases} 0, & x < 0 \\ 1 - p, & 0 \le x < 1 \\ 1, & x \ge 1 \end{cases}$$

# **Input Parameters**

method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
P	DOUBLE PRECISION, INTENT(IN). Success probability $p$ of a trial.
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	int. Number of random values to be generated.
Р	double. Success probability $p$ of a trial.

Output Parameters FORTRAN:	
r	<b>INTEGER</b> , <b>INTENT</b> (OUT). Vector of <i>n</i> Bernoulli distributed pseudorandom values.
C:	
r	<b>int</b> *. Vector of <i>n</i> Bernoulli distributed pseudorandom values.

# Geometric

*Generates geometrically distributed pseudorandom values.* 

### Fortran:

call virnggeometric( method, stream, n, r, p )

#### C:

viRngGeometric( method, stream, n, r, p )

### **Discussion**

This function generates geometrically distributed pseudorandom numbers with probability *p* of a single trial success, where  $p \in R$ ; 0 .

A geometrically distributed variate represents the number of independent Bernoulli trials preceding the first success. The probability of a single Bernoulli trial success is *p*.

The probability distribution is given by:

$$P(X = k) = p \cdot (1-p)^{k}, \ k \in \{0, 1, 2, ...\}$$

The cumulative distribution function is as follows:

$$F_{p}(x) = \begin{cases} 0, & x < 0 \\ & 1 - (1-p)^{\lfloor x+1 \rfloor}, & x \ge 0 \end{cases}, x \in \mathbb{R}.$$

# Input Parameters

method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
P	DOUBLE PRECISION, INTENT(IN). Success probability $p$ of a trial.
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	int. Number of random values to be generated.
p	double. Success probability $p$ of a trial.
Output Parameters FORTRAN:	
r	<b>INTEGER</b> , <b>INTENT</b> (OUT). Vector of <i>n</i> geometrically distributed pseudorandom values.
C:	
r	<b>int</b> *. Vector of <i>n</i> geometrically distributed pseudorandom values.

# **Binomial**

Generates binomially distributed pseudorandom numbers.

### Fortran:

call virngbinomial( method, stream, n, r, ntrial, p )

### **C**:

```
viRngBinomial( method, stream, n, r, ntrial, p )
```

# Discussion

This function generates binomially distributed pseudorandom numbers with number of independent Bernoulli trials m, and with probability p of a single trial success, where  $p \in R$ ;  $0 \le p \le 1$ ,  $m \in N$ .

A binomially distributed variate represents the number of successes in m independent Bernoulli trials with probability of a single trial success p.

The probability distribution is given by:

$$P(X = k) = C_m^k p^k (1-p)^{m-k}, \ k \in \{0, 1, ..., m\}.$$

The cumulative distribution function is as follows:

$$F_{m, p}(x) = \begin{cases} 0, & x < 0\\ \lfloor x \rfloor \\ \sum_{k=0}^{k} C_{m}^{k} p^{k} (1-p)^{m-k}, & 0 \le x < m \\ 1, & x \ge m \end{cases}$$

## **Input Parameters**

method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.

n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
ntrial	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of independent trials <i>m</i> .
P	DOUBLE PRECISION, INTENT(IN). Success probability $p$ of a single trial.
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	int. Number of random values to be generated.
ntrial	int. Number of independent trials <i>m</i> .
p	double. Success probability p of a single trial.

# **Output Parameters**

r	<b>INTEGER</b> , <b>INTENT</b> ( <b>OUT</b> ). Vector of <i>n</i> binomially distributed pseudorandom values.
C:	
r	int*. Vector of <i>n</i> binomially distributed pseudorandom values.

# Hypergeometric

Generates hypergeometrically distributed pseudorandom values.

### Fortran:

call virnghypergeometric( method, stream, n, r, l, s, m )

### **C**:

viRngHypergeometric( method, stream, n, r, l, s, m )

### **Discussion**

This function generates hypergeometrically distributed pseudorandom values with lot size l, size of sampling s, and number of marked elements in the lot m, where l, m,  $s \in N \cup \{0\}$ ;  $l \ge max(s, m)$ .

Consider a lot of 1 elements comprising m "marked" and 1-m "unmarked" elements. A trial sampling without replacement of exactly s elements from this lot helps to define the hypergeometric distribution, which is the probability that the group of s elements contains exactly k marked elements.

The probability distribution is given by:

$$P(X = k) = \frac{C_m^k C_{l-m}^{s-k}}{C_l^s}, \ k \in \{max(0, \ s+m-l), \ ..., \ min(s, \ m)\}.$$

The cumulative distribution function is as follows:

$$F_{l, s, m}(x) = \begin{cases} 0, & x < max(0, s + m - l) \\ \sum_{k=max(0, s + m - l)} \frac{C_m^k C_{l-m}^{s-k}}{C_l^s} , max(0, s + m - l) \le x \le min(s, m) \\ 1, & x > min(s, m) \end{cases}$$

# **Input Parameters**

FORTRAN:	
method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
1	INTEGER, INTENT(IN). Lot size 1.
S	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Size of sampling without replacement <i>s</i> .
m	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of marked elements <i>m</i> .
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	int. Number of random values to be generated.
1	int. Lot size 1.
S	int. Size of sampling without replacement s.
m	int. Number of marked elements <i>m</i> .

# **Output Parameters**

FORTRAN:

r

**INTEGER**, **INTENT**(**OUT**). Vector of *n* hypergeometrically distributed pseudorandom values.

rint*.Vector of n hypergeometrically<br/>distributed pseudorandom values.

# Poisson

Generates Poisson distributed pseudorandom values.

C:

### Fortran:

call virngpoisson( method, stream, n, r, lambda )

### **C**:

viRngPoisson( method, stream, n, r, lambda )

### **Discussion**

This function generates Poisson distributed pseudorandom numbers with distribution parameter  $\lambda$ , where  $\lambda \in R$ ;  $\lambda > 0$ .

The probability distribution is given by:

$$P(X = k) = \frac{\lambda^k e^{-\lambda}}{k!}, \quad k \in \{0, 1, 2, ...\}$$

The cumulative distribution function is as follows:

$$F_{\lambda}(x) = \begin{cases} \sum_{k=0}^{\lfloor x \rfloor} \frac{\lambda^{k} e^{-\lambda}}{k!}, & x \ge 0\\ 0, & x < 0 \end{cases}, \quad x \in \mathbb{R}.$$

r

# **Input Parameters**

FORTRAN:	
method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE), INTENT(IN). Descriptor of the stream state structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
lambda	DOUBLE PRECISION, INTENT(IN). Distribution parameter $\lambda$ .
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	<b>int</b> . Number of random values to be generated.
lambda	double. Distribution parameter $\lambda$ .
Output Parameters	
FORTRAN:	
r	<b>INTEGER</b> , <b>INTENT</b> (OUT). Vector of $n$ Poisson distributed pseudorandom values.
C:	

int*. Vector of *n* Poisson distributed values.

# **NegBinomial**

Generates pseudorandom numbers with negative binomial distribution.

### Fortran:

call virngnegbinomial( method, stream, n, r, a, p )

### **C**:

```
viRngNegBinomial( method, stream, n, r, a, p )
```

### **Discussion**

This function generates pseudorandom numbers with negative binomial distribution and distribution parameters **a** and **p**., where **p**,  $a \in R$ ; 0 ; <math>a > 0.

If the first distribution parameter  $a \in N$ , this distribution is the same as Pascal distribution. If  $a \in N$ , the distribution can be interpreted as the expected time of a -th success in a sequence of Bernoulli trials, when the probability of success is p.

The probability distribution is given by:

$$P(X = k) = C_{a+k-1}^{k} p^{a} (1-p)^{k}, \ k \in \{0, 1, 2, ..\}$$

The cumulative distribution function is as follows:

$$F_{a, p}(x) = \begin{cases} \sum_{k=0}^{\lfloor x \rfloor} C_{a+k-1}^{k} p^{a} (1-p)^{k}, & x \ge 0 \\ 0, & x < 0 \end{cases}, \quad x \in \mathbb{R}.$$

### **Input Parameters**

FORTRAN:	
method	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Generation method.
stream	TYPE (VSL_STREAM_STATE),         INTENT(IN).         Descriptor of the stream state         structure.
n	<b>INTEGER</b> , <b>INTENT</b> ( <b>IN</b> ). Number of random values to be generated.
a	DOUBLE PRECISION, INTENT(IN). The first distribution parameter a.
p	DOUBLE PRECISION, INTENT(IN). The second distribution parameter <i>p</i> .
C:	
method	int. Generation method.
stream	VSLStreamStatePtr. Pointer to the stream state structure.
n	int. Number of random values to be generated.
a	double. The first distribution parameter a.
a p	double. The first distribution parameter <i>a</i> . double. The second distribution parameter <i>p</i> .
	•
P	•

C: r int*. Vector of n pseudorandom values with negative binomial distribution.

# **Advanced Service Subroutines**

This section describes service subroutines for registering a basic generator and obtaining properties of the previously registered basic generators.

 Table 8-4
 Advanced Service Subroutines

Subroutine	Short Description
RegisterBrng	Registers a user-designed basic generator.
<u>GetBrngProperties</u>	Returns the structure with properties of the basic generator with a given number.

## Data types

The subroutines of this section refer to a structure defining the properties of the basic generator:

#### Example 8-5 Fortran Version

TYPE VSL_BRNG_PROPER	TIES
INTEGER	streamstatesize
INTEGER	nseeds
INTEGER	includeszero
INTEGER	wordsize
INTEGER	nbits
INTEGER	initstream
INTEGER	sbrng
INTEGER	dbrng
INTEGER	ibrng
END TYPE VSL_BRNG_PR	OPERTIES

### Example 8-6 C Version

typedef struct _VSLBRngProp	perties {
int	StreamStateSize;
int	NSeeds;
int	IncludesZero;
int	WordSize;
int	NBits;
InitStreamPtr	InitStream;
sBRngPtr	sBRng;
dBRngPtr	dBRng;
iBRngPtr	iBRng;
<pre>} VSLBRngProperties;</pre>	

### Example 8-7 Pointers to Functions

typedef	<pre>int (*InitStreamPtr)( int method, void * stream, int n,</pre>
	<pre>const unsigned int params[] );</pre>
typedef	<pre>void (*sBRngPtr)( void * stream, int n, float r[],</pre>
	float a, float b );
typedef	void (*dBRngPtr)( void * stream, int n, double r[],
	double a, double b );
typedef	<pre>void (*iBRngPtr)( void * stream, int n,</pre>
0720001	unsigned int r[] );

# Table 8-5 Field Descriptions

Field	Short Description
FORTRAN:	The size, in bytes, of the stream state structure for a given basic generator.
streamstatesize	
C:	
StreamStateSize	
FORTRAN:	The number of 32-bit initial conditions (seeds)
nseeds	necessary to initialize the stream state structure
C:	for a given basic generator.
NSeeds	
FORTRAN:	Flag value indicating whether the generator can produce a pseudorandom 0 ¹ .
includeszero	
C:	
IncludesZero	
FORTRAN:	Machine word size, in bytes, used in
wordsize	integer-value computations. Possible values: 4, 8, and 16 for 32, 64, and 128-bit generators,
C:	respectively.
WordSize	
FORTRAN:	The number of bits required to represent a pseudorandom value in integer arithmetic. Note that, for instance, 48-bit pseudorandom values are stored to 64-bit (8 byte) memory locations. In this case, WordSize is equal to 8 (number of bytes used to store the pseudorandom value), while NBits contains the actual number of bits occupied by the value (in this example, 48).
nbits	
C:	
NBits	

#### Table 8-5 Field Descriptions (continued)

Field	Short Description
FORTRAN:	Contains the pointer to the initialization
initstream	subroutine of a given basic generator.
C:	
InitStream	
FORTRAN:	Contains the pointer to the basic generator of
sbrng	single precision real numbers uniformly distributed over the interval ( <i>a,b</i> ) (REAL in FORTRAN and float in C).
C:	
sBRng	,
FORTRAN:	Contains the pointer to the basic generator of
dbrng	double precision real numbers uniformly
C:	distributed over the interval ( <i>a,b</i> ) (DOUBLE PRECISION in FORTRAN and double in C).
dBRng	
FORTRAN:	Contains the pointer to the basic generator of
ibrng	integer numbers with uniform bit distribution ² (INTEGER in FORTRAN and unsigned int in C).
C:	
iBRng	,

1. Certain types of generators, for example, generalized feedback shift registers can potentially generate a pseudorandom 0. On the other hand, generators like multiplicative congruential generators never generate such a number. In most cases this information is irrelevant because the probability of generating a zero value is extremely small. However, in certain non-uniform distribution generators the possibility for a basic generator to produce a pseudorandom zero may lead to generation of an infinitely large number (overflow). Even though the software handles overflows correctly, so that they may be interpreted as +∞ and -∞, the user has to be careful and verify the final results. If an infinitely large number may affect the computation, the user should either remove such numbers from the generated vector, or use safe generators, which do not produce pseudorandom 0.

2. A specific generator that permits operations over single bits and bit groups of pseudorandom numbers.

# **RegisterBrng**

Registers user-defined basic generator.

#### Fortran:

brng = vslregisterbrng( properties )

C: brng = vslRegisterBrng( properties )

### Discussion

An example of a registration procedure can be found in the respective directory  $vsl\examples$ .

### **Input Parameters**

FORTRAN:

properties	TYPE (VSL_BRNG_PROPERTIES), INTENT(IN). Structure containing properties of the basic generator to be registered.
C:	
properties	VSLBrngProperties*. Structure containing properties of the basic generator to be registered.
Output Parameters FORTRAN:	
brng	<b>INTEGER.</b> The number (index) of the registered basic generator; used for

registration error.

identification. Negative values indicate the

int. The number (index) of the registered basic generator; used for identification. Negative values indicate the registration error.

# **GetBrngProperties**

C:

brng

*Returns structure with properties of a given basic generator.* 

# Fortran: call vslgetbrngproperties( brng, properties ) **C**: call vslGetBrngProperties( brng, properties ) **Input Parameters** FORTRAN: INTEGER, INTENT(IN). Number brng (index) of the registered basic generator. C: int. Number (index) of the registered brng basic generator. **Output Parameters** FORTRAN: TYPE (VSL_BRNG_PROPERTIES), properties **INTENT(OUT)**. Structure containing properties of the generator with number brng.

C:

properties

VSLBrngProperties*. Structure containing properties of the generator with number *brng*.

# **Formats for User-Designed Generators**

To register a user-designed basic generator using RegisterBrng function, you need to pass the pointer *iBrng* to the integer-value implementation of the generator; the pointers *sBrng* and *dBrng* to the generator implementations for single and double precision values, respectively; and pass the pointer *InitStream* to the stream initialization subroutine. This section contains recommendations on defining such functions with input and output arguments. An example of the registration procedure for a user-designed generator can be found in the respective directory vsl\examples.

#### **InitStream**

#### FORTRAN:

```
INTEGER FUNCTION mybrnginitstream( method, stream, n, params )
        INTEGER, INTENT (IN) :: method
        TYPE(MYSTREAM_STATE), INTENT (INOUT):: stream
        INTEGER, INTENT (IN) :: n
        INTEGER, INTENT (IN) :: params
! Initialize the stream
        ...
END SUBROUTINE mybrnginitstream
        C:
int MyBrngInitStream( int method, VSLStreamStatePtr stream,
        int n, const unsigned int params[] )
{
```

/* Initialize the stream */

#### } /* MyBrngInitStream */

#### **Discussion**

The initialization subroutine of a user-designed generator must initialize *stream* according to the specified initialization *method*, initial conditions *params* and the argument *n*. The value of *method* determines the initialization method to be used.

- If *method* is equal to 0, the initialization is by the standard generation method, which must be supported by all basic generators. In this case the function assumes that the *stream* structure was not previously initialized. The value of *n* is used as the actual number of 32-bit values passed as initial conditions through *params*. Note, that the situation when the actual number of initial conditions passed to the function is not sufficient to initialize the generator is not an error. Whenever it occurs, the basic generator must initialize the missing conditions using default settings.
- If *method* is equal to 1, the generation is by the leapfrog method, where *n* specifies the number of computational nodes (independent streams). Here the function assumes that the *stream* was previously initialized by the standard generation method. In this case *params* contains only one element, which identifies the computational node. If the generator does not support the leapfrog method, the function must return the error code VSL_ERROR_LEAPFROG_UNSUPPORTED.
- If *method* is equal to 2, the generation is by the block-splitting method. Same as above, the *stream* is assumed to be previously initialized by the standard generation method; *params* is not used, *n* identifies the number of skipped elements. If the generator does not support the block-splitting method, the function must return the error code VSL_ERROR_SKIPAHEAD_UNSUPPORTED.

For a more detailed description of the leapfrog and the block-splitting methods, refer to the description of LeapfrogStream and SkipAheadStream, respectively.

Stream state structure is individual for every generator. However, each structure has a number of fields that are the same for all the generators:

#### FORTRAN:

```
type(mystream_state)
      INTEGER*4
                  reserved1
       INTEGER*4
                 reserved2
      INTEGER*4 reserved3
       INTEGER*4
                 reserved4
       [ fields specific for the given generator ]
end type mystream_state
C:
typedef struct
{
      uint64 Reserved1;
      uint64 Reserved2;
      [ fields specific for the given generator ]
} MyStreamState
```

The fields *Reserved1* and *Reserved2* are reserved for private needs only, and must not be modified by the user. When including specific fields into the structure, follow the rules below:

- The fields must fully describe the current state of the generator. For example, the state of a linear congruential generator can be identified by only one initial condition;
- If the generator can use both the leapfrog and the block-splitting methods, additional fields should be introduced to identify the independent streams. For example, in LCG(a, c, m), apart from the initial conditions, two more fields should be specified: the value of the multiplier  $a^k$  and the value of the increment  $(a^k 1)c/(a 1)$ .

For a more detailed discussion, refer to [Knuth81], and [Gentle98]. An example of the registration procedure can be found in the respective directory vsl\examples.

## iBRng

#### FORTRAN:

SUBROUTINE imybrng( stream, n, r )

```
TYPE(MYSTREAM_STATE), INTENT(INOUT):: stream
     INTEGER, INTENT(IN) :: n
     INTEGER, DIMENSION(*), INTENT(OUT) :: r
! Generating integer random numbers
! Pay attention to word size needed to
! store one random number
     DO i = 1, n
           R(I) = ...
     END DO
! Update stream state
END SUBROUTINE imybrng
           C:
void iMyBrng( VSLStreamStatePtr stream, int n,
              unsigned int r[] )
{
      int
               i;
                    /* Loop variable */
     /* Generating integer random numbers */
     /* Pay attention to word size needed to
        store only random number */
     for(i = 0; i < n; i++)
      {
               r[i] = ...
      }
     /* Update stream state */
     ....
} /* iMyBrng */
```



**NOTE.** When using 64 and 128-bit generators, consider digit capacity to store the numbers to the pseudorandom vector  $\mathbf{r}$  correctly. For example, storing one 64-bit value requires two elements of  $\mathbf{r}$ , the first to store the lower 32 bits and the second to store the higher 32 bits. Similarly, use 4 elements of  $\mathbf{r}$  to store a 128-bit value.

### sBRng

```
SUBROUTINE smybrng( stream, n, r, a, b)
     TYPE(MYSTREAM_STATE), INTENT(INOUT):: stream
                          :: n
     INTEGER, INTENT(IN)
     REAL, DIMENSION(n), INTENT(OUT) :: r
     REAL, INTENT(IN) :: a
     REAL, INTENT(IN)
                        :: b
! Generating real (a,b) random numbers
     DO i = 1, n
            R(I) = ...
     END DO
! Update stream state
END SUBROUTINE smybrng
            C:
void sMyBrng( VSLStreamStatePtr stream, int n, float r[],
              float a, float b )
{
      int
               i;
                      /* Loop variable */
      /* Generating float (a,b) random numbers */
     for (i = 0; i < n; i++)
      Ł
               r[i] = ...
      }
      /* Update stream state */
```

```
} /* sMyBrng */
```

# dBRng

### FORTRAN:

```
SUBROUTINE dmybrng( stream, n, r, a, b)
     TYPE(MYSTREAM_STATE), INTENT(INOUT) :: stream
     INTEGER, INTENT(IN) :: n
     DOUBLE PRECISION, DIMENSION(n), INTENT(OUT) :: r
     REAL, INTENT(IN) :: a
     REAL, INTENT(IN) :: b
! Generating double precision (a,b) random numbers
     DO i = 1, n
           R(I) = ...
     END DO
! Update stream state
            ....
END SUBROUTINE dmybrng
           C:
void dMyBrng( VSLStreamStatePtr stream, int n, double r[],
              double a, double b )
{
      int
             i; /* Loop variable */
     /* Generating double (a,b) random numbers */
     for (i = 0; i < n; i++)
      {
               r[i] = ...
      }
     /* Update stream state */
     ••••
} /* dMyBrng */
```

# Advanced DFT Functions



The Fast Fourier Transform (FFT) algorithm that calculates the Discrete Fourier Transform (DFT) is an indispensable tool in a vast number of fields. This chapter describes the set of new DFT functions implemented in Intel[®] MKL, which present a uniform and easy-to-use Applications Programmer Interface (API) providing fast computation of DFT via FFT.

The Discrete Fourier Transform function library of Intel MKL provides one-dimensional, two-dimensional, and multi-dimensional (up to the order of 7) routines.

Both Fortran- and C-interfaces exist for all transform functions.

Although Intel MKL still supports the FFT interface described in chapter 3 of this manual, users are encouraged to migrate to the new advanced DFT functions in their application programs. Unlike the older FFT routines, the DFT routines support transform lengths of other than powers of 2 mixed radix.

The full list of DFT functions implemented in Intel MKL is given in the table below:

#### Table 9-1 DFT Functions in Intel MKL

Function Name	Operation
Descriptor Manipulation Functions	
DftiCreateDescriptor	Allocates memory for the descriptor data structure and instantiates it with default configuration settings.
DftiCommitDescriptor	Performs all initialization that facilitates the actual DFT computation.
DftiCopyDescriptor	Copies an existing descriptor.
DftiFreeDescriptor	Frees memory allocated for a descriptor.

Function Name	Operation
DFT Computation Function	ns
DftiComputeForward	Computes the forward DFT.
DftiComputeBackward	Computes the backward DFT.
Descriptor Configuration	Functions
DftiSetValue	Sets one particular configuration parameter with the specified configuration value.
DftiGetValue	Gets the configuration value of one particular configuration parameter.
Status Checking Function	15
DftiErrorClass	Checks if the status reflects an error of a predefined class.
DftiErrorMessage	Generates an error message.

Table 9-1DFT Functions in Intel MKL (continued)

Description of DFT functions is followed by discussion of configuration settings (see <u>Configuration Settings</u>) and various configuration parameters used.

# **Computing DFT**

DFT functions described later in this chapter are implemented in Fortran and C interface. Fortran stands for Fortran 95. DFT interface relies critically on many modern features offered in Fortran 95 that have no counterpart in Fortran 77



**NOTE.** Following the explicit function interface in Fortran, data array must be defined as one-dimensional for any transformation type.

The materials presented in this chapter assume the availability of native complex types in C as they are specified in C9X.

Before the presenting every function, a couple of usage examples are given.

For most common situations, we expect a DFT computation can be effected by four function calls. Here are the examples of two one-dimensional computations.

#### Example 9-1 One-dimensional DFT (Fortran-interface)

```
! Fortran example.
! 1D complex to complex, and real to conjugate even
Use MKL_DFTI
Complex :: X(32)
Real :: Y(34)
type(DFTI_DESCRIPTOR), POINTER :: My_Desc1_Handle, My_Desc2_Handle
Integer :: Status
...put input data into X(1),...,X(32); Y(1),...,Y(32)
! Perform a complex to complex transform
Status = DftiCreateDescriptor( My_Desc1_Handle, DFTI_SINGLE,
          DFTI_COMPLEX, 1, 32 )
Status = DftiCommitDescriptor( My_Desc1_Handle )
Status = DftiComputeForward( My_Desc1_Handle, X )
Status = DftiFreeDescriptor(My_Desc1_Handle)
! result is given by \{X(1), X(2), ..., X(32)\}
! Perform a real to complex conjugate even transform
Status = DftiCreateDescriptor(My_Desc2_Handle, DFTI_SINGLE,
          DFTI_REAL, 1, 32)
Status = DftiCommitDescriptor(My Desc2 Handle)
Status = DftiComputeForward(My Desc2 Handle, Y)
Status = DftiFreeDescriptor(My Desc2 Handle)
! result is given by \{Y(1)+iY(2), Y(3)+iY(4), \ldots, Y(33)+iY(34), \}
! Y(31)-iY(32), Y(29)-iY(30), \ldots, Y(3)-iY(4).
```

#### Example 9-2 One-dimensional DFT (C-interface)

```
/* C example, float _Complex is defined in C9X */
#include "mkl_dfti.h"
float _Complex x[32];
float y[34];
DFTI DESCRIPTOR *my_desc1_handle, *my_desc2_handle;
/* .... or alternatively
DFTI DESCRIPTOR HANDLE my desc1 handle, my desc2 handle; */
long status;
...put input data into x[0],...,x[31]; y[0],...,y[31]
status = DftiCreateDescriptor( &my_desc1_handle, DFTI_SINGLE,
          DFTI_COMPLEX, 1, 32);
status = DftiCommitDescriptor( my_desc1_handle );
status = DftiComputeForward( my_desc1_handle, x);
status = DftiFreeDescriptor(&my_desc1_handle);
/* result is x[0], ..., x[31] */
status = DftiCreateDescriptor( &my_desc2_handle, DFTI_SINGLE,
          DFTI_REAL, 1, 32);
status = DftiCommitDescriptor( my_desc2_handle);
status = DftiComputeForward( my_desc2_handle, y);
status = DftiFreeDescriptor(&my_desc2_handle);
/* y[0]+iy[1], ..., y[32]+iy[33], y[30]-iy[31], ..., y[2]-iy[3] */
```

The following is an example of two simple two-dimensional transforms. Notice that the data and result parameters in computation functions are all declared as assumed-size rank-1 array DIMENSION(0:*). Therefore two-dimensional array must be transformed to one-dimensional array by EQUIVALENCE statement or other facilities of Fortran.

#### Example 9-3 Two-dimensional DFT (Fortran-interface)

```
! Fortran example.
! 2D complex to complex, and real to conjugate even
Use MKL DFTI
Complex :: X_2D(32,100)
Real :: Y_2D(34, 102)
Complex :: X(3200)
Real :: Y(3468)
Equivalence (X_2D, X)
Equivalence (Y_2D, Y)
type(DFTI_DESCRIPTOR), POINTER :: My_Desc1_Handle, My_Desc2_Handle
Integer :: Status, L(2)
...put input data into X_2D(j,k), Y_2D(j,k), 1<=j=32,1<=k<=100
...set L(1) = 32, L(2) = 100
... the transform is a 32-by-100
! Perform a complex to complex transform
Status = DftiCreateDescriptor( My_Desc1_Handle, DFTI_SINGLE,
          DFTI_COMPLEX, 2, L)
Status = DftiCommitDescriptor( My Desc1 Handle)
Status = DftiComputeForward( My_Desc1_Handle, X)
Status = DftiFreeDescriptor(My_Desc1_Handle)
! result is given by X_{2D}(j,k), 1 <= j <= 32, 1 <= k <= 100
! Perform a real to complex conjugate even transform
Status = DftiCreateDescriptor( My_Desc2_Handle, DFTI_SINGLE,
          DFTI_REAL, 2, L)
Status = DftiCommitDescriptor( My_Desc2_Handle)
Status = DftiComputeForward( My_Desc2_Handle, Y)
Status = DftiFreeDescriptor(My_Desc2_Handle)
! result is given by the complex value z(j,k) 1<=j<=32; 1<=k<=100 where
! z(j,k) = Y_2D(2j-1,k) + iY_2D(2j,k) 1<=j<=17; 1<=k<=100
! z(j,k) = Y_2D(2(34-j)-1,k) - iY_2D(2(34-j),k) 18<=j<=32; 1<=k<=100
```

#### Example 9-4 Two-dimensional DFT (C-interface)

```
/* C example */
#include "mkl_dfti.h"
float _Complex x[32][100];
float y[34][102];
DFTI_DESCRIPTOR_HANDLE my_desc1_handle, my_desc2_handle;
/* or alternatively
DFTI_DESCRIPTOR *my_desc1_handle, *my_desc2_handle; */
long status, 1[2];
...put input data into x[j][k] 0<=j<=31, 0<=k<=99
...put input data into y[j][k] 0<=j<=31, 0<=k<=99
1[0] = 32; 1[1] = 100;
status = DftiCreateDescriptor( &my_desc1_handle, DFTI_SINGLE,
          DFTI_COMPLEX, 2, 1);
status = DftiCommitDescriptor( my_desc1_handle);
status = DftiComputeForward( my_desc1_handle, x);
status = DftiFreeDescriptor(&my_desc1_handle);
/* result is the complex value x[j][k], 0<=j<=31, 0<=k<=99 */
status = DftiCreateDescriptor( &my_desc2_handle, DFTI_SINGLE,
          DFTI_REAL, 2, 1);
status = DftiCommitDescriptor( my_desc2_handle);
status = DftiComputeForward( my_desc2_handle, y);
status = DftiFreeDescriptor(&my_desc2_handle);
/* result is the complex value z(j,k) = 0 <= j <= 31; = 0 <= k <= 99
/* z(j,k) = y[2j][k] + iy[2j+1][k] 0<=j<=16; 0<=k<=99 */</pre>
/* z(j,k) = y[2(32-j)][k] - iy[2(32-j)+1][k] 17<=j<=31; 1<=k<=100 */</pre>
```

The record of type DFTI_DESCRIPTOR, when created, contains information about the length and domain of the DFT to be computed. Moreover, it contains the setting of a rather large number of configuration parameters. The examples above use the default settings for all of these parameters, which include, for example, the following:

the DFT to be computed does not have a scale factor;

- there is only one set of data to be transformed;
- the data is stored contiguously in memory;
- the forward transform is defined to be the formula using  $e^{-i2\pi jk/n}$  rather than  $e^{+i2\pi jk/n}$ ;
- complex data is stored in the native complex data type;
- the computed result overwrites (in place) the input data; etc.

Should any one of these many default settings be inappropriate, they can be changed one-at-a-time through the function <u>DftiSetValue</u>. For example, to preserve the input data after the DFT computation, the configuration of the F should be changed to "not in place" from the default choice of "in place." The code below illustrates how this can be done:

### Example 9-5 Changing Default Settings (Fortran)

#### Example 9-6 Changing Default Settings (C)

```
/* C example */
#include "mkl dfti.h"
float _Complex x_in[32], x_out[32];
DFTI_DESCRIPTOR_HANDLE my_desc_handle;
/* or alternatively
DFTI_DESCRIPTOR *my_desc_handle; */
long status;
...put input data into x_in[j], 0 <= j < 32
status = DftiCreateDescriptor( &my_desc_handle, DFTI_SINGLE,
DFTI_COMPLEX, 1, 32);
status = DftiSetValue( my_desc_handle, DFTI_PLACEMENT,
DFTI_NOT_INPLACE);
status = DftiCommitDescriptor( my_desc_handle);
status = DftiComputeForward( my_desc_handle, x_in, x_out);
status = DftiFreeDescriptor(&my_desc_handle);
/* result is x_out[0], x_out[1], ..., x_out[31] */
```

The approach adopted in Intel MKL for DFT computation uses one single data structure, the descriptor, to record flexible configuration whose parameters can be changed independently. This results in enhanced functionality and ease of use.

# **DFT Interface**

To use the advanced DFT functions, the user needs to access the module MKL_DFTI through the "use" statement in Fortran; or access the header file mkl_dfti.h through "include" in C.

The Fortran interface provides a derived type DFTI_DESCRIPTOR; a number of named constants representing various names of configuration parameters and their possible values; and a number of overloaded functions through the generic functionality of Fortran 95.

The C interface provides a structure type DFTI_DESCRIPTOR, a macro definition

#define DFTI_DESCRIPTOR_HANDLE DFTI_DESCRIPTOR *;

a number of named constants of two enumeration types DFTI_CONFIG_PARAM and DFTI_CONFIG_VALUE; and a number of functions, some of which accept different number of input arguments.



**NOTE.** Some of the functions and/or functionality described in the subsequent sections of this chapter may not be supported by the currently available implementation of the library. You can find the complete list of the implementation-specific exceptions in the release notes to your version of the library.

There are four main categories of DFT functions in Intel MKL:

1. **Descriptor Manipulation.** There are four functions in this category. The first one creates a DFT descriptor whose storage is allocated dynamically by the routine. This function configures the descriptor with default settings corresponding to a few input values supplied by the user.

The second "commits" the descriptor to all its setting. In practice, this usually means that all the necessary precomputation will be performed. This may include factorization of the input length and

computation of all the required twiddle factors. The third function makes an extra copy of a descriptor, and the fourth function frees up all the memory allocated for the descriptor information.

- 2. **DFT Computation**. There are two functions in this category. The first effects a forward DFT computation, and the second a backward DFT computation.
- 3. **Descriptor configuration**. There are two functions in this category. One function sets one specific value to one of the many configuration parameters that are changeable (a few are not); the other gets the current value of any one of these configuration parameters (all are readable). These parameters, though many, are handled one-at-a-time.
- 4. **Status Checking**. The functions described in the three categories return an integer value denoting the status of the operation. In particular, a non-zero return value always indicates a problem of some sort. Envisioned to be further enhanced in later releases of Intel MKL, DFT interface at present provides for one logical status class function and a simple status message generation function.

# **Status Checking Functions**

All of the descriptor manipulation, DFT computation, and descriptor configuration functions return an integer value denoting the status of the operation. Two functions serve to check the status. The first function is a logical function that checks if the status reflects an error of a predefined class, and the second is an error message function that returns a character string.

# **ErrorClass**

Checks if the status reflects an error of a predefined class.

## Usage

```
! Fortran
Predicate = DftiErrorClass( Status, Error_Class )
/* C */
predicate = DftiErrorClass( status, error_class );
```

## **Discussion**

DFT interface in Intel MKL provides a set of predefined error class listed in <u>Table 9-2</u>. These are named constants and have the type **INTEGER** in Fortran and long in C.

Named Constants	Comments
DFTI_NO_ERROR	No error
DFTI_MEMORY_ERROR	Usually associated with memory allocation
DFTI_INVALID_CONFIGURATION	Invalid settings of one or more configuration parameters
DFTI_INCONSISTENT_CONFIGURATION	Inconsistent configuration or input parameters
DFTI_MULTITHREADED_ERROR	Usually associated with OMP routine's error return value
DFTI_BAD_DESCRIPTOR	Descriptor is unusable for computation
DFTI_UNIMPLEMENTED	Unimplemented legitimate settings; implementation dependent
DFTI_MKL_INTERNAL_ERROR	Internal library error

## Table 9-2 Predefined Error Class

Note that the correct usage is to check if the status returns .TRUE. or .FALSE. through the use of DFTI_ERROR_CLASS with a specific error class. Direct comparison of a status with the predefined class is an incorrect usage.

#### Example 9-7 Using Status Checking Function

```
from C language:
DFTI_DESCRIPTOR_HANDLE desc;
long status, class_error, value;
char* error_message;
 . . . descriptor creation and other code
status = DftiGetValue( desc, DFTI_PRECISION, &value); //
//or any DFTI function
class error = DftiErrorClass(status, DFTI ERROR CLASS);
if (! class_error) {
printf ("status is not a member of Predefined Error
Class\n");
} else {
error_message = DftiErrorMessage(status);
printf("error_message = %s \n", error_message);
. . .
from Fortran:
type(DFTI_DESCRIPTOR), POINTER :: desc
integer value, status
character(DFTI_MAX_MESSAGE_LENGTH) error_message
logical class_error
 . . . descriptor creation and other code
status = DftiGetValue( desc, DFTI_PRECISION, value)
class_error = DftiErrorClass(status, DFTI_ERROR_CLASS)
if (.not. class_error) then
print *, 'status is not a member of Predefined Error
Class '
else
error_message = DftiErrorMessage(status)
print *, 'error_message = ', error_message
endif
```

#### Interface and prototype

```
//Fortran interface
INTERFACE DftiErrorClass
//Note that the body provided here is to illustrate the different
```

```
//argument list and types of dummy arguments. The interface
//does not guarantee what the actual function names are.
//Users can only rely on the function name following the
//keyword INTERFACE
FUNCTION some_actual_function_8( Status, Error_Class )
LOGICAL some_actual_function_8
INTEGER, INTENT(IN) :: Status, Error_Class
END FUNCTION some_actual_function_8
END INTERFACE DftiErrorClass
/* C prototype */
long DftiErrorClass( long , long );
```

# **ErrorMessage**

Generates an error message.

### Usage

```
! Fortran
ERROR_MESSAGE = DftiErrorMessage( Status )
/* C */
error_message = DftiErrorMessage( status );
```

#### **Discussion**

The error message function generates an error message character string. The maximum length of the string in Fortran is given by the named constant DFTI_MAX_MESSAGE_LENGTH. The actual error message is implementation dependent. In Fortran, the user needs to use a character string of length DFTI_MAX_MESSAGE_LENGTH as the target. In C, the function returns a pointer to a character string, that is, a character array with the delimiter '0'.

Example 9-7 shows how this function can be implemented.

#### Interface and prototype

```
//Fortran interface
INTERFACE DftiErrorMessage
//Note that the body provided here is to illustrate the different
//argument list and types of dummy arguments. The interface
//does not guarantee what the actual function names are.
//Users can only rely on the function name following the
//keyword INTERFACE
FUNCTION some_actual_function_9( Status, Error_Class )
CHARACTER(LEN=DFTI_MAX_MESSAGE_LENGTH) some_actual_function_9( Status )
INTEGER, INTENT(IN) :: Status
END FUNCTION some_actual_function_9
END INTERFACE DftiErrorMessage
```

```
/* C prototype */
char *DftiErrorMessage( long );
```

# **Descriptor Manipulation**

There are four functions in this category: create a descriptor, commit a descriptor, copy a descriptor, and free a descriptor.

# CreateDescriptor

Allocates memory for the descriptor data structure and instantiates it with default configuration settings.

# Usage

! Fortran		
<pre>Status = DftiCreateDescriptor(</pre>	Desc_Handle,	&
	Precision,	&
	Forward_Domain,	&
	Dimension,	&
	Length )	

### **Discussion**

This function allocates memory for the descriptor data structure and instantiates it with all the default configuration settings with respect to the precision, domain, dimension, and length of the desired transform. The domain is understood to be the domain of the forward transform. Since memory is allocated dynamically, the result is actually a pointer to the created descriptor. This function is slightly different from the "initialization" routine in more traditional software packages or libraries used for computing DFT. In all likelihood, this function will not perform any significant computation work such as twiddle factors computation, as the default configuration settings can still be changed upon user's request through the value setting function <u>DftiSetValue</u>.

The precision and (forward) domain are specified through named constants provided in DFT interface for the configuration values. The choices for precision are DFTI_SINGLE and DFTI_DOUBLE; and the choices for (forward) domain are DFTI_COMPLEX, DFTI_REAL, and DFTI_CONJUGATE_EVEN. See <u>Table 9-5</u> for the complete table of named constants for configuration values.

Dimension is a simple positive integer indicating the dimension of the transform. Length is either a simple positive integer for one-dimensional transform, or an integer array (pointer in C) containing the positive integers corresponding to the lengths dimensions for multi-dimensional transform.

The function returns DFTI_NO_ERROR when completes successfully. See <u>"Status Checking Functions"</u> for more information on returned status.

#### Interface and prototype

```
!Fortran interface.
INTERFACE DftiCreateDescriptor
!Note that the body provided here is to illustrate the different
!argument list and types of dummy arguments. The interface
!does not guarantee what the actual function names are.
!Users can only rely on the function name following the
 !keyword INTERFACE
 FUNCTION some_actual_function_1D( Desc_Handle, Prec, Dom, Dim, Length )
   INTEGER :: some_actual_function_1D
   TYPE(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
   INTEGER, INTENT(IN) :: Prec, Dom
   INTEGER, INTENT(IN) :: Dim, Length
 END FUNCTION some actual function 1D
 FUNCTION some_actual_function_HIGHD( Desc_Handle, Prec, Dom, Dim, Length )
   INTEGER :: some_actual_function_HIGHD
   TYPE(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
   INTEGER, INTENT(IN) :: Prec, Dom
```

```
INTEGER, INTENT(IN) :: Dim, Length(*)
```

```
END FUNCTION some_actual_function_HIGHD
END INTERFACE DftiCreateDescriptor
```

Note that the function is overloaded as the actual argument for Length can be a scalar or a a rank-one array.

```
/* C prototype */
```

The variable arguments facility is used to cope with the argument for lengths that can be a scalar (long), or an array (long *).

# CommitDescriptor

*Performs all initialization that facilitates the actual DFT computation.* 

### Usage

```
! Fortran
Status = DftiCommitDescriptor( Desc_Handle )
/* C */
status = DftiCommitDescriptor( desc_handle );
```

### **Discussion**

The interface requires a function that commits a previously created descriptor be invoked before the descriptor can be used for DFT computations. Typically, this committal performs all initialization that facilitates the actual DFT computation. For a modern implementation, it may involve exploring many different factorizations of the input length to search for highly efficient computation method.

Any changes of configuration parameters of a committed descriptor via the set value function (see <u>"Descriptor Configuration"</u>) requires a re-committal of the descriptor before a computation function can be invoked. Typically, this committal function call is immediately followed by a computation function call (see <u>"DFT Computation"</u>).

The function returns DFTI_NO_ERROR when completes successfully. See <u>"Status Checking Functions"</u> for more information on returned status.

#### Interface and prototype

```
! Fortran interface
```

```
INTERFACE DftiCommitDescriptor
```

```
!Note that the body provided here is to illustrate the different
!argument list and types of dummy arguments. The interface
!does not guarantee what the actual function names are.
!Users can only rely on the function name following the
!keyword INTERFACE
FUNCTION some_actual function_1 ( Desc_Handle )
    INTEGER :: some_actual function_1
    TYPE(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
END FUNCTION some_actual function_1
END INTERFACE DftiCommitDescriptor
```

```
/* C prototype */
long DftiCommitDescriptor( DFTI_DESCRIPTOR_HANDLE );
```

# CopyDescriptor

Copies an existing descriptor.

### Usage

! Fortran

#### **Discussion**

This function makes a copy of an existing descriptor and provides a pointer to it. The purpose is that all information of the original descriptor will be maintained even if the original is destroyed via the free descriptor function DftiFreeDescriptor.

The function returns DFTI_NO_ERROR when completes successfully. See <u>"Status Checking Functions"</u> for more information on returned status.

### Interface and prototype

```
/* C prototype */
long DftiCopyDescriptor( DFTI_DESCRIPTOR_HANLDE, DFTI_DESCRIPTOR_HANDLE * );
```

# **FreeDescriptor**

*Frees memory allocated for a descriptor.* 

## Usage

```
! Fortran
Status = DftiFreeDescriptor( Desc_Handle )
/* C */
status = DftiFreeDescriptor( &desc_handle );
```

## **Discussion**

This function frees up all memory space allocated for a descriptor.

The function returns DFTI_NO_ERROR when completes successfully. See <u>"Status Checking Functions"</u> for more information on returned status.

#### Interface and prototype

```
! Fortran interface
INTERFACE DftiFreeDescriptor
//Note that the body provided here is to illustrate the different
//argument list and types of dummy arguments. The interface
//does not guarantee what the actual function names are.
//Users can only rely on the function name following the
//keyword INTERFACE
FUNCTION some_actual_function_3( Desc_Handle )
INTEGER :: some_actual_function_3
TYPE(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
END FUNCTION some_actual_function_3
END INTERFACE DftiFreeDescriptor
/* C prototype */
long DftiFreeDescriptor( DFTI_DESCRIPTOR_HANDLE * );
```

# **DFT Computation**

There are two functions in this category: compute the forward transform, and compute the backward transform.

# **ComputeForward**

Computes the forward DFT.

#### Usage

```
! Fortran
Status = DftiComputeForward( Desc_Handle, X_inout )
Status = DftiComputeForward( Desc_Handle, X_in, X_out )
Status = DftiComputeForward( Desc_Handle, X_inout, Y_inout )
Status = DftiComputeForward( Desc_Handle, X_in, Y_in, X_out, Y_out )
/* C */
status = DftiComputeForward( desc_handle, x_inout );
status = DftiComputeForward( desc_handle, x_in, x_out );
status = DftiComputeForward( desc_handle, x_inout, y_inout );
status = DftiComputeForward( desc_handle, x_in, y_in, x_out, y_out );
```

### **Discussion**

As soon as a descriptor is configured and committed successfully, actual computation of DFT can be performed. The DftiComputeForward function computes the forward DFT. By default, this is the transform using the factor  $e^{-i2\pi/n}$  (instead of the one with a positive sign). Because of the flexibility in configuration, input data can be represented in various ways as well as output result can be placed differently. Consequently, the number of input parameters as well as their type vary. This variation is accommodated by the generic function facility of Fortran 95. Data and result parameters are all declared as assumed-size rank-1 array DIMENSION(0:*).

The function returns DFTI_NO_ERROR when completes successfully. See

"Status Checking Functions" for more information on returned status.

#### Interface and prototype

//Fortran interface. INTERFACE DftiComputeFoward //Note that the body provided here is to illustrate the different //argument list and types of dummy arguments. The interface //does not guarantee what the actual function names are. //Users can only rely on the function name following the //keyword INTERFACE // One argument single precision complex FUNCTION some_actual_function_4_C( Desc_Handle, X ) INTEGER :: some_actual_function_4_C TYPE(DFTI_DESCRIPTOR), POINTER :: Desc_Handle COMPLEX, INTENT(INOUT) :: X(*) END FUNCTION some_actual_function_4_C // One argument double precision complex FUNCTION some_actual_function_4_Z( Desc_Handle, X ) INTEGER :: some_actual_function_4_Z TYPE(DFTI_DESCRIPTOR), POINTER :: Desc_Handle COMPLEX (Kind((0D0,0D0))), INTENT(INOUT) :: X(*) END FUNCTION some_actual_function_4_Z // One argument single precision real FUNCTION some_actual_function_4_R( Desc_Handle, X ) INTEGER :: some_actual_function_4_R TYPE(DFTI_DESCRIPTOR), POINTER :: Desc_Handle REAL, INTENT(INOUT) :: X(*) END FUNCTION some_actual_function_4_R // One argument double precision real // Two argument single precision complex . . . // Four argument double precision real FUNCTION some_actual_function_4_DDDD( Desc_Handle, X1_In, X2_In, Y1_Out, Y2_Out )

```
...);
```

The implementations of DFT interface expect the data be treated as data stored linearly in memory with a regular "stride" pattern (discussed more fully in <u>"Strides"</u>, see also [3]). The function expects the starting address of the first element. Hence we use the assume-size declaration in Fortran.

The descriptor by itself contains sufficient information to determine exactly how many arguments and of what type should be present. The implementation could use this information to check against possible input inconsistency.

# **ComputeBackward**

Computes the backward DFT.

#### Usage

```
! Fortran
Status = DftiComputeBackward( Desc_Handle, X_inout )
Status = DftiComputeBackward( Desc_Handle, X_in, X_out )
Status = DftiComputeBackward( Desc_Handle, X_inout, Y_inout )
Status = DftiComputeBackward( Desc_Handle, X_in, Y_in, X_out, Y_out )
/* C */
status = DftiComputeBackward( desc_handle, x_inout );
status = DftiComputeBackward( desc_handle, x_in, x_out );
```

```
status = DftiComputeBackward( desc_handle, x_inout, y_inout );
status = DftiComputeBackward( desc_handle, x_in, y_in, x_out, y_out );
```

#### **Discussion**

As soon as a descriptor is configured and committed successfully, actual computation of DFT can be performed. The DftiComputeBackward function computes the backward DFT. By default, this is the transform using the factor  $e^{i2\pi/n}$  (instead of the one with a negative sign). Because of the flexibility in configuration, input data can be represented in various ways as well as output result can be placed differently. Consequently, the number of input parameters as well as their type vary. This variation is accommodated by the generic function facility of Fortran 95. Data and result parameters are all declared as assumed-size rank-1 array DIMENSION(0:*).

The function returns DFTI_NO_ERROR when completes successfully. See <u>"Status Checking Functions"</u> for more information on returned status.

#### Interface and prototype

```
//Fortran interface.
```

INTERFACE DftiComputeBackward //Note that the body provided here is to illustrate the different //argument list and types of dummy arguments. The interface //does not guarantee what the actual function names are. //Users can only rely on the function name following the //keyword INTERFACE // One argument single precision complex FUNCTION some_actual_function_5_C( Desc_Handle, X ) INTEGER :: some_actual_function_5_C TYPE(DFTI_DESCRIPTOR), POINTER :: Desc_Handle COMPLEX, INTENT(INOUT) :: X(*) END FUNCTION some_actual_function_5_C // One argument double precision complex FUNCTION some_actual_function_5_Z( Desc_Handle, X ) INTEGER :: some_actual_function_5_Z TYPE(DFTI_DESCRIPTOR), POINTER :: Desc_Handle COMPLEX (Kind((0D0,0D0))), INTENT(INOUT) :: X(*)

```
END FUNCTION some_actual_function_5_Z
 // One argument single precision real
 FUNCTION some actual function 5 R( Desc Handle, X )
    INTEGER :: some_actual_function_5_R
   TYPE(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
   REAL, INTENT(INOUT) :: X(*)
 END FUNCTION some actual function 5 R
 // One argument double precision real
 // Two argument single precision complex
 . . .
 . . .
 // Four argument double precision real
 FUNCTION some actual function 5 DDDD( Desc Handle, X1 In, X2 In,
                                          Y1_Out, Y2_Out )
    INTEGER :: some_actual_function_5_DDDD
   TYPE(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
   REAL (Kind(0D0)), INTENT(IN) :: X1_In(*), X2_In(*)
    REAL (Kind(0D0)), INTENT(OUT) :: Y1_Out(*), Y2_Out(*)
 END FUNCTION some_actual_function_5_DDDD
END INTERFACE DftiComputeBackward
```

The implementations of DFT interface expect the data be treated as data stored linearly in memory with a regular "stride" pattern (discussed more fully in <u>"Strides"</u>, see also [3]). The function expects the starting address of the first element. Hence we use the assume-size declaration in Fortran.

The descriptor by itself contains sufficient information to determine exactly how many arguments and of what type should be present. The implementation could use this information to check against possible input inconsistency.

# **Descriptor Configuration**

There are two functions in this category: the value setting function DftiSetValue sets one particular configuration parameter to an appropriate value, and the value getting function DftiGetValue reads the values of one particular configuration parameter. While all configuration parameters are readable, a few of them cannot be set by user. Some of these contain fixed information of a particular implementation such as version number, or dynamic information, but nevertheless are derived by the implementation during execution of one of the functions.

#### Table 9-3 Settable Configuration Parameters

Named Constants	Value Type	Comments	

#### Most common configurations, no default, must be set explicitly

DFTI_PRECISION	Named constant	Precision of computation
DFTI_FORWARD_DOMAIN	Named constant	Domain for the forward transform
DFTI_DIMENSION	Integer scalar	Dimension of the transform
DFTI_LENGTHS	Integer scalar/array	Lengths of each dimension

#### Common configurations including multiple transform and data representation

	•	-
DFTI_NUMBER_OF_TRANSFORMS	Integer scalar	For multiple number of transforms
DFTI_FORWARD_SIGN	Named constant	The definition for forward transform
DFTI_FORWARD_SCALE	Floating-point scalar	Scale factor for forward transform
DFTI_BACKWARD_SCALE	Floating-point scalar	Scale factor for backward transform
DFTI_PLACEMENT	Named constant	Placement of the computation result
DFTI_COMPLEX_STORAGE	Named constant	Storage method, complex domain data
DFTI_REAL_STORAGE	Named constant	Storage method, real domain data
DFTI_CONJUGATE_EVEN_STORAGE	Named constant	Storage method, conjugate even domain data
DFTI_DESCRIPTOR_NAME	Character string	No longer than DFTI_MAX_NAME_LENGTH
DFTI_PACKED_FORMAT	Named constant	Packed format, real domain data

Named Constants	Value Type	Comments
Configurations regarding stride of c	lata	
DFTI_INPUT_DISTANCE	Integer scalar	Multiple transforms, distance of first elements
DFTI_OUTPUT_DISTANCE	Integer scalar	Multiple transforms, distance of first elements
DFTI_INPUT_STRIDES	Integer array	Stride information of input data
DFTI_OUTPUT_STRIDES	Integer array	Stride information of output data
Advanced configuration		
DFTI_INITIALIZATION_EFFORT	Named constant	Dynamic search for computation method
DFTI_ORDERING	Named constant	Scrambling of data order
DFTI_WORKSPACE	Named constant	Computation without auxiliary storage
DFTI_TRANSPOSE	Named constant	Scrambling of dimension

#### Table 9-3 Settable Configuration Parameters (continued)

Each of these configuration parameters is identified by a named constant in the MKL_DFTI module. In C, these named constants have the enumeration type DFTI_CONFIG_PARAM. The list of configuration parameters whose values can be set by user is given in <u>Table 9-3</u>; the list of configuration parameters that are read-only is given in <u>Table 9-4</u>. All parameters are readable. Most of these parameters are self-explanatory, while some others are discussed more fully in the description of the relevant functions.

# Table 9-4 Read-Only Configuration Parameters

Named Constants	Value Type	Comments
DFTI_COMMIT_STATUS	Name constant	Whether descriptor has been committed
DFTI_VERSION	String	Intel MKL library version number
DFTI_FORWARD_ORDERING	Integer pointer	Pointer to an integer array (see <u>"Ordering"</u> )
DFTI_BACKWARD_ORDERING	Integer pointer	Pointer to an integer array (see <u>"Ordering"</u> )

The configuration parameters are set by various values. Some of these values are specified by native data types such as an integer value (for example, number of simultaneous transforms requested), or a single-precision number (for example, the scale factor one would like to apply on a forward transform).

Other configuration values are discrete in nature (for example, the domain of the forward transform) and are thus provided in the DFTI module as named constants. In C, these named constants have the enumeration type DFTI_CONFIG_VALUE. The complete list of named constants used for this kind of configuration values is given in <u>Table 9-5</u>.

#### Table 9-5 Named Constant Configuration Values

Named Constant	Comments
DFTI_SINGLE	Single precision
DFTI_DOUBLE	Double precision
DFTI_COMPLEX	Complex domain
DFTI_REAL	Real domain
DFTI_CONJUGATE_EVEN	Conjugate even domain
DFTI_NEGATIVE	Sign used to define the forward transform
DFTI_POSITIVE	Sign used to define the forward transform
DFTI_INPLACE	Output overwrites input
DFTI_NOT_INPLACE	Output does not overwrite input
DFTI_COMPLEX_COMPLEX	Storage method (see <u>"Storage schemes"</u> )
DFTI_REAL_REAL	Storage method (see <u>"Storage schemes"</u> )
DFTI_COMPLEX_REAL	Storage method (see <u>"Storage schemes"</u> )
DFTI_REAL_COMPLEX	Storage method (see <u>"Storage schemes"</u> )
DFTI_HIGH	A high setting, related to initialization effort
DFTI_MEDIUM	A medium setting, related to initialization effort
DFTI_LOW	A low setting, related to initialization effort
DFTI_COMMITTED	Committal status of a descriptor
DFTI_UNCOMMITTED	Committal status of a descriptor
DFTI_ORDERED	Data ordered in both forward and backward domains
DFTI_BACKWARD_SCRAMBLED	Data scrambled in backward domain (by forward transform)

Named Constant	Comments
DFTI_FORWARD_SCRAMBLED	Data scrambled in forward domain (by backward transform)
DFTI_ALLOW	Allow certain request or usage if useful
DFTI_AVOID	Avoid certain request or usage if practical
DFTI_NONE	Used to specify no transposition
DFTI_CCS_FORMAT	Packed format, real data (see <u>"Packed formats"</u> )
DFTI_PACK_FORMAT	Packed format, real data (see <u>"Packed formats"</u> )
DFTI_PERM_FORMAT	Packed format, real data (see <u>"Packed formats"</u> )
DFTI_VERSION_LENGTH	Number of characters for library version length
DFTI_MAX_NAME_LENGTH	Maximum descriptor name length
DFTI_MAX_MESSAGE_LENGTH	Maximum status message length

# Table 9-5 Named Constant Configuration Values (continued)

<u>Table 9-6</u> lists the possible values for those configuration parameters that are discrete in nature.

Named Constant	Possible Values
DFTI_PRECISION	DFTI_SINGLE, or
	DFTI_DOUBLE (no default)
DFTI_FORWARD_DOMAIN	DFTI_COMPLEX, or
	DFTI_REAL, or
	DFTI_CONJUGATE_EVEN (no default)
DFTI_FORWARD_SIGN	DFTI_NEGATIVE (default), or
	DFTI_POSITIVE
DFTI_PLACEMENT	DFTI_INPLACE (default), or
	DFTI_NOT_INPLACE
DFTI_COMPLEX_STORAGE	DFTI_COMPLEX_COMPLEX (default), or
	DFTI_COMPLEX REAL, or
	DFTI_REAL_REAL
DFTI_REAL_STORAGE	DFTI_REAL_REAL (default), or
	DFTI_REAL_COMPLEX
DFTI_CONJUGATE_EVEN_STORAGE	DFTI_COMPLEX_COMPLEX, or

# Table 9-6 Settings for Discrete Configuration Parameters

Named Constant	Possible Values
	DFTI_COMPLEX_REAL (default), or
	DFTI_REAL_REAL (1-D transform only)
DFTI_PACKED_FORMAT	DFTI_CCS_FORMAT (default) or,
	DFTI_PACK_FORMAT or,
	DFTI_PERM_FORMAT

# Table 9-6 Settings for Discrete Configuration Parameters (continued)

Table 9-7 lists the default values of the settable configuration parameters.

# Table 9-7 Default Configuration Values of Settable Parameters

Named Constants	Default Value
DFTI_NUMBER_OF_TRANSFORMS	1
DFTI_FORWARD_SIGN	DFTI_NEGATIVE
DFTI_FORWARD_SCALE	1.0
DFTI_BACKWARD_SCALE	1.0
DFTI_PLACEMENT	DFTI_INPLACE
DFTI_COMPLEX_STORAGE	DFTI_COMPLEX_COMPLEX
DFTI_REAL_STORAGE	DFTI_REAL_REAL
DFTI_CONJUGATE_EVEN_STORAGE	DFTI_COMPLEX_REAL
DFTI_PACKED_FORMAT	DFTI_CCS_FORMAT
DFTI_DESCRIPTOR_NAME	no name, string of zero length
DFTI_INPUT_DISTANCE	0
DFTI_OUTPUT_DISTANCE	0
DFTI_INPUT_STRIDES	Tightly packed according to dimension, lengths, and storage
DFTI_OUTPUT_STRIDES	Same as above. See <u>"Strides"</u> for details
DFTI_INITIALIZATION_EFFORT	DFTI_MEDIUM
DFTI_ORDERING	DFTI_ORDERED
DFTI_WORKSPACE	DFTI_ALLOW
DFTI_TRANSPOSE	DFTI_NONE

# **SetValue**

Sets one particular configuration parameter with the specified configuration value.

## Usage

## **Discussion**

This function sets one particular configuration parameter with the specified configuration value. The configuration parameter is one of the named constants listed in <u>Table 9-3</u>, and the configuration value is the corresponding appropriate type, which can be a named constant or a native type. See <u>"Configuration Settings"</u> for details of the meaning of the setting.

The function returns DFTI_NO_ERROR when completes successfully. See <u>"Status Checking Functions"</u> for more information on returned status.

# Interface and prototype

- ! Fortran interface
- INTERFACE DftiSetValue

//Note that the body provided here is to illustrate the different
//argument list and types of dummy arguments. The interface
//does not guarantee what the actual function names are.

//Users can only rely on the function name following the

```
//keyword INTERFACE
 FUNCTION some actual function 6 INTVAL( Desc Handle, Config Param,
INTVAL )
   INTEGER :: some_actual_function_6_INTVAL
   Type(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
   INTEGER, INTENT(IN) :: Config Param
   INTEGER, INTENT(IN) :: INTVAL
 END FUNCTION some_actual_function_6_INTVAL
 FUNCTION some_actual_function_6_SGLVAL( Desc_Handle, Config_Param,
SGLVAL )
   INTEGER :: some actual function 6 SGLVAL
   Type(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
   INTEGER, INTENT(IN) :: Config_Param
   REAL, INTENT(IN) :: SGLVAL
 END FUNCTION some actual function 6 SGLVAL
 FUNCTION some_actual_function_6_DBLVAL( Desc_Handle, Config_Param,
DBLVAL )
   INTEGER :: some_actual_function_6_DBLVAL
   Type(DFTI DESCRIPTOR), POINTER :: Desc Handle
   INTEGER, INTENT(IN) :: Config_Param
   REAL (KIND(0D0)), INTENT(IN) :: DBLVAL
 END FUNCTION some_actual_function_6_DBLVAL
 FUNCTION some actual function 6 INTVEC( Desc Handle, Config Param,
INTVEC )
   INTEGER :: some actual function 6 INTVEC
   Type(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
   INTEGER, INTENT(IN) :: Config_Param
   INTEGER, INTENT(IN) :: INTVEC(*)
 END FUNCTION some actual function 6 INTVEC
 FUNCTION some_actual_function_6_CHARS( Desc_Handle, Config_Param,
CHARS )
   INTEGER :: some actual function 6 CHARS
   Type(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
```

```
INTEGER, INTENT(IN) :: Config_Param
CHARCTER(*), INTENT(IN) :: CHARS
END FUNCTION some_actual_function_6_CHARS
END INTERFACE DftiSetValue
```

# **GetValue**

*Gets the configuration value of one particular configuration parameter.* 

## Usage

#### **Discussion**

This function gets the configuration value of one particular configuration parameter. The configuration parameter is one of the named constants listed in <u>Table 9-3</u> and <u>Table 9-4</u>, and the configuration value is the corresponding appropriate type, which can be a named constant or a native type.

The function returns DFTI_NO_ERROR when completes successfully. See <u>"Status Checking Functions"</u> for more information on returned status.

#### Interface and prototype

```
! Fortran interface
INTERFACE DftiGetValue
//Note that the body provided here is to illustrate the different
//argument list and types of dummy arguments. The interface
//does not guarantee what the actual function names are.
//Users can only rely on the function name following the
//keyword INTERFACE
 FUNCTION some_actual_function_7_INTVAL( Desc_Handle, Config_Param,
INTVAL )
    INTEGER :: some_actual_function_7_INTVAL
    Type(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
    INTEGER, INTENT(IN) :: Config_Param
    INTEGER, INTENT(OUT) :: INTVAL
 END FUNCTION DFTI_GET_VALUE_INTVAL
 FUNCTION some actual function 7 SGLVAL( Desc Handle, Config Param,
SGLVAL )
    INTEGER :: some_actual_function_7_SGLVAL
    Type(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
    INTEGER, INTENT(IN) :: Config_Param
    REAL, INTENT(OUT) :: SGLVAL
 END FUNCTION some_actual_function_7_SGLVAL
 FUNCTION some_actual_function_7_DBLVAL( Desc_Handle, Config_Param,
DBLVAL )
    INTEGER :: some_actual_function_7_DBLVAL
    Type(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
    INTEGER, INTENT(IN) :: Config_Param
    REAL (KIND(0D0)), INTENT(OUT) :: DBLVAL
 END FUNCTION some actual function 7 DBLVAL
 FUNCTION some_actual_function_7_INTVEC( Desc_Handle, Config_Param,
INTVEC )
    INTEGER :: some_actual_function_7_INTVEC
    Type(DFTI DESCRIPTOR), POINTER :: Desc Handle
    INTEGER, INTENT(IN) :: Config_Param
```

```
INTEGER, INTENT(OUT) :: INTVEC(*)
 END FUNCTION some actual function 7 INTVEC
 FUNCTION some_actual_function_7_INTPNT( Desc_Handle, Config_Param,
INTPNT )
    INTEGER :: some_actual_function_7_INTPNT
   Type(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
    INTEGER, INTENT(IN) :: Config_Param
    INTEGER, DIMENSION(*), POINTER :: INTPNT
 END FUNCTION some_actual_function_7_INTPNT
 FUNCTION some_actual_function_7_CHARS( Desc_Handle, Config_Param,
CHARS )
    INTEGER :: some_actual_function_7_CHARS
   Type(DFTI_DESCRIPTOR), POINTER :: Desc_Handle
   INTEGER, INTENT(IN) :: Config_Param
    CHARCTER(*), INTENT(OUT):: CHARS
 END FUNCTION some_actual_function_7_CHARS
END INTERFACE DftiGetValue
/* C prototype */
long DftiGetValue( DFTI_DESCRIPTOR_HANDLE,
                   DFTI CONFIG PARAM ,
                    ...);
```

# **Configuration Settings**

#### **Precision of transform**

The configuration parameter DFTI_PRECISION denotes the floating-point precision in which the transform is to be carried out. A setting of DFTI_SINGLE stands for single precision, and a setting of DFTI_DOUBLE stands for double precision. The data is meant to be presented in this precision; the computation will be carried out in this precision; and the result will be delivered in this precision. This is one of the four settable configuration parameters that do not have default values. The user must set them explicitly, most conveniently at the call to descriptor creation function DftiCreateDescriptor.

# Forward domain of transform

The general form of the discrete Fourier transform is

$$z_{k_{1}, k_{2}, \dots, k_{d}} = \sigma \times \sum_{j_{d}=0}^{n_{d}-1} \sum_{j_{2}=0}^{n_{1}-1} \sum_{j_{1}=0}^{n_{1}-1} w_{j_{1}, j_{2}, \dots, j_{d}} \exp\left(\delta i 2\pi \sum_{l=1}^{d} j_{l} k_{l} / n_{l}\right)$$
(7.1)

for  $k_1 = 0, \pm 1, \pm 2, ...,$  where  $\sigma$  is an arbitrary real-valued scale factor and  $\delta = \pm 1$ . By default, the forward transform is defined by  $\sigma = 1$  and  $\delta = -1$ . In most common situations, the domain of the forward transform, that is, the set where the input (periodic) sequence  $\{w_{j_1}, j_2, ..., j_d\}$  belongs, can be either the set of complex-valued sequences, real-valued sequences, and complex-valued conjugate even sequences. The configuration parameter DFTI_FORWARD_DOMAIN indicates the domain for the forward transform. Note that this implicitly specifies the domain for the backward transform because of mathematical property of the DFT. See Table 9-8 for details.

# Table 9-8 Correspondence of Forward and Backward Domain

Forw	ard Domain	Implied Backward Domain
Complex	(DFTI_COMPLEX)	Complex
Real	(DFTI_REAL)	Conjugate Even
Conjugate Even	(DFTI_CONJUGATE_EVEN)	Real

On transforms in the real domain, some software packages only offer one "real-to-complex" transform. This in essence omits the conjugate even domain for the forward transform. The forward domain configuration parameter DFTI_FORWARD_DOMAIN is the second of four configuration parameters without default value.

# **Transform dimension and lengths**

The dimension of the transform is a positive integer value represented in an integer scalar of type Integer. For one-dimensional transform, the transform length is specified by a positive integer value represented in an integer scalar of type Integer. For multi-dimensional ( $\geq 2$ ) transform, the

lengths of each of the dimension is supplied in an integer array. DFTI_DIMENSION and DFTI_LENGTHS are the remaining two of four configuration parameters without default.

As mentioned, these four configuration parameters do not have default value. They are most conveniently set at the descriptor creation function. For dimension and length configuration, they can only be set in the descriptor creation function, and not by the function DftiSetValue. The other two configuration values can be changed through the function DftiSetValue, although this is not deemed common.



**CAUTION.** Changing the dimension and length would likely render the stride value inappropriate. Unless certain of otherwise, the user is advised to reconfigure the stride (see <u>"Strides"</u>).

# Number of transforms

In some situations, the user may need to perform a number of DFT transforms of the same dimension and lengths. The most common situation would be to transform a number of one-dimensional data of the same length. This parameter has the default value of 1, and can be set to positive integer value by an **Integer** data type in Fortran and **long** data type in C. Data sets have no common elements. The distance parameter is obligatory if multiple number is more than one.

# Sign and scale

The general form of the discrete Fourier transform is given by (7.1), for  $k_1 = 0, \pm 1, \pm 2, ...$ , where  $\sigma$  is an arbitrary real-valued scale factor and  $\delta = \pm 1$ . By default, the forward transform is defined by  $\sigma = 1$  and  $\delta = -1$ , and the backward transform is defined by  $\sigma = 1$  and  $\delta = 1$ . The user can change the definition of forward transform via setting the sign  $\delta$  to be DFTI_NEGATIVE (default) or DFTI_POSITIVE. The sign of the backward transform is implicitly defined to be the negative of the sign for the forward transform.

The forward transform and backward transform are each associated with a scale factor  $\sigma$  of its own with default value of 1. The user can set one or both of them via the two configuration parameters DFTI_FORWARD_SCALE and DFTI_BACKWARD_SCALE. For example, for a one-dimensional transform of length *n*, one can use the default scale of 1 for the forward transform while setting the scale factor for backward transform to be 1/n, making the backward transform the inverse of the forward transform.

The scale factor configuration parameter should be set by a real floating-point data type of the same precision as the value for DFTI_PRECISION.



**NOTE.** The sign configuration is not supported. The forward transform is defined as  $\delta = -1$ .

# **Placement of result**

By default, the computational functions overwrite the input data with the output result. That is, the default setting of the configuration parameter DFTI_PLACEMENT is DFTI_INPLACE. The user can change that by setting it to DFTI_NOT_INPLACE.

# **Packed formats**

The result of the forward transform (i.e. in the frequency-domain) of real data is represented in several possible packed formats: *Pack*, *Perm*, or *CCS*. The data can be packed due to the symmetry property of the DFT transform of a real data.

The *ccs* format stores the values of the first half of the output complex signal resulted from the forward DFT. Note that the signal stored in CCS format is one complex element longer. In CCS format, the output samples of the DFT are arranged as shown in <u>Table 9-9</u>.

The **Pack** format is a compact representation of a complex conjugate-symmetric sequence. The disadvantage of this format is that it is not the natural format used by the real DFT algorithms ("natural" in the sense that array is natural for complex DFTs). In Pack format, the output samples of the DFT are arranged as shown in <u>Table 9-9</u>.

The **Perm** format is an arbitrary permutation of the Pack format for even lengths and one is the same as the Pack format for odd lengths. In Perm format, the output samples of the DFT are arranged as shown in <u>Table 9-9</u>.

For (N	= S*2)										
DFT Re	al	0	1	2	3		N-2	N-1	Ν	N	+1
		0	1					(2S-1)	2S	(2	2S+1)
CCS		R ₀	0	R ₁	I ₁		R _{N/2-1}	I _{N/2-1}	R _{N/2}	2 0	
Pack		R ₀	R ₁	l ₁	$R_2$		I _{N/2-1}	R _{N/2}			
Perm		R ₀	R _{n/2}	R ₁	I ₁		R _{N/2-1}	I _{N/2-1}			
For (N DFT		-									
Pool	<b>N</b>	- 1	2	2		NL-4	NL2	NL-2	N_1	N	N. 1
Real	0	1	2	3		N-4	N-3	N-2	N-1 25	N (25±1)	N+1
	0	1							2S	(2S+1)	
Real CCS Pack			2 R ₁ I ₁	3   ₁   ₂	••• •••	N-4 I _{S_2} R _{S-1}	<b>N-3</b> R _{S-1} I _{S_1}	N-2 I _{S_1} R _{S-1}			

# Table 9-9 Packed Format Output Samples

See also Table 9-10 and Table 9-11.

# **Storage schemes**

For each of the three domains DFTI_COMPLEX, DFTI_REAL, and DFTI_CONJUGATE_EVEN (for the forward as well as the backward operator), a subset of the four storage schemes DFTI_COMPLEX_COMPLEX, DFTI_COMPLEX_REAL, DFTI_REAL_COMPLEX, and DFTI_REAL_REAL. Specific examples are presented here to illustrate the storage schemes. See the document [3] for the rationale behind this definition of the storage schemes.



**NOTE.** *The data is stored in the Fortran style only, that is, the real and imaginary parts are stored side by side.* 

## Storage scheme for complex domain

This setting is recorded in the configuration parameter DFTI_COMPLEX_STORAGE. The three values that can be set are DFTI_COMPLEX_COMPLEX, DFTI_COMPLEX_REAL, and DFTI_REAL_REAL. Consider a one-dimensional *n*-length transform of the form

$$z_{k} = \sum_{j=0}^{n-1} w_{j} e^{-i2\pi j k/n}, \qquad w_{j}, \ z_{k} \in \mathbb{C}.$$

Assume the stride has default value (unit stride) and DFTI_PLACEMENT has the default in-place setting.

**1. DFTI_COMPLEX_COMPLEX storage scheme.** A typical usage will be as follows.

```
COMPLEX :: X(0:n-1)
...some other code...
Status = DftiComputeForward( Desc_Handle, X )
O :
```

On input,

 $X(j) = w_{j}, j = 0, 1, ..., n-1$ .

On output,

 $X(k) = z_k, k = 0, 1, ..., n-1$ .

**2. DFTI_COMPLEX_REAL storage scheme**. A typical usage will be as follows.

```
REAL :: X(0:2*n-1)
...some other code...
Status = DftiComputeForward( Desc_Handle, X )
On input,
```

 $X(2*j) = \operatorname{Re}(w_j), X(2*j+1) = \operatorname{Im}(w_j), j = 0,1,...,n-1$ .

On output,

 $X(2*k) = \operatorname{Re}(z_k), X(2*k+1) = \operatorname{Im}(z_k), k = 0, 1, \dots, n-1$ .

The notations  $\operatorname{Re}(w_j)$  and  $\operatorname{Im}(w_j)$  are the real and imaginary parts of the complex number  $w_j$ .

3. DFTI_REAL_REAL storage scheme. A typical usage will be as follows.
REAL :: X(0:n-1), Y(0:n-1)
...some other code...
Status = DftiComputeForward( Desc_Handle, X, Y )

On input,

$$\mathbf{X}(j) = \operatorname{Re}(w_{j}), \mathbf{Y}(j) = \operatorname{Im}(w_{j}), j = 0, 1, ..., n-1$$

On output,

 $\mathbf{X}(k) = \operatorname{Re}(z_k), \mathbf{Y}(k) = \operatorname{Im}(z_k), k = 0, 1, ..., n-1$ .

#### Storage scheme for the real and conjugate even domains

This setting for the storage schemes for these domains are recorded in the configuration parameters DFTI_REAL_STORAGE and DFTI_CONJUGATE_EVEN. Since a forward real domain corresponds to a conjugate even backward domain, they are considered together. The example uses a one-dimensional real to conjugate even transform. In-place computation is assumed whenever possible (that is, when the input data type matches with the output data type).

Consider a one-dimensional *n*-length transform of the form

$$z_{k} = \sum_{j=0}^{n-1} w_{j} e^{-i2\pi jk/n} , \qquad w_{j} \in \mathbf{R}, \ z_{k} \in \mathbf{C}.$$

There is a symmetry:

For even n: z(n/2+i) = conjg(z(n/2-i)),  $1 \le i \le n/2 - 1$ , and moreover z(0) and z(n/2) are real values.

For odd n:  $z(m+i) = conjg(z(m-i+1)), 1 \le i \le m$ , and moreover z(0) is real value.

_

m = floor(n/2).

# Table 9-10Comparison of the Storage Effects of Complex-to-Complex and<br/>Real-to-Complex DFTs for Forward Transform

N=8							
	Input Vectors			Output V	/ectors		
Com	olex DFT	Real DFT	comp	lex DFT	real	DFT	
Com	plex Data	Real Data	Com	plex Data	Real D	ata	
Real	Imaginary		Real	Imaginary	CCS	Pack	Perm
w0	0.000000	w0	z0	0.000000	z0	z0	z0
w1	0.000000	w1	Re(z1)	lm(z1)	0.000000	Re(z1)	z4
w2	0.000000	w2	Re(z2)	lm(z2)	Re(z1)	lm(z1)	Re(z1)
w3	0.000000	w3	Re(z3)	lm(z3)	lm(z1)	Re(z2)	lm(z1)
w4	0.000000	w4	z4	0.000000	Re(z2)	lm(z2)	Re(z2)
w5	0.000000	w5	Re(z3)	-Im(z3)	lm(z2)	Re(z3)	lm(z2)
w6	0.000000	w6	Re(z2)	-Im(z2)	Re(z3)	lm(z3)	Re(z3)
w7	0.000000	w7	Re(z1)	-lm(z1)	lm(z3)	z4	lm(z3)
					z4		
					0.000000		

#### N=7

	Input Vectors			Output	Vectors		
Comp	lex DFT	Real DFT	comp	lex DFT	:	real DFT	
Com	plex Data	Real Data	Com	plex Data	I	Real Data	
Real	Imaginary		Real	Imaginary	CCS	Pack	Perm
w0	0.000000	w0	z0	0.000000	z0	z0	z0
w1	0.000000	w1	Re(z1)	lm(z1)	0.000000	Re(z1)	Re(z1)
w2	0.000000	w2	Re(z2)	lm(z2)	Re(z1)	lm(z1)	lm(z1)

	Input Vectors			Output V	ectors		
Com	plex DFT	Real DFT	comp	lex DFT		real DFT	
Com	plex Data	Real Data	Com	plex Data		Real Data	
Real	Imaginary		Real	Imaginary	CCS	Pack	Perm
w3	0.000000	w3	Re(z3)	lm(z3)	lm(z1)	Re(z2)	Re(z2)
w4	0.000000	w4	Re(z3)	-lm(z3)	Re(z2)	lm(z2)	lm(z2)
w5	0.000000	w5	Re(z2)	-lm(z2)	lm(z2)	Re(z3)	Re(z3)
w6	0.000000	w6	Re(z1)	-lm(z1)	Re(z3)	lm(z3)	lm(z3)
					lm(z3)		

# N=7

# Table 9-11Comparison of the Storage Effects of Complex-to-Complex and<br/>Complex-to-Real DFTs for Backward Transform

#### N=8

C	<b>Dutput Vectors</b>	3		Input V	ectors		
Com	plex DFT	Real DFT Real Data	-	lex DFT plex Data			
Real	Imaginary		Real	Imaginary	ccs	Pack	Perm
w0	0.000000	w0	z0	0.000000	z0	z0	z0
w1	0.000000	w1	Re(z1)	lm(z1)	0.000000	Re(z1)	z4
w2	0.000000	w2	Re(z2)	lm(z2)	Re(z1)	lm(z1)	Re(z1)
w3	0.000000	w3	Re(z3)	lm(z3)	lm(z1)	Re(z2)	lm(z1)
w4	0.000000	w4	z4		Re(z2)	lm(z2)	Re(z2)
w5	0.000000	w5	Re(z3)	-lm(z3)	lm(z2)	Re(z3)	lm(z2)
w6	0.000000	w6	Re(z2)	-lm(z2)	Re(z3)	lm(z3)	Re(z3)
w7	0.00000	w7	Re(z1)	-lm(z1)	lm(z3)	z4	lm(z3)
					z4		
					0.000000		

## N=7

C	Output Vectors	5		Input V	ectors		
Comp	lex DFT	Real DFT	comp	lex DFT	r	eal DFT	
Com	plex Data	Real Data	Com	olex Data	I	Real Data	
Real	Imaginary		Real	Imaginary	CCS	Pack	Perm
w0	0.000000	w0	z0	0.000000	z0	z0	z0
w1	0.000000	w1	Re(z1)	lm(z1)	0.000000	Re(z1)	Re(z1)
w2	0.000000	w2	Re(z2)	lm(z2)	Re(z1)	lm(z1)	lm(z1)
w3	0.000000	w3	Re(z3)	lm(z3)	lm(z1)	Re(z2)	Re(z2)
w4	0.000000	w4	Re(z3)	-Im(z3)	Re(z2)	lm(z2)	lm(z2)
w5	0.000000	w5	Re(z2)	-Im(z2)	lm(z2)	Re(z3)	Re(z3)

C	Output Vectors	5		Input Ve	ectors		
Com	plex DFT	Real DFT	comp	lex DFT	:	real DFT	
		Real					
Com	plex Data	Data	Com	plex Data		Real Data	
Real	Imaginary		Real	Imaginary	CCS	Pack	Perm
w6	0.000000	w6	Re(z1)	-lm(z1)	Re(z3)	lm(z3)	lm(z3)
					lm(z3)		

Assume that the stride has the default value (unit stride).

This complex conjugate-symmetric vector can be stored in the complex array of size m+1 or in the real array of size 2m+2 Or 2m depending on packed format.

1. DFTI_REAL_REAL for real domain, DFTI_COMPLEX_COMPLEX for conjugate even domain. A typical usage will be as follows.

```
//m = floor(n/2)
REAL :: X(0:n-1)
COMPLEX :: Y(0:m)
...some other code...
... out of place transform ...
Status = DftiComputeForward( Desc_Handle, X, Y )
```

On input,

 $X(j) = w_{j}, j = 0, 1, ..., n-1$ .

On output,

 $Y(k) = z_k, k = 0, 1, ..., m$ .

2. DFTI_REAL_REAL for real domain, DFTI_COMPLEX_REAL for conjugate even domain. A typical usage will be as follows.

```
//m = floor(n/2)
REAL :: X(0:2*m+1)
...some other code...
...assuming inplace...
Status = DftiComputeForward( Desc_Handle, X )
```

.. _

On input,

 $X(j) = w_{j}, j = 0, 1, ..., n-1$ .

On output,

Output data stored in one of formats: Pack, Perm or CCS (see <u>"Packed formats"</u>).

CCS format:  $x(2*k) = \text{Re}(z_k)$ ,  $x(2*k+1) = \text{Im}(z_k)$ , k = 0, 1, ..., m.

Pack format: even n:  $\mathbf{x}(0) = \operatorname{Re}(z_0)$ ,  $\mathbf{x}(2*k-1) = \operatorname{Re}(z_k)$ ,  $\mathbf{x}(2*k) = \operatorname{Im}(z_k)$ , k = 1,...,m-1, and  $\mathbf{x}(n-1) = \operatorname{Re}(z_m)$ 

odd n:  $\mathbf{x}(0) = \operatorname{Re}(z_0), \ \mathbf{x}(2^{*}k-1) = \operatorname{Re}(z_k), \ \mathbf{x}(2^{*}k) = \operatorname{Im}(z_k), \ k = 1,...,m$ 

Perm format: even n:  $\mathbf{x}(0) = \text{Re}(z_0)$ ,  $\mathbf{x}(1) = \text{Re}(z_m)$ ,  $\mathbf{x}(2^*k) = \text{Re}(z_k)$ ,  $\mathbf{x}(2^*k+1) = \text{Im}(z_k)$ , k = 1,...,m-1,

odd n:  $x(0) = \text{Re}(z_0), x(2*k-1) = \text{Re}(z_k), x(2*k) = \text{Im}(z_k), k = 1,...,m.$ 

3. DFTI_REAL_REAL for real domain, DFTI_REAL_REAL for conjugate even domain. This storage scheme for conjugate even domain is applicable for one-dimensional transform only. A typical usage will be as follows.

```
// m = floor( n/2 )
REAL :: X(0:n-1)
...some other code...
...assuming inplace...
Status = DftiComputeForward( Desc_Handle, X )
On input,
X(j) = w<sub>j</sub>, j = 0,1,...,n-1.
On output,
```

 $\mathbf{X}(k) = \operatorname{Re}(z_k), k = 0, 1, ..., \mathbf{m}.$ 

and

 $X(n-k) = \text{Im}(z_k), k = 1, 2, ..., m-1.$ 

**4. DFTI_REAL_COMPLEX for real domain, DFTI_COMPLEX_COMPLEX for conjugate even domain.** A typical usage will be as follows.

```
// m = floor( n/2 )
COMPLEX :: X(0:n-1)
...some other code...
...inplace transform...
```

```
Status = DftiComputeForward( Desc_Handle, X )
```

On input,

 $X(j) = w_{j}, j = 0, 1, ..., n-1$ .

That is, the imaginary parts of  $\mathbf{X}(j)$  are zero. On output,

 $Y(k) = z_k, k = 0, 1, ..., m$ .

where m is  $\lfloor n/2 \rfloor$ .

**5. DFTI_REAL_COMPLEX for real domain, DFTI_COMPLEX_REAL for conjugate even domain.** A typical usage will be as follows.

```
// m = floor( n/2 )
COMPLEX :: X(0:n-1)
REAL :: Y(0:2*m+1)
...some other code...
...not inplace...
Status = DftiComputeForward( Desc_Handle, X, Y )
Optimize
```

On input,

 $X(j) = w_{j}, j = 0, 1, ..., n-1$ .

On output,

Output data stored in one of formats: Pack, Perm or CCS (see <u>"Packed formats"</u>).

CCS format:  $\mathbf{Y}(2^*k) = \operatorname{Re}(z_k)$ ,  $\mathbf{Y}(2^*k+1) = \operatorname{Im}(z_k)$ , k = 0,1,...,m. Pack format: even n:  $\mathbf{Y}(0) = \operatorname{Re}(z_0)$ ,  $\mathbf{Y}(2^*k-1) = \operatorname{Re}(z_k)$ ,  $\mathbf{Y}(2^*k) = \operatorname{Im}(z_k)$ , k = 1,...,m-1, and  $\mathbf{Y}(n-1) = \operatorname{Re}(z_m)$ odd n:  $\mathbf{Y}(0) = \operatorname{Re}(z_0)$ ,  $\mathbf{Y}(2^*k-1) = \operatorname{Re}(z_k)$ ,  $\mathbf{Y}(2^*k) = \operatorname{Im}(z_k)$ , k = 1,...,mPerm format: even n:  $\mathbf{Y}(0) = \operatorname{Re}(z_0)$ ,  $\mathbf{Y}(1) = \operatorname{Re}(z_m)$ ,  $\mathbf{Y}(2^*k) = \operatorname{Re}(z_k)$ , ,  $\mathbf{Y}(2^*k+1) = \operatorname{Im}(z_k)$ , k = 1,...,m-1, odd n:  $\mathbf{Y}(0) = \operatorname{Re}(z_0)$ ,  $\mathbf{Y}(2^*k-1) = \operatorname{Re}(z_k)$ ,  $\mathbf{Y}(2^*k) = \operatorname{Im}(z_k)$ , k = 1,...,m. **6.** DFTI_REAL_COMPLEX for real domain, DFTI_REAL_REAL for

**conjugate even domain.** This storage scheme for conjugate even domain is applicable for one-dimensional transform only. A typical usage will be as follows.

// m = floor( n/2 )
COMPLEX :: X(0:n-1)

```
REAL :: Y(0:n-1)
...some other code...
...not inplace...
Status = DftiComputeForward( Desc_Handle, X, Y )
On input,
X(j) = w_j, j = 0,1,...,n-1.
On output,
Y(k) = \operatorname{Re}(z_k), k = 0,1,...,m.
and
Y(n-k) = \operatorname{Im}(z_k), k = 1,2,...,m-1.
```

# Input and output distances

DFT interface in Intel MKL allows the computation of multiple number of transforms. Consequently, the user needs to be able to specify the data distribution of these multiple sets of data. This is accomplished by the distance between the first data element of the consecutive data sets. This parameter is obligatory if multiple number is more than one. Data sets don't have any common elements. The following example illustrates the specification. Consider computing the forward DFT on three 32-length complex sequences stored in X(0:31, 1), X(0:31, 2), and X(0:31, 3). Suppose the results are to be stored in the locations Y(0:31, k), k = 1, 2, 3, of the array Y(0:63, 3). Thus the input distance is 32, while the output distance is 64. Notice that the data and result parameters in computation functions are all declared as assumed-size rank-1 array DIMENSION(0:*). Therefore two-dimensional array must be transformed to one-dimensional array by EQUIVALENCE statement or other facilities of Fortran. Here is the code fragment:

```
Complex :: X_2D(0:31,3), Y_2D(0:63, 3)
Complex :: X(96), Y(192)
Equivalence (X_2D, X)
Equivalence (Y_2D, Y)
.....Status = DftiCreateDescriptor(Desc_Handle, DFTI_SINGLE,
DFTI_COMPLEX, 1, 32)
Status = DftiSetValue(Desc Handle, DFTI NUMBER OF TRANSFORM, 3)
```

```
Status = DftiSetValue(Desc_Handle, DFTI_INPUT_DISTANCE, 32)
Status = DftiSetValue(Desc_Handle, DFTI_OUTPUT_DISTANCE, 64)
Status = DftiSetValue(Desc_Handle, DFTI_PLACEMENT, DFTI_NOT_INPLACE)
Status = DftiCommitDescriptor(Desc_Handle)
Status = DftiComputeForward(Desc_Handle, X, Y)
Status = DftiFreeDescriptor(Desc Handle)
```

# **Strides**

In addition to supporting transforms of multiple number of datasets, DFT interface supports non-unit stride distribution of data within each data set. Consider the following situation where a 32-length DFT is to be computed on the sequence  $x_j$ ,  $0 \le j < 32$ . The actual location of these values are in X(5), X(7), ..., X(67) of an array X(1:68). The stride accommodated by DFT interface consists of a displacement from the first element of the data array  $L_0$ , (4 in this case), and a constant distance of consecutive elements  $L_1$  (2 in this case). Thus for the Fortran array X

 $x_i = \mathbf{x}(1 + L_0 + L_1 * j) = \mathbf{x}(5 + L_1 * j)$ .

This stride vector (4,2) is provided by a length-2 rank-1 integer array:

```
COMPLEX :: X(68)
INTEGER :: Stride(2)
. . . . . . . . . . . . . . . . . . . .
Status = DftiCreateDescriptor(Desc_Handle, DFTI_SINGLE,
                                       DFTI_COMPLEX, 1, 32)
Stride = (/ 4, 2 /)
Status = DftiSetValue(Desc_Handle, DFTI_INPUT_STRIDE, Stride)
Status = DftiSetValue(Desc_Handle, DFTI_OUTPUT_STRIDE, Stride)
Status = DftiCommitDescriptor(Desc_Handle)
Status = DftiComputeForward(Desc_Handle, X)
Status = DftiFreeDescriptor(Desc Handle)
              In general, for a d-dimensional transform, the stride is provided by a
              d +1-length integer vector (L_0, L_1, L_2, ..., L_d) with the meaning:
              L_0 = displacement from the first array element
              L_1 = distance between consecutive data elements in the first dimension
              L_2 = distance between consecutive data elements in the second dimension
```

... = ...

 $L_d$  = distance between consecutive data elements in the *d*-th dimension.

A d-dimensional data sequence

 $\mathbf{x}_{\mathbf{j}_1, \mathbf{j}_2, \dots, \mathbf{j}_d}, \quad 0 \leq j_i < J_i, \quad 1 \leq i \leq d$ 

will be stored in the rank-1 array  $\mathbf{x}$  by the mapping

$$\mathbf{x}_{j_1, j_2, \dots, j_d} = \mathbf{x}(\text{first index} + L_0 + j_1 L_1 + j_2 L_2 + \dots + j_d L_d)$$

For multiple transforms, the value  $L_0$  applies to the first data sequence, and  $L_i$ , j = 1, 2, ..., d apply to all the data sequences.

In the case of a single one-dimensional sequence,  $L_I$  is simply the usual stride. The default setting of strides in the general multi-dimensional situation corresponds to the case where the sequences are distributed tightly into the array:

$$L_1 = 1, L_2 = J_1, L_3 = J_1 J_2, ..., L_d = \prod_{i=1}^{J_i} J_i$$

Both the input data and output data have a stride associated with it. The default is set in accordance with the data to be stored contiguously in memory in a way that is natural to the language.

Finally, consider a contrived example where a 20-by-40 two-dimensional DFT is computed explicitly using one-dimensional transforms. Notice that the data and result parameters in computation functions are all declared as assumed-size rank-1 array DIMENSION(0:*). Therefore two-dimensional array must be transformed to one-dimensional array by EQUIVALENCE statement or other facilities of Fortran.

```
! Fortran
```

```
Complex :: X_2D(20,40),
Complex :: X(800)
Equivalence (X_2D, X)
INTEGER :: STRIDE(2)
type(DFTI_DESCRIPTOR), POINTER :: Desc_Handle_Dim1
type(DFTI_DESCRIPTOR), POINTER :: Desc_Handle_Dim2
...
Status = DftiCreateDescriptor( Desc_Handle_Dim1, DFTI_SINGLE,
DFTI_COMPLEX, 1, 20 )
```

```
Status = DftiCreateDescriptor( Desc Handle Dim2, DFTI SINGLE,
                                 DFTI COMPLEX, 1, 40)
! perform 40 one-dimensional transforms along 1st dimension
Status = DftiSetValue( Desc_Handle_Dim1, DFTI_NUMBER_OF_TRANSFORMS, 40 )
Status = DftiSetValue( Desc Handle Dim1, DFTI INPUT DISTANCE, 20 )
Status = DftiSetValue( Desc_Handle_Dim1, DFTI_OUTPUT_DISTANCE, 20 )
Status = DftiCommitDescriptor( Desc_Handle_Dim1 )
Status = DftiComputeForward( Desc_Handle_Dim1, X )
! perform 20 one-dimensional transforms along 2nd dimension
Stride(1) = 0; Stride(2) = 20
Status = DftiSetValue( Desc Handle Dim2, DFTI NUMBER OF TRANSFORMS, 20 )
Status = DftiSetValue( Desc Handle Dim2, DFTI INPUT DISTANCE, 1 )
Status = DftiSetValue( Desc Handle Dim2, DFTI OUTPUT DISTANCE, 1 )
Status = DftiSetValue( Desc Handle Dim2, DFTI INPUT STRIDES, Stride )
Status = DftiSetValue( Desc Handle Dim2, DFTI OUTPUT STRIDES, Stride )
Status = DftiCommitDescriptor( Desc Handle Dim2 )
Status = DftiComputeForward( Desc Handle Dim2, X )
Status = DftiFreeDescriptor( Desc_Handle_Dim1 )
Status = DftiFreeDescriptor( Desc Handle Dim2 )
/* C */
float _Complex x[20][40];
long stride[2];
DFTI_DESCRIPTOR_HANDLE Desc_Handle_Dim1;
DFTI_DESCRIPTOR_HANDLE Desc_Handle_Dim2;
status = DftiCreateDescriptor( &desc handle dim1, DFTI SINGLE,
                                 DFTI_COMPLEX, 1, 20 );
status = DftiCreateDescriptor( &desc_handle_dim2, DFTI_SINGLE,
                                 DFTI_COMPLEX, 1, 40 );
/* perform 40 one-dimensional transforms along 1st dimension */
/* note that the 1st dimension data are not unit-stride */
stride[0] = 0; stride[1] = 40;
status = DftiSetValue( desc handle dim1, DFTI NUMBER OF TRANSFORMS, 40 );
```

```
status = DftiSetValue( desc_handle_dim1, DFTI_INPUT_DISTANCE, 1 );
status = DftiSetValue( desc_handle_dim1, DFTI_OUTPUT_DISTANCE, 1 );
status = DftiSetValue( desc_handle_dim1, DFTI_INPUT_STRIDES, stride );
status = DftiSetValue( desc_handle_dim1, DFTI_OUTPUT_STRIDES, stride );
status = DftiCommitDescriptor( desc_handle_dim1 );
status = DftiComputeForward( desc_handle_dim1, x );
/* perform 20 one-dimensional transforms along 2nd dimension */
/* note that the 2nd dimension is unit stride */
status = DftiSetValue( desc_handle_dim2, DFTI_NUMBER_OF_TRANSFORMS, 20 );
status = DftiSetValue( desc_handle_dim2, DFTI_INPUT_DISTANCE, 40 );
status = DftiSetValue( desc_handle_dim2, DFTI_OUTPUT_DISTANCE, 40 );
status = DftiCommitDescriptor( desc_handle_dim2 );
status = DftiCommitDescriptor( desc_handle_dim2, x );
status = DftiFreeDescriptor( &Desc_Handle_Dim1 );
status = DftiFreeDescriptor( &Desc_Handle_Dim1 );
```

## **Initialization Effort**

In modern approaches to constructing fast algorithms (FFT) for DFT computations, one often has a flexibility of spending more effort in initializing (preparing for) an FFT algorithm to buy higher efficiency in the computation on actual data to follow. Advanced DFT functions in Intel MKL accommodate this situation through the configuration parameter DFTI_INITIALIZATION_EFFORT. The three configuration values are DFTI_LOW, DFTI_MEDIUM (default), and DFTI_HIGH. Note that specific implementations of DFT interface may or may not make use of this setting (see *MKL Release Notes* for implementation details).

# Ordering

It is well known that a number of FFT algorithms apply an explicit permutation stage that is time consuming [4]. The exclusion of this step is similar to applying DFT to input data whose order is scrambled, or allowing a scrambled order of the DFT results. In applications such as convolution and power spectrum calculation, the order of result or data is unimportant and thus permission of scrambled order is attractive if it leads to higher performance. Three following options are available in Intel MKL:

- 1. DFTI_ORDERED: Forward transform data ordered, backward transform data ordered (default option).
- 2. DFTI_BACKWARD_SCRAMBLED: Forward transform data ordered, backward transform data scrambled.
- 3. DFTI_FORWARD_SCRAMBLED: Forward transform data scrambled, backward transform data ordered.

Table 9-12 tabulates the effect on this configuration setting.

# Table 9-12 Scrambled Order Transform

	DftiComputeForward	DftiComputeBackward
DFTI_ORDERING	Input —Output	Input —Output
DFTI_ORDERED	ordered>ordered	ordered>ordered
DFTI_BACKWARD_SCRAMBLED	ordered>scrambled	scrambled $\rightarrow$ ordered
DFTI_FORWARD_SCRAMBLED	scrambled>ordered	ordered —scrambled

Note that meaning of the latter two options are "allow scrambled order if practical." There are situations where in fact allowing out of order data gives no performance advantage, and thus an implementation may choose to ignore the suggestion. Strictly speaking, the normal order is also a scrambled order, the trivial one.

When the ordering setting is other than the default DFTI_ORDERED, the user may need to know the actual ordering of the input and output data. The ordering of the data in the forward domain is obtained through reading (getting) the configuration parameter DFTI_FORWARD_ORDERING; and the ordering of the data in the reverse domain is obtained through reading (getting) the configuration parameter DFTI_BACKWARD_ORDERING. The configuration values are integer vectors, thus provided by pointer to any integer array. We now describe how these integer values specify the actual scrambling of data.

All scramblings involved are digit reversal along one single dimension. Precisely, a length *J* is factored into *K* ordered factors  $D_1, D_2, ..., D_K$ . Any index *i*,  $0 \le i < n$ , can be expressed uniquely as *K* digits  $i_1, i_2, ..., i_K$  where  $0 \le i_l < D_l$  and

 $i = i_1 + i_2 D_1 + i_3 D_1 D_2 + \dots + i_K D_1 D_2 \dots D_{K-1} .$ 

A digit reversal permutation scram(i) is given by

$$scram(i) = i_K + i_{K-1}D_K + i_{K-2}D_KD_{K-1} + \dots + i_1D_KD_{K-1} \dots D_2$$

Factoring *J* into one factor *J* leads to no scrambling at all, that is, scram(*i*) = *i*. Note that the factoring does not need to correspond exactly to the number of "butterfly" stages to be carried out. In fact, the computation routine in its initialization stage determines if a scrambled order in some or all of the dimensions can result in performance gain. The digits of the digit reversal are recorded and stored in the descriptor. These digits can be obtained by calling a corresponding inquiry routine that returns a pointer to an integer array. The first element is  $K^{(1)}$ , which is the number of digits for the first dimension, followed by  $K^{(1)}$  values of the corresponding digits. If the dimension is higher than one, the next integer value is  $K^{(2)}$ , etc.

Simple permutation such as mod-p sort [4] is a special case of digit reversal. Hence this option could be useful for high-performance implementation of one-dimensional DFT via a "six-step" or "four-step" framework [4].

The user can check the scrambling setting on the forward data and reverse data. This information is returned as an integer vector containing a number of sequence  $(K, D_1, D_2, ..., D_K)$ , one for each dimension. Thus the first element indicates how many *D*'s will follow. The inquiry routine allocates memory, fills it will this information, and returns a pointer to the memory location.

# Workspace

Some FFT algorithms do not require a scratch space for permutation purposes. The user can choose between the setting of DFTI_ALLOW (default) and DFTI_AVOID for the option DFTI_WORKSPACE. Note that the setting DFTI_AVOID is meant to be "avoid if practical," hence allowing the implementation the flexibility to use workspace regardless of the setting.

# **Transposition**

This is an option that allows for the result of a high-dimensional transform to be presented in a transposed manner. The default setting is DFTI_NONE and can be set to DFTI_ALLOW. Similar to that of scrambled order, sometimes in higher dimension transform, performance can be gained if the

result is delivered in a transposed manner. DFT interface offers an option for the output be returned in a transposed form if performance gain is possible. Since the generic stride specification is naturally suited for representation of transposition, this option allows the strides for the output to be possibly different from those originally specified by the user. Consider an example where a two-dimensional result  $\mathbf{y}_{j_1, j_2}$ ,  $0 \leq j_i < n_i$ , is expected. Originally the user specified that the result be distributed in the (flat) array  $\mathbf{y}$  in with generic strides  $L_1 = 1$  and  $L_2 = n_1$ . With the transposition option, the computation may actually return the result into  $\mathbf{y}$ with stride  $L_1 = n_2$  and  $L_2 = 1$ . These strides can be obtained from an appropriate inquiry function. Note also that in dimension 3 and above, transposition means an arbitrary permutation of the dimension.

# Routine and Function Arguments



The major arguments in the BLAS routines are vector and matrix, whereas VML functions work on vector arguments only. The sections that follow discuss each of these arguments and provide examples.

# **Vector Arguments in BLAS**

Vector arguments are passed in one-dimensional arrays. The array dimension (length) and vector increment are passed as integer variables. The length determines the number of elements in the vector. The increment (also called stride) determines the spacing between vector elements and the order of the elements in the array in which the vector is passed.

A vector of length n and increment *incx* is passed in a one-dimensional array x whose values are defined as

```
x(1), x(1+|incx|), ..., x(1+(n-1)*|incx|)
```

If *incx* is positive, then the elements in array x are stored in increasing order. If *incx* is negative, the elements in array x are stored in decreasing order with the first element defined as x(1+(n-1)*|incx|). If *incx* is zero, then all elements of the vector have the same value, x(1). The dimension of the one-dimensional array that stores the vector must always be at least

idimx = 1 + (n-1)* |incx|

# Example A-1 One-dimensional Real Array

Let $x(1:7)$ be the one-dimensional real array
x = (1.0, 3.0, 5.0, 7.0, 9.0, 11.0, 13.0).
If $incx = 2$ and $n = 3$ , then the vector argument with elements in order from first to last is $(1.0, 5.0, 9.0)$ .
If $incx = -2$ and $n = 4$ , then the vector elements in order from first
to last is (13.0, 9.0, 5.0, 1.0).
If $incx = 0$ and $n = 4$ , then the vector elements in order from first to
last is (1.0, 1.0, 1.0, 1.0).

One-dimensional substructures of a matrix, such as the rows, columns, and diagonals, can be passed as vector arguments with the starting address and increment specified. In Fortran, storing the m by n matrix is based on column-major ordering where the increment between elements in the same column is 1, the increment between elements in the same row is m, and the increment between elements on the same diagonal is m + 1.

# Example A-2 Two-dimensional Real Matrix

```
Let a be the real 5 x 4 matrix declared as REAL A (5,4).
To scale the third column of a by 2.0, use the BLAS routine sscal
with the following calling sequence:
call sscal (5, 2.0, a(1,3), 1).
To scale the second row, use the statement:
call sscal (4, 2.0, a(2,1), 5).
To scale the main diagonal of A by 2.0, use the statement:
call sscal (5, 2.0, a(1,1), 6).
```



**NOTE.** *The default vector argument is assumed to be 1.* 

# **Vector Arguments in VML**

Vector arguments of VML mathematical functions are passed in one-dimensional arrays with unit vector increment. It means that a vector of length n is passed contiguously in an array a whose values are defined as  $a[0], a[1], \ldots, a[n-1]$  (for C- interface).

To accommodate for arrays with other increments, or more complicated indexing, VML contains auxiliary pack/unpack functions that gather the array elements into a contiguous vector and then scatter them after the computation is complete.

Generally, if the vector elements are stored in a one-dimensional array a as

 $a[m_0], a[m_1], \ldots, a[m_{n-1}]$ 

and need to be regrouped into an array y as

 $y[k_0], y[k_1], \ldots, y[k_{n-1}],$ 

VML pack/unpack functions can use one of the following indexing methods:

# **Positive Increment Indexing**

 $k_j = incy * j, m_j = inca * j, j = 0, ..., n-1$ 

Constraint: incy > 0 and inca > 0.

For example, setting incy = 1 specifies gathering array elements into a contiguous vector.

This method is similar to that used in BLAS, with the exception that negative and zero increments are not permitted.

## **Index Vector Indexing**

 $k_{j} = iy[j], m_{j} = ia[j], j = 0, ..., n-1,$ 

where ia and iy are arrays of length n that contain index vectors for the input and output arrays a and y, respectively.

## **Mask Vector Indexing**

Indices  $k_{i}$ ,  $m_{i}$  are such that:

 $my[k_j] \neq 0, ma[m_j] \neq 0, j = 0, ..., n-1,$ 

where ma and my are arrays that contain mask vectors for the input and output arrays a and y, respectively.

# **Matrix Arguments**

Matrix arguments of the Intel[®] Math Kernel Library routines can be stored in either one- or two-dimensional arrays, using the following storage schemes:

- conventional full storage (in a two-dimensional array)
- packed storage for Hermitian, symmetric, or triangular matrices (in a one-dimensional array)
- band storage for band matrices (in a two-dimensional array).

**Full storage** is the following obvious scheme: a matrix *A* is stored in a two-dimensional array *a*, with the matrix element  $a_{ij}$  stored in the array element a(i, j).

If a matrix is *triangular* (upper or lower, as specified by the argument *uplo*), only the elements of the relevant triangle are stored; the remaining elements of the array need not be set.

Routines that handle symmetric or Hermitian matrices allow for either the upper or lower triangle of the matrix to be stored in the corresponding elements of the array:

if <i>uplo</i> = 'U',	$a_{ij}$ is stored in $a(i, j)$ for $i \leq j$ , other elements of a need not be set.
if <i>uplo</i> = 'L',	$a_{ij}$ is stored in $a(i, j)$ for $j \le i$ , other elements of $a$ need not be set.

**Packed storage** allows you to store symmetric, Hermitian, or triangular matrices more compactly: the relevant triangle (again, as specified by the argument uplo) is packed by columns in a one-dimensional array ap:

if uplo = 'U',  $a_{ij}$  is stored in ap(i+j(j-1)/2) for  $i \le j$ 

if uplo = 'L',  $a_{ij}$  is stored in ap(i+(2*n-j)*(j-1)/2) for  $j \le i$ .

In descriptions of LAPACK routines, arrays with packed matrices have names ending in *p*.

**Band storage** is as follows: an *m* by *n* band matrix with kl non-zero sub-diagonals and *ku* non-zero super-diagonals is stored compactly in a two-dimensional array *ab* with kl+ku+l rows and *n* columns. Columns of the matrix are stored in the corresponding columns of the array, and diagonals of the matrix are stored in rows of the array. Thus,

Band storage of A

 $a_{ij}$  is stored in ab(kl+ku+1+i-j, j) for  $max(n, j-ku) \le i \le min(n, j+kl)$ .

Use the band storage scheme only when kl and ku are much less than the matrix size n. (Although the routines work correctly for all values of kl and ku, it's inefficient to use the band storage if your matrices are not really banded).

When a general band matrix is supplied for *LU factorization*, space must be allowed to store kl additional super-diagonals generated by fill-in as a result of row interchanges. This means that the matrix is stored according to the above scheme, but with kl + ku super-diagonals.

The band storage scheme is illustrated by the following example, when m = n = 6, kl = 2, ku = 1:

Banded matrix A

111	<b>a</b> ₁₂	0	0	0	0
	a ₂₂			0	0
<b>a</b> ₃₁	<b>a</b> ₃₂	<b>a</b> ₃₃	<mark>a</mark> 34	0	0
0	<b>a</b> ₄₂	<b>a</b> ₄₃	<b>a</b> ₄₄	<b>a</b> ₄₅	0
0	0	a ₅₃	a ₅₄	a ₅₅	a ₅₆
0	0	0	<b>a</b> ₆₄	a ₆₅	a ₆₆

Array elements marked * are not used by the routines; elements marked + need not be set on entry, but are required by the LU factorization routines to store the results. The input array will be overwritten on exit by the details of the LU factorization as follows:

where  $u_{ij}$  are the elements of the upper triangular matrix U, and  $m_{ij}$  are the multipliers used during factorization.

Triangular band matrices are stored in the same format, with either kl = 0 if upper triangular, or ku = 0 if lower triangular. For symmetric or Hermitian band matrices with k sub-diagonals or super-diagonals, you need to store only the upper or lower triangle, as specified by the argument uplo:

if uplo = U',  $a_{ij}$  is stored in ab(k+1+i-j, j) for  $max(1, j-k) \le i \le j$ if uplo = L',  $a_{ij}$  is stored in ab(1+i-j, j) for  $j \le i \le min(n, j+k)$ .

In descriptions of LAPACK routines, arrays that hold matrices in band storage have names ending in *b*.

In Fortran, column-major ordering of storage is assumed. This means that elements of the same column occupy successive storage locations.

Three quantities are usually associated with a two-dimensional array argument: its leading dimension, which specifies the number of storage locations between elements in the same row, its number of rows, and its number of columns. For a matrix in full storage, the leading dimension of the array must be at least as large as the number of rows in the matrix.

A character transposition parameter is often passed to indicate whether the matrix argument is to be used in normal or transposed form or, for a complex matrix, if the conjugate transpose of the matrix is to be used. The values of the transposition parameter for these three cases are the following:

'N' or 'n'	normal (no conjugation, no transposition)
'T' or 't'	transpose
'C' or 'c'	conjugate transpose.

# **Example A-3 Two-Dimensional Complex Array**

Suppose A (1:5, 1:4) is the complex two-dimensional array presented by matrix

Let transa be the transposition parameter, m be the number of rows, n be the number of columns, and lda be the leading dimension. Then if

transa = 'N', m = 4, n = 2, and 1da = 5, the matrix argument would be

 $\begin{bmatrix} (1.1, 0.11) & (1.2, 0.12) \\ (2.1, 0.21) & (2.2, 0.22) \\ (3.1, 0.31) & (3.2, 0.32) \\ (4.1, 0.41) & (4.2, 0.42) \end{bmatrix}$ 

If transa = 'T', m = 4, n = 2, and 1da = 5, the matrix argument would be

 $\begin{array}{c} (1.1, \ 0.11) \ (2.1, \ 0.21) \ (3.1, \ 0.31) \ (4.1, \ 0.41) \\ (1.2, \ 0.12) \ (2.2, \ 0.22) \ (3.2, \ 0.32) \ (4.2, \ 0.42) \end{array}$ 

If transa = 'C', m = 4, n = 2, and 1da = 5,

the matrix argument would be

 $\begin{bmatrix} (1.1, -0.11) & (2.1, -0.21) & (3.1, -0.31) & (4.1, -0.41) \\ (1.2, -0.12) & (2.2, -0.22) & (3.2, -0.32) & (4.2, -0.42) \end{bmatrix}$ 

Note that care should be taken when using a leading dimension value which is different from the number of rows specified in the declaration of the two-dimensional array. For example, suppose the array A above is declared as COMPLEX A (5, 4).

continued *

Then if transa = 'N', m = 3, n = 4, and 1da = 4, the matrix argument will be

 $\begin{bmatrix} (1.1, 0.11) (5.1, 0.51) (4.2, 0.42) (3.3, 0.33) \\ (2.1, 0.21) (1.2, 0.12) (5.2, 0.52) (4.3, 0.43) \\ (3.1, 0.31) (2.2, 0.22) (1.3, 0.13) (5.3, 0.53) \end{bmatrix}$ 

# Code Examples

# B

This appendix presents code examples of using BLAS routines and functions.

# Example B-1 Using BLAS Level 1 Function



The following example illustrates a call to the BLAS Level 1 function sdot. This function performs a vector-vector operation of computing a scalar product of two single-precision real vectors  $\mathbf{x}$  and  $\mathbf{y}$ .

# **Parameters**

п	Specifies the order of vectors $\mathbf{x}$ and $\mathbf{y}$ .	
incx	Specifies the increment for the elements of $\mathbf{x}$ .	
incy	Specifies the increment for the elements of <i>y</i> .	
<pre>program dot_main real x(10), y(10), sdot, res integer n, incx, incy, i external sdot n = 5</pre>		
<pre>incx = 2 incy = 1</pre>		
do i = 1, 10 x(i) = 2.0e0 y(i) = 1.0e0 end do		

continued *

# Example B-1 Using BLAS Level 1 Function (continued)

```
res = sdot (n, x, incx, y, incy)
print*, `SDOT = `, res
end
As a result of this program execution, the following line is printed:
SDOT = 10.000
```

# Example B-2 Using BLAS Level 1 Routine



The following example illustrates a call to the BLAS Level 1 routine scopy. This routine performs a vector-vector operation of copying a single-precision real vector **x** to a vector **y**.

# **Parameters**

п	Specifies the order of vectors $\mathbf{x}$ and $\mathbf{y}$ .
incx	Specifies the increment for the elements of $\mathbf{x}$ .
incy	Specifies the increment for the elements of <i>y</i> .

```
program copy_main
real x(10), y(10)
integer n, incx, incy, i
n = 3
incx = 3
incy = 1
do i = 1, 10
    x(i) = i
end do
call scopy (n, x, incx, y, incy)
print*, 'Y = ', (y(i), i = 1, n)
end
```

As a result of this program execution, the following line is printed:

 $Y = 1.00000 \; 4.00000 \; 7.00000$ 

# Example B-3 Using BLAS Level 2 Routine



The following example illustrates a call to the BLAS Level 2 routine sger. This routine performs a matrix-vector operation

a := alpha*x*y' + a.

# **Parameters**

alpha	Specifies a scalar <i>alpha</i> .	
x	<i>m</i> -element vector.	
У	<i>n</i> -element vector.	
a	<i>m</i> by <i>n</i> matrix.	
<pre>a</pre>		

continued *

# Example B-3 Using BLAS Level 2 Routine (continued)

As a result of this program execution, matrix *a* is printed as follows: Matrix A: 1.50000 2.50000 3.50000 1.50000 2.50000 3.50000

# Example B-4 Using BLAS Level 3 Routine



The following example illustrates a call to the BLAS Level 3 routine ssymm. This routine performs a matrix-matrix operation

c := alpha*a*b' + beta*c.

# **Parameters**

alpha	Specifies a scalar alpha.
beta	Specifies a scalar beta.
a	Symmetric matrix.
b	<i>m</i> by <i>n</i> matrix.
С	<i>m</i> by <i>n</i> matrix.
<pre>program symm_main real a(3,3), b(3,2), c(3,3), alpha, beta integer m, n, lda, ldb, ldc, i, j character uplo, side uplo = 'u' side = 'l' m = 3 n = 2 lda = 3 ldb = 3 ldb = 3 ldc = 3 alpha = 0.5 beta = 2.0</pre>	

continued *

# Example B-4 Using BLAS Level 3 Routine (continued)

```
do i = 1, m
  do j = 1, m
    a(i,j) = 1.0
  end do
end do
do i = 1, m
  do j = 1, n
    c(i,j) = 1.0
    b(i,j) = 2.0
  end do
end do
call ssymm (side, uplo, m, n, alpha, a, lda, b, ldb,
beta, c, ldc)
print*, 'Matrix C: '
do i = 1, m
  print*, (c(i,j), j = 1, n)
end do
end
As a result of this program execution, matrix c is printed as follows:
Matrix C:
5.00000 5.00000
5.00000 5.00000
5.00000 5.00000
```

# Example B-5 Calling a Complex BLAS Level 1 Function from C

The following example illustrates a call from a C program to the complex BLAS Level 1 function zdotc(). This function computes the dot product of two double-precision complex vectors.

In this example, the complex dot product is returned in the structure c.

```
#define N 5
void main()
{
    int n, inca = 1, incb = 1, i;
    typedef struct{ double re; double im; } complex16;
    complex16 a[N], b[N], c;
    void zdotc();
    n = N;
    for( i = 0; i < n; i++ ){
        a[i].re = (double)i; a[i].im = (double)i * 2.0;
        b[i].re = (double)(n - i); b[i].im = (double)i * 2.0;
    }
    zdotc( &c, &n, a, &inca, b, &incb );
    printf( "The complex dot product is: ( %6.2f, %6.2f
)\n", c.re, c.im );
}</pre>
```



**NOTE.** Instead of calling BLAS directly from C programs, you might wish to use the CBLAS interface; this is the supported way of calling BLAS from C. For more information about CBLAS, see Appendix C, <u>"CBLAS Interface to the BLAS"</u>.

# CBLAS Interface to the BLAS

# C

This appendix presents CBLAS, the C interface to the Basic Linear Algebra Subprograms (BLAS) implemented in Intel[®] MKL.

Similar to BLAS, the CBLAS interface includes the following levels of functions:

- <u>Level 1 CBLAS</u> (vector-vector operations)
- <u>Level 2 CBLAS</u> (matrix-vector operations)
- <u>Level 3 CBLAS</u> (matrix-matrix operations).
- <u>Sparse CBLAS</u> (operations on sparse vectors).

To obtain the C interface, the Fortran routine names are prefixed with cblas_ (for example, dasum becomes cblas_dasum). Names of all CBLAS functions are in lowercase letters.

Complex functions ?dotc and ?dotu become CBLAS subroutines (void functions); they return the complex result via a void pointer, added as the last parameter. CBLAS names of these functions are suffixed with _sub. For example, the BLAS function cdotc corresponds to cblas_cdotc_sub.

# **CBLAS Arguments**

The arguments of CBLAS functions obey the following rules:

- Input arguments are declared with the **const** modifier.
- Non-complex scalar input arguments are passed by value.
- Complex scalar input arguments are passed as void pointers.
- Array arguments are passed by address.
- Output scalar arguments are passed by address.

- BLAS character arguments are replaced by the appropriate enumerated type.
- Level 2 and Level 3 routines acquire an additional parameter of type CBLAS_ORDER as their first argument. This parameter specifies whether two-dimensional arrays are row-major (CblasRowMajor) or column-major (CblasColMajor).

# **Enumerated Types**

The CBLAS interface uses the following enumerated types:

```
enum CBLAS_ORDER {
  CblasRowMajor=101, /* row-major arrays */
  CblasColMajor=102}; /* column-major arrays */
enum CBLAS_TRANSPOSE {
  CblasNoTrans=111, /* trans='N' */
  CblasTrans=112,
                      /* trans='T' */
  CblasConjTrans=113; /* trans='C' */
enum CBLAS_UPLO {
  CblasUpper=121,
                       /* uplo ='U' */
  CblasLower=122};
                       /* uplo ='L' */
enum CBLAS_DIAG {
  CblasNonUnit=131,
                      /* diag ='N' */
  CblasUnit=132};
                        /* diag ='U' */
enum CBLAS_SIDE {
  CblasLeft=141,
                       /* side ='L' */
  CblasRight=142};
                      /* side ='R' */
```

# Level 1 CBLAS

This is an interface to <u>BLAS Level 1 Routines and Functions</u>, which perform basic vector-vector operations.

#### <u>?asum</u>

float cblas_sasum(const int N, const float *X, const int incX); double cblas_dasum(const int N, const double *X, const int incX);

float cblas_scasum(const int N, const void *X, const int incX); double cblas_dzasum(const int N, const void *X, const int incX);

#### <u>?axpy</u>

void cblas_saxpy(const int N, const float alpha, const float *X, const int incX, float *Y, const int incY);

void cblas_daxpy(const int N, const double alpha, const double
*X, const int incX, double *Y, const int incY);

void cblas_caxpy(const int N, const void *alpha, const void *X, const int incX, void *Y, const int incY);

void cblas_zaxpy(const int N, const void *alpha, const void *X, const int incX, void *Y, const int incY);

# <u>?copy</u>

void cblas_scopy(const int N, const float *X, const int incX, float *Y, const int incY);

void cblas_dcopy(const int N, const double *X, const int incX, double *Y, const int incY);

void cblas_ccopy(const int N, const void *X, const int incX, void *Y, const int incY);

void cblas_zcopy(const int N, const void *X, const int incX, void *Y, const int incY);

# <u>?dot</u>

float cblas_sdot(const int N, const float *X, const int incX, const float *Y, const int incY);

double cblas_ddot(const int N, const double *X, const int incX, const double *Y, const int incY);

#### <u>?sdot</u>

float cblas_sdsdot(const int N, const float *SB, const float *SX, const int incX, const float *SY, const int incY); double cblas_dsdot(const int N, const float *SX, const int incX, const float *SY, const int incY);

#### <u>?dotc</u>

void cblas_cdotc_sub(const int N, const void *X, const int incX, const void *Y, const int incY, void *dotc); void cblas_zdotc_sub(const int N, const void *X, const int incX, const void *Y, const int incY, void *dotc);

#### <u>?dotu</u>

void cblas_cdotu_sub(const int N, const void *X, const int incX, const void *Y, const int incY, void *dotu);

void cblas_zdotu_sub(const int N, const void *X, const int incX, const void *Y, const int incY, void *dotu);

#### <u>?nrm2</u>

float cblas_snrm2(const int N, const float *X, const int incX); double cblas_dnrm2(const int N, const double *X, const int incX);

float cblas_scnrm2(const int N, const void *X, const int incX); double cblas_dznrm2(const int N, const void *X, const int incX);

#### <u>?rot</u>

void cblas_srot(const int N, float *X, const int incX, float *Y, const int incY, const float c, const float s);

void cblas_drot(const int N, double *X, const int incX, double *Y,const int incY, const double c, const double s);

#### <u>?rotg</u>

void cblas_srotg(float *a, float *b, float *c, float *s);

void cblas_drotg(double *a, double *b, double *c, double *s);

#### <u>?rotm</u>

void cblas_srotm(const int N, float *X, const int incX, float *Y, const int incY, const float *P);

void cblas_drotm(const int N, double *X, const int incX, double *Y, const int incY, const double *P);

#### <u>?rotmg</u>

void cblas_srotmg(float *d1, float *d2, float *b1, const float b2, float *P);

void cblas_drotmg(double *d1, double *d2, double *b1, const double b2, double *P);

#### <u>?scal</u>

void cblas_sscal(const int N, const float alpha, float *X, const int incX);

void cblas_dscal(const int N, const double alpha, double *X, const int incX);

void cblas_cscal(const int N, const void *alpha, void *X, const int incX);

void cblas_zscal(const int N, const void *alpha, void *X, const int incX);

void cblas_csscal(const int N, const float alpha, void *X, const int incX);

void cblas_zdscal(const int N, const double alpha, void *X, const int incX);

#### <u>?swap</u>

void cblas_sswap(const int N, float *X, const int incX, float *Y, const int incY);

void cblas_dswap(const int N, double *X, const int incX, double *Y, const int incY);

void cblas_cswap(const int N, void *X, const int incX, void *Y, const int incY);

void cblas_zswap(const int N, void *X, const int incX, void *Y, const int incY);

#### <u>i?amax</u>

CBLAS_INDEX cblas_isamax(const int N, const float *X, const int incX);

CBLAS_INDEX cblas_idamax(const int N, const double *X, const int incX);

CBLAS_INDEX cblas_icamax(const int N, const void *X, const int incX);

CBLAS_INDEX cblas_izamax(const int N, const void *X, const int incX);

#### <u>i?amin</u>

CBLAS_INDEX cblas_isamin(const int N, const float *X, const int incX);

CBLAS_INDEX cblas_idamin(const int N, const double *X, const int incX);

CBLAS_INDEX cblas_icamin(const int N, const void *X, const int incX);

CBLAS_INDEX cblas_izamin(const int N, const void *X, const int incX);

# Level 2 CBLAS

This is an interface to <u>BLAS Level 2 Routines</u>, which perform basic matrix-vector operations. Each C routine in this group has an additional parameter of type <u>CBLAS_ORDER</u> (the first argument) that determines whether the two-dimensional arrays use column-major or row-major storage.

#### ?gbmv

void cblas_sgbmv(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const int KL, const int KU, const float alpha, const float *A, const int lda, const float *X, const int incX, const float beta, float *Y, const int incY);

void cblas_dgbmv(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const int KL, const int KU, const double alpha, const double *A, const int lda, const double *X, const int incX, const double beta, double *Y, const int incY);

void cblas_cgbmv(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const int KL, const int KU, const void *alpha, const void *A, const int lda, const void *X, const int incX, const void *beta, void *Y, const int incY);

void cblas_zgbmv(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const int KL, const int KU, const void *alpha, const void *A, const int lda, const void *X, const int incX, const void *beta, void *Y, const int incY);

#### ?gemv

void cblas_sgemv(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const float alpha, const float *A, const int lda, const float *X, const int incX, const float beta, float *Y, const int incY);

void cblas_dgemv(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const double alpha, const double *A, const int lda, const double *X, const int incX, const double beta, double *Y, const int incY);

void cblas_cgemv(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const void *alpha, const void *A, const int lda, const void *X, const int incX, const void *beta, void *Y, const int incY); void cblas_zgemv(const enum CBLAS_ORDER order, const enum CBLAS_TRANSPOSE TransA, const int M, const int N, const void *alpha, const void *A, const int lda, const void *X, const int incX, const void *beta, void *Y, const int incY);

#### ?ger

void cblas_sger(const enum CBLAS_ORDER order, const int M, const int N, const float alpha, const float *X, const int incX, const float *Y, const int incY, float *A, const int lda);

void cblas_dger(const enum CBLAS_ORDER order, const int M, const int N, const double alpha, const double *X, const int incX, const double *Y, const int incY, double *A, const int lda);

#### ?gerc

void cblas_cgerc(const enum CBLAS_ORDER order, const int M, const int N, const void *alpha, const void *X, const int incX, const void *Y, const int incY, void *A, const int lda);

void cblas_zgerc(const enum CBLAS_ORDER order, const int M, const int N, const void *alpha, const void *X, const int incX, const void *Y, const int incY, void *A, const int lda);

#### <u>?geru</u>

void cblas_cgeru(const enum CBLAS_ORDER order, const int M, const int N, const void *alpha, const void *X, const int incX, const void *Y, const int incY, void *A, const int lda);

void cblas_zgeru(const enum CBLAS_ORDER order, const int M, const int N, const void *alpha, const void *X, const int incX, const void *Y, const int incY, void *A, const int lda);

#### <u>?hbmv</u>

void cblas_chbmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const int K, const void *alpha, const void *A, const int lda, const void *X, const int incX, const void *beta, void *Y, const int incY);

void cblas_zhbmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const int K, const void *alpha, const void *A, const int lda, const void *X, const int incX, const void *beta, void *Y, const int incY);

#### <u>?hemv</u>

void cblas_chemv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *A, const int lda, const void *X, const int incX, const void *beta, void *Y, const int incY); void cblas_zhemv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *A, const int lda, const void *X, const int incX, const void *beta, void *Y, const int incY);

#### <u>?her</u>

void cblas_cher(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const void *X, const int incX, void *A, const int lda);

void cblas_zher(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const void *X, const int incX, void *A, const int lda);

#### ?her2

void cblas_cher2(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *X, const int incX, const void *Y, const int incY, void *A, const int lda);

void cblas_zher2(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *X, const int incX, const void *Y, const int incY, void *A, const int lda);

#### <u>?hpmv</u>

void cblas_chpmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *Ap, const void *X, const int incX, const void *beta, void *Y, const int incY);

void cblas_zhpmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *Ap, const void *X, const int incX, const void *beta, void *Y, const int incY);

#### <u>?hpr</u>

void cblas_chpr(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const void *X, const int incX, void *A);

void cblas_zhpr(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const void *X, const int incX, void *A);

#### <u>?hpr2</u>

void cblas_chpr2(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *X, const int incX, const void *Y, const int incY, void *Ap); void cblas_zhpr2(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const void *alpha, const void *X, const int incX, const void *Y, const int incY, void *Ap);

#### <u>?sbmv</u>

void cblas_ssbmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const int K, const float alpha, const float *A, const int lda, const float *X, const int incX, const float beta, float *Y, const int incY);

void cblas_dsbmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const int K, const double alpha, const double *A, const int lda, const double *X, const int incX, const double beta, double *Y, const int incY);

#### <u>?spmv</u>

void cblas_sspmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *Ap, const float *X, const int incX, const float beta, float *Y, const int incY);

void cblas_dspmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *Ap, const double *X, const int incX, const double beta, double *Y, const int incY);

#### <u>?spr</u>

void cblas_sspr(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *X, const int incX, float *Ap);

void cblas_dspr(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *X, const int incX, double *Ap);

#### <u>?spr2</u>

void cblas_sspr2(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *X, const int incX, const float *Y, const int incY, float *A);

void cblas_dspr2(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *X, const int incX, const double *Y, const int incY, double *A);

#### <u>?symv</u>

void cblas_ssymv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *A, const int lda, const float *X, const int incX, const float beta, float *Y, const int incY);

void cblas_dsymv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *A, const int lda, const double *X, const int incX, const double beta, double *Y, const int incY);

#### <u>?syr</u>

void cblas_ssyr(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *X, const int incX, float *A, const int lda);

void cblas_dsyr(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *X, const int incX, double *A, const int lda);

#### <u>?syr2</u>

void cblas_ssyr2(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const float alpha, const float *X, const int incX, const float *Y, const int incY, float *A, const int lda);

void cblas_dsyr2(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const int N, const double alpha, const double *X, const int incX, const double *Y, const int incY, double *A, const int lda);

#### <u>?tbmv</u>

void cblas_stbmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const float *A, const int lda, float *X, const int incX);

void cblas_dtbmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const double *A, const int lda, double *X, const int incX);

void cblas_ctbmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const void *A, const int lda, void *X, const int incX); void cblas_ztbmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const void *A, const int lda, void *X, const int incX);

#### <u>?tbsv</u>

void cblas_stbsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const float *A, const int lda, float *X, const int incX);

void cblas_dtbsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const double *A, const int lda, double *X, const int incX);

void cblas_ctbsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const void *A, const int lda, void *X, const int incX);

void cblas_ztbsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const int K, const void *A, const int lda, void *X, const int incX);

#### <u>?tpmv</u>

void cblas_stpmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const float *Ap, float *X, const int incX);

void cblas_dtpmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N, const double *Ap, double *X, const int incX);

void cblas_ctpmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const void *Ap, void *X, const int incX);

void cblas_ztpmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const void *Ap, void *X, const int incX);

#### <u>?tpsv</u>

void cblas_stpsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const float *Ap, float *X, const int incX);

void cblas_dtpsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const double *Ap, double *X, const int incX);

void cblas_ctpsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const void *Ap, void *X, const int incX);

void cblas_ztpsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const void *Ap, void *X, const int incX);

#### <u>?trmv</u>

void cblas_strmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const float *A, const int lda, float *X, const int incX);

void cblas_dtrmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const double *A, const int lda, double *X, const int incX);

void cblas_ctrmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const void *A, const int lda, void *X, const int incX);

void cblas_ztrmv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const void *A, const int lda, void *X, const int incX);

#### <u>?trsv</u>

void cblas_strsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const float *A, const int lda, float *X, const int incX); void cblas_dtrsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const double *A, const int lda, double *X, const int incX);

void cblas_ctrsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const void *A, const int lda, void *X, const int incX);

void cblas_ztrsv(const enum CBLAS_ORDER order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int N,const void *A, const int lda, void *X, const int incX);

# Level 3 CBLAS

This is an interface to <u>BLAS Level 3 Routines</u>, which perform basic matrix-matrix operations. Each C routine in this group has an additional parameter of type <u>CBLAS_ORDER</u> (the first argument) that determines whether the two-dimensional arrays use column-major or row-major storage.

#### ?gemm

void cblas_sgemm(const enum CBLAS_ORDER Order, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_TRANSPOSE TransB, const int M, const int N, const int K, const float alpha, const float *A, const int lda, const float *B, const int ldb, const float beta, float *C, const int ldc);

void cblas_dgemm(const enum CBLAS_ORDER Order, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_TRANSPOSE TransB, const int M, const int N, const int K, const double alpha, const double *A, const int lda, const double *B, const int ldb, const double beta, double *C, const int ldc);

void cblas_cgemm(const enum CBLAS_ORDER Order, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_TRANSPOSE TransB, const int M, const int N, const int K, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc);

void cblas_zgemm(const enum CBLAS_ORDER Order, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_TRANSPOSE TransB, const int M, const int N, const int K, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc);

#### <u>?hemm</u>

void cblas_chemm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc);

void cblas_zhemm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc);

#### <u>?herk</u>

void cblas_cherk(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const float alpha, const void *A, const int lda, const float beta, void *C, const int ldc);

void cblas_zherk(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const double alpha, const void *A, const int lda, const double beta, void *C, const int ldc);

#### <u>?her2k</u>

void cblas_cher2k(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const float beta, void *C, const int ldc);

void cblas_zher2k(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const double beta, void *C, const int ldc);

#### ?symm

void cblas_ssymm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const float alpha, const float *A, const int lda, const float *B, const int ldb, const float beta, float *C, const int ldc);

void cblas_dsymm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const double alpha, const double *A, const int lda, const double *B, const int ldb, const double beta, double *C, const int ldc);

void cblas_csymm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc);

void cblas_zsymm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const int M, const int N, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc);

#### <u>?syrk</u>

void cblas_ssyrk(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const float alpha, const float *A, const int lda, const float beta, float *C, const int ldc);

void cblas_dsyrk(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const double alpha, const double *A, const int lda, const double beta, double *C, const int ldc);

void cblas_csyrk(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const void *alpha, const void *A, const int lda, const void *beta, void *C, const int ldc);

void cblas_zsyrk(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const void *alpha, const void *A, const int lda, const void *beta, void *C, const int ldc);

#### <u>?syr2k</u>

void cblas_ssyr2k(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const float alpha,const float *A, const int lda, const float *B, const int ldb, const float beta, float *C, const int ldc);

void cblas_dsyr2k(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const double alpha, const double *A, const int lda, const double *B, const int ldb, const double beta, double *C, const int ldc);

void cblas_csyr2k(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSP SE Trans, const int N, const int K, const void *alpha,const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc);

void cblas_zsyr2k(const enum CBLAS_ORDER Order, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE Trans, const int N, const int K, const void *alpha, const void *A, const int lda, const void *B, const int ldb, const void *beta, void *C, const int ldc);

#### <u>?trmm</u>

void cblas_strmm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const float alpha, const float *A, const int lda, float *B, const int ldb);

void cblas_dtrmm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const double alpha, const double *A, const int lda, double *B, const int ldb);

void cblas_ctrmm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const void *alpha, const void *A, const int lda, void *B, const int ldb);

void cblas_ztrmm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const void *alpha, const void *A, const int lda, void *B, const int ldb);

#### <u>?trsm</u>

void cblas_strsm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const float alpha, const float *A, const int lda, float *B, const int ldb);

void cblas_dtrsm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const double alpha, const double *A, const int lda, double *B, const int ldb);

void cblas_ctrsm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const void *alpha, const void *A, const int lda, void *B, const int ldb);

void cblas_ztrsm(const enum CBLAS_ORDER Order, const enum CBLAS_SIDE Side, const enum CBLAS_UPLO Uplo, const enum CBLAS_TRANSPOSE TransA, const enum CBLAS_DIAG Diag, const int M, const int N, const void *alpha, const void *A, const int lda, void *B, const int ldb);

# **Sparse CBLAS**

This is an interface to <u>Sparse BLAS Routines and Functions</u>, which perform a number of common vector operations on sparse vectors stored in compressed form.

Note that all index parameters, *indx*, are in C-type notation and vary in the range [0 . .N-1].

## <u>?axpyi</u>

void cblas_saxpyi(const int N, const float alpha, const float *X, const int *indx, float *Y); void cblas_daxpyi(const int N, const double alpha, const double *X, const int *indx, double *Y); void cblas_caxpyi(const int N, const void *alpha, const void *X, const int *indx, void *Y);

void cblas_zaxpyi(const int N, const void *alpha, const void *X, const int *indx, void *Y);

#### <u>?doti</u>

float cblas_sdoti(const int N, const float *X, const int *indx, const float *Y);

double cblas_ddoti(const int N, const double *X, const int *indx, const double *Y);

#### <u>?dotci</u>

void cblas_cdotci_sub(const int N, const void *X, const int *indx, const void *Y, void *dotui); void cblas_zdotci_sub(const int N, const void *X, const int *indx, const void *Y, void *dotui);

#### <u>?dotui</u>

void cblas_cdotui_sub(const int N, const void *X, const int *indx, const void *Y, void *dotui); void cblas_zdotui_sub(const int N, const void *X, const int *indx, const void *Y, void *dotui);

#### <u>?gthr</u>

void cblas_sgthr(const int N, const float *Y, float *X, const int *indx); void cblas_dgthr(const int N, const double *Y, double *X, const int *indx); void cblas_cgthr(const int N, const void *Y, void *X, const int *indx); void cblas_zgthr(const int N, const void *Y, void *X, const int *indx);

#### <u>?gthrz</u>

void cblas_sgthrz(const int N, float *Y, float *X, const int *indx); void cblas_dgthrz(const int N, double *Y, double *X, const int *indx); void cblas_cgthrz(const int N, void *Y, void *X, const int *indx); void cblas_zgthrz(const int N, void *Y, void *X, const int *indx);

## <u>?roti</u>

void cblas_sroti(const int N, float *X, const int *indx, float *Y, const float c, const float s);

void cblas_droti(const int N, double *X, const int *indx, double *Y, const double c, const double s);

#### <u>?sctr</u>

void cblas_ssctr(const int N, const float *X, const int *indx, float *Y);

void cblas_dsctr(const int N, const double *X, const int *indx, double *Y);

void cblas_csctr(const int N, const void *X, const int *indx, void *Y);

void cblas_zsctr(const int N, const void *X, const int *indx, void *Y);

# Glossary

$A^H$	Denotes the conjugate of a general matrix <i>A</i> . <i>See also</i> conjugate matrix.
$A^T$	Denotes the transpose of a general matrix <i>A</i> . <i>See also</i> transpose.
band matrix	A general <i>m</i> by <i>n</i> matrix <i>A</i> such that $a_{ij} = 0$ for $ i - j  > l$ , where $1 < l < \min(m, n)$ . For example, any tridiagonal matrix is a band matrix.
band storage	A special storage scheme for band matrices. A matrix is stored in a two-dimensional array: columns of the matrix are stored in the corresponding columns of the array, and <i>diagonals</i> of the matrix are stored in rows of the array.
BLAS	Abbreviation for Basic Linear Algebra Subprograms. These subprograms implement vector, matrix-vector, and matrix-matrix operations.
Bunch-Kaufman factorization	Representation of a real symmetric or complex Hermitian matrix A in the form $A = PUDU^{H}P^{T}$ (or $A = PLDL^{H}P^{T}$ ) where P is a permutation matrix, U and L are upper and lower triangular matrices with unit diagonal, and D is a Hermitian block-diagonal matrix with 1-by-1 and 2-by-2 diagonal blocks. U and L have 2-by-2 unit diagonal blocks corresponding to the 2-by-2 blocks of D.

с	When found as the first letter of routine names, c indicates the usage of single-precision complex data type.
CBLAS	C interface to the BLAS. See BLAS.
Cholesky factorization	Representation of a symmetric positive-definite or, for complex data, Hermitian positive-definite matrix $A$ in the form $A = U^H U$ or $A = LL^H$ , where $L$ is a lower triangular matrix and $U$ is an upper triangular matrix.
condition number	The number $\kappa(A)$ defined for a given square matrix <i>A</i> as follows: $\kappa(A) =   A     A^{-1}  $ .
conjugate matrix	The matrix $A^H$ defined for a given general matrix $A$ as follows: $(A^H)_{ij} = (a_{ji})^*$ .
conjugate number	The conjugate of a complex number $z = a + bi$ is $z^* = a - bi$ .
d	When found as the first letter of routine names, d indicates the usage of double-precision real data type.
dot product	The number denoted $x \cdot y$ and defined for given vectors x and y as follows: $x \cdot y = \sum_i x_i y_i$ . Here $x_i$ and $y_i$ stand for the <i>i</i> th elements of x and y, respectively.
double precision	A floating-point data type. On Intel [®] processors, this data type allows you to store real numbers <i>x</i> such that $2.23*10^{-308} <  x  < 1.79*10^{308}$ . For this data type, the machine precision $\varepsilon$ is approximately $10^{-15}$ , which means that double-precision numbers usually contain no more than 15 significant decimal digits. For more information, refer to <i>Pentium[®] Processor</i> <i>Family Developer's Manual, Volume 3: Architecture</i> <i>and Programming Manual.</i>
eigenvalue	See eigenvalue problem.

eigenvalue problem	A problem of finding non-zero vectors <i>x</i> and numbers $\lambda$ (for a given square matrix <i>A</i> ) such that <i>Ax</i> = $\lambda x$ . Here the numbers $\lambda$ are called the <i>eigenvalues</i> of the matrix <i>A</i> and the vectors <i>x</i> are called the <i>eigenvectors</i> of the matrix <i>A</i> .
eigenvector	See eigenvalue problem.
elementary reflector (Householder matrix)	Matrix of a general form $H = I - \tau v v^T$ , where v is a column vector and $\tau$ is a scalar. In LAPACK elementary reflectors are used, for example, to represent the matrix Q in the QR factorization (the matrix Q is represented as a product of elementary reflectors).
factorization	Representation of a matrix as a product of matrices. See also Bunch-Kaufman factorization, Cholesky factorization, LU factorization, LQ factorization, QR factorization, Schur factorization.
FFTs	Abbreviation for Fast Fourier Transforms. <i>See</i> Chapter 3 of this book.
full storage	A storage scheme allowing you to store matrices of any kind. A matrix A is stored in a two-dimensional array <b>a</b> , with the matrix element $a_{ij}$ stored in the array element <b>a</b> ( <i>i</i> , <i>j</i> ).
Hermitian matrix	A square matrix <i>A</i> that is equal to its conjugate matrix $A^H$ . The conjugate $A^H$ is defined as follows: $(A^H)_{ij} = (a_{ji})^*$ .
Ι	See identity matrix.
identity matrix	A square matrix <i>I</i> whose diagonal elements are 1, and off-diagonal elements are 0. For any matrix <i>A</i> , AI = A and $IA = A$ .
in-place	Qualifier of an operation. A function that performs its operation in-place takes its input from an array and returns its output to the same array.

inverse matrix	The matrix denoted as $A^{-1}$ and defined for a given square matrix A as follows: $AA^{-1} = A^{-1}A = I$ . $A^{-1}$ does not exist for singular matrices A.
LQ factorization	Representation of an <i>m</i> by <i>n</i> matrix <i>A</i> as $A = LQ$ or $A = (L 0)Q$ . Here <i>Q</i> is an <i>n</i> by <i>n</i> orthogonal (unitary) matrix. For $m \le n, L$ is an <i>m</i> by <i>m</i> lower triangular matrix with real diagonal elements; for $m > n$ ,
	$L = \begin{bmatrix} L_1 \\ L_2 \end{bmatrix}$
	where $L_1$ is an <i>n</i> by <i>n</i> lower triangular matrix, and $L_2$ is a rectangular matrix.
<i>LU</i> factorization	Representation of a general <i>m</i> by <i>n</i> matrix <i>A</i> as $A = PLU$ , where <i>P</i> is a permutation matrix, <i>L</i> is lower triangular with unit diagonal elements (lower trapezoidal if $m > n$ ) and <i>U</i> is upper triangular (upper trapezoidal if $m < n$ ).
machine precision	The number $\varepsilon$ determining the precision of the machine representation of real numbers. For Intel [®] architecture, the machine precision is approximately $10^{-7}$ for single-precision data, and approximately $10^{-15}$ for double-precision data. The precision also determines the number of significant decimal digits in the machine representation of real numbers. <i>See also</i> double precision and single precision.
MKL	Abbreviation for Math Kernel Library.
orthogonal matrix	A real square matrix A whose transpose and inverse are equal, that is, $A^T = A^{-1}$ , and therefore $AA^T = A^TA = I$ . All eigenvalues of an orthogonal matrix have the absolute value 1.
packed storage	A storage scheme allowing you to store symmetric, Hermitian, or triangular matrices more compactly. The upper or lower triangle of a matrix is packed by columns in a one-dimensional array.

positive-definite matrix	A square matrix A such that $Ax \cdot x > 0$ for any non-zero vector x. Here $\cdot$ denotes the dot product.
QR factorization	Representation of an <i>m</i> by <i>n</i> matrix <i>A</i> as $A = QR$ , where <i>Q</i> is an <i>m</i> by <i>m</i> orthogonal (unitary) matrix, and <i>R</i> is <i>n</i> by <i>n</i> upper triangular with real diagonal elements (if $m \ge n$ ) or trapezoidal (if $m < n$ ) matrix.
S	When found as the first letter of routine names, s indicates the usage of single-precision real data type.
Schur factorization	Representation of a square matrix A in the form $A = ZTZ^{H}$ . Here T is an upper quasi-triangular matrix (for complex A, triangular matrix) called the Schur form of A; the matrix Z is orthogonal (for complex A, unitary). Columns of Z are called Schur vectors.
single precision	A floating-point data type. On Intel [®] processors, this data type allows you to store real numbers <i>x</i> such that $1.18*10^{-38} <  x  < 3.40*10^{-38}$ . For this data type, the machine precision ( $\varepsilon$ ) is approximately $10^{-7}$ , which means that single-precision numbers usually contain no more than 7 significant decimal digits. For more information, refer to <i>Pentium[®] Processor Family</i> <i>Developer's Manual, Volume 3: Architecture and</i> <i>Programming Manual.</i>
singular matrix	A matrix whose determinant is zero. If <i>A</i> is a singular matrix, the inverse $A^{-1}$ does not exist, and the system of equations $Ax = b$ does not have a unique solution (that is, there exist no solutions or an infinite number of solutions).
singular value	The numbers defined for a given general matrix $A$ as the eigenvalues of the matrix $AA^{H}$ . See also SVD.
SMP	Abbreviation for Symmetric MultiProcessing. The MKL offers performance gains through parallelism provided by the SMP feature.

sparse BLAS	Routines performing basic vector operations on sparse vectors. Sparse BLAS routines take advantage of vectors' sparsity: they allow you to store only non-zero elements of vectors. <i>See</i> BLAS.
sparse vectors	Vectors in which most of the components are zeros.
storage scheme	The way of storing matrices. <i>See</i> full storage, packed storage, and band storage.
SVD	Abbreviation for Singular Value Decomposition. See also Singular value decomposition section in Chapter 5.
symmetric matrix	A square matrix A such that $a_{ij} = a_{ji}$ .
transpose	The transpose of a given matrix A is a matrix $A^T$ such that $(A^T)_{ij} = a_{ji}$ (rows of A become columns of $A^T$ , and columns of A become rows of $A^T$ ).
trapezoidal matrix	A matrix A such that $A = (A_1A_2)$ , where $A_1$ is an upper triangular matrix, $A_2$ is a rectangular matrix.
triangular matrix	A matrix <i>A</i> is called an upper (lower) triangular matrix if all its subdiagonal elements (superdiagonal elements) are zeros. Thus, for an upper triangular matrix $a_{ij} = 0$ when $i > j$ ; for a lower triangular matrix $a_{ij} = 0$ when $i < j$ .
tridiagonal matrix	A matrix whose non-zero elements are in three diagonals only: the leading diagonal, the first subdiagonal, and the first super-diagonal.
unitary matrix	A complex square matrix A whose conjugate and inverse are equal, that is, that is, $A^H = A^{-1}$ , and therefore $AA^H = A^H A = I$ . All eigenvalues of a unitary matrix have the absolute value 1.
VML	Abbreviation for Vector Mathematical Library. <i>See</i> Chapter 6 of this book.
Ζ	When found as the first letter of routine names, z indicates the usage of double-precision complex data type.

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