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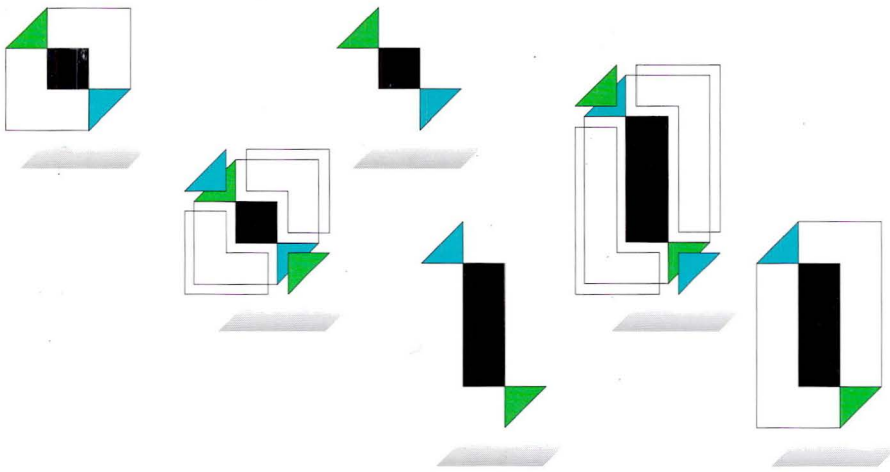

HP MLIB LAPACK
User's Guide

Third Edition

Hewlett-Packard Company
Convex Division
3000 Waterview Parkway
P.O. Box 833851
Richardson, TX 75083-3851
United States of America

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Preface

Purpose and Audience

This guide describes the Hewlett-Packard Linear Algebra Package (LAPACK) software library and shows how to use it. Hewlett-Packard LAPACK (hereafter referred to as LAPACK) is a collection of Fortran-callable subprograms that provides mathematical software for application programs involving linear algebra, including linear equations, least squares, eigenvalue problems, and the singular value decomposition. The package is designed to supersede LINPACK and EISPACK. The National Science Foundation, the Defense Advanced Research Projects Agency, and the Department of Energy supported the development of the public-domain version of LAPACK, from which the Hewlett-Packard version of LAPACK was derived.

Much of the information in this manual was derived from the source code and its comments, and from various LAPACK working notes. These sources are in the public domain.

The *HP MLIB LAPACK User's Guide* addresses experienced Fortran programmers who:

- Convert, develop, or optimize programs for use on Hewlett-Packard supercomputers and workstations
- Optimize existing software to improve performance and increase productivity

Organization

To learn fundamental information necessary for using the LAPACK library, read Chapter 1 and the introductory sections of the other chapters. These sections of background information will help you efficiently use the LAPACK library subprograms.

To learn more about the subject of any given chapter, refer to the literature cited in the "Overview" section of each chapter.

To find the page number on which a subprogram is described, use the Index or refer to the "Subprogram Descriptions" section in the chapter introduction.

This guide is organized into the following chapters:

- Chapter 1 introduces general concepts about LAPACK.
- Chapter 2 describes simple drivers for linear equations.
- Chapter 3 explains expert drivers for linear equations.
- Chapter 4 describes computational linear equation subprograms.
- Chapter 5 explains the least squares capabilities of LAPACK.
- Chapter 6 describes computational subprograms for computing and using orthogonal factorizations.
- Chapter 7 explains the simple driver subprograms for ordinary eigenanalysis.
- Chapter 8 describes the expert driver subprograms for ordinary eigenanalysis.
- Chapter 9 explains the generalized eigenvalue subprograms.
- Chapter 10 describes singular value decomposition subprograms.
- Chapter 11 describes user-visible auxiliary subprograms in LAPACK.
- An index is included at the back of the manual.

Notational Conventions

The following conventions are used in this manual:

- *Italics* within text may indicate mathematical entities used or manipulated by the program. For example, solve the n-by-n system of linear equations $Ax = b$.

  Italics within text may also indicate the first occurrence of a new term.

  Italics within command lines indicate generic commands, file names, or subprogram names. Substitute actual commands, file names, or subprograms for the *italicized* words. For example, the command line

  fc *prog_name*.**o**

  instructs you to type the command *fc*, followed by the name of a program or subprogram object file.

- **UPPERCASE BOLDFACE** within text and in prototype Fortran statements indicates Fortran keywords and subprogram names that must be typed just as they appear. For example, **CALL SGESV**.

- Type in **lowercase boldface** indicates Fortran generic variable or array names. You should substitute actual variable or array names. The *italicized* mathematical entities and the **lowercase boldface** variable and array names usually correspond. For example, A is a matrix and **a** is the Fortran array containing the matrix:

  CALL SGESV (n, nrhs, a, lda, ipvt, b, ldb, info)

  Within command lines, **lowercase boldface** indicates ASCII characters that must be typed just as they appear. For example, the command line

  fc *prog_name*.**o**

  instructs you to type the command *fc*, followed by the name of a program or subprogram file.

- `UPPERCASE CONSTANT WIDTH` represents Fortran programs.

- Brackets ([ ]) enclose optional entries.

Associated Documents

Using this guide successfully may require information not specific to the tasks described herein or not within the scope of this guide. The following documents are provided to help you:

- *HP MLIB VECLIB User's Guide* (B5649-90003). This guide provides definitions for many additional subprograms available to SCILIB users through inclusion of VECLIB, but not documented in the *HP MLIB SCILIB User's Guide*.
- *HP MLIB SCILIB User's Guide* (B5649-90002). This guide provides information on the subprograms provided with the LAPACK library.
- *Exemplar Programming Guide: S-Class and X-Class Servers* (B5600-90001). This manual describes efficient programming techniques for the Exemplar family of computers.
- *Exemplar C and Fortran 77 Programmer's Guide* (B5600-90002), *Release Notice, Fortran 77 Compiler V1.0*, and *Release Notice, C Compiler V1.0*. These documents describe the Exemplar Fortran 77 and C compilers.
- *HP C/HP-UX Reference Manual* (92453-90024). This manual presents reference information on the C programming language, as implemented by Hewlett-Packard.
- *HP C/HP-UX Programmer's Guide* (92434-90002). This guide contains detailed discussions of selected C topics.
- *Fortran/9000 Programmer's Reference* (B3906-90002). This book is a language reference for Hewlett-Packard Fortran 77.
- *Fortran/9000 Programmer's Guide* (B3906-90001). This manual is a task reference. It describes features and requirements in terms of the tasks a programmer might perform. These tasks include how to compile, link, run, debug, and optimize programs.
- *Programming on HP-UX* (B2355-90652). This book describes how to develop software on HP-UX using the HP compilers, assemblers, linker, libraries, and object files.
- *Exemplar SPP1000 Series Architecture* (DHW-014). This book describes the SPP1200 and SPP1600 architectures.
- *Exemplar Architecture: S-Class and X-Class Servers* (A4716-90001). This book describes the architectures of the S2000 and X2000 servers.

- *CXpa Reference: Exemplar S-Class and X-Class Servers* (B5639-90002). This guide explains the operation of the CXpa Performance Analyzer and the steps needed to create and interpret a CXpa profile.
- *CXdb Quick Reference: Exemplar S-Class and X-Class Servers* (B5639-90001). This book describes prominent features of the CXdb visual debugger.
- *CXdb Online Help*. This document describes the CXdb visual debugger. Also, see the xcdb(1) man page.
- *HP MPI User's Guide: S-, X-, D-, and K-Class Servers* (B6011-90001). This book discusses message-passing programming using the Message-Passing Interface library.
- *HP PVM User's Guide: S-Class and X-Class Servers* (B5885-90001). This book discusses message-passing programming using the Parallel Virtual Machine library.
- *HP Fortran 90 Programmer's Reference* (B5876-90001). This book is a complete Fortran 90 language reference. It also covers compiler options, compiler directives, and library information.
- *HP Fortran 90 Programmer's Notes* (B5876-90002). This book provides extensive usage information, including how to compile and link, suggestions and tools for migrating to HP Fortran 90, and how to call C and HP-UX routines from HP Fortran 90.
- *Exemplar C++ Programming Guide: S-Class and X-Class Servers* (B5630-90001). This book describes the Exemplar C++ compiler.
- *HP-UX Assembly Language Reference Manual* (92432-90001). This manual describes the HP-UX Assembler for the PA-RISC processor.
- *HP PA-RISC 2.0 Architecture Reference* (B5655-90009). This manual describes the architecture of the Hewlett-Packard PA-RISC 2.0 processor.
- *HP PA-RISC 1.1 Architecture and Instruction Set Reference Manual* (DHP-181). This manual describes the architecture and the instruction set of the Hewlett-Packard PA-RISC 1.1 processor.
- *PA-RISC Procedure Calling Conventions Reference* (09740-90015). This manual describes the conventions for creating PA-RISC assembly language procedure calls.

Ordering Documentation

To order additional copies of this document or other documents listed in "Associated Documents," send requests to:

Hewlett-Packard Company
Convex Division
Customer Service
P.O. Box 833851
Richardson, TX 75083-3851 USA

Please include the order number (xxxxx-9xxxx number) or the exact title of the document.

Technical Assistance

If you have questions that are not answered in this book, contact the Hewlett-Packard Convex Technical Assistance Center (TAC) at the following locations:

- Within the continental U.S., call 1 (800) 952-0379.
- From Canada, call 1 (800) 345-2384.
- All other locations, contact your local Hewlett-Packard office.

You can also use the `contact` utility, if you would like to report any problems you may have with HP MLIB LAPACK or its associated documentation.

1 Introduction to LAPACK

Overview

LAPACK, a component of HP MLIB, is a collection of Fortran-callable subprograms that provides mathematical software for application programs involving linear algebra, including linear equations, least squares, eigenvalue problems, and the singular value decomposition. The package is designed to supersede LINPACK and EISPACK. The National Science Foundation, the Defense Advanced Research Projects Agency, and the Department of Energy supported the development of the public-domain version of LAPACK, from which the Hewlett-Packard version of LAPACK was derived.

Although LAPACK was designed for use with Fortran programs, C programs can call LAPACK subprograms as described in appendix A of the HP MLIB VECLIB User's Guide, which is included in this documentation set.

This chapter provides information necessary for efficient use of LAPACK. It includes discussions of LAPACK conformance to public-domain LAPACK standards, the LAPACK and LAPACK8 library files, accessing LAPACK subprograms, optimizations, including parallel processing and interactions with other analysis and optimization products, supported floating-point formats, roundoff effects, and the naming convention. It also contains information on the LAPACK library contents, how to use the two libraries and various compiler options, and error handling. The chapter also covers online documentation and HP support services.

The MLIB documentation set includes the *HP MLIB VECLIB User's Guide*, the *HP MLIB SCILIB User's Guide*, and the *HP MLIB LAPACK User's Guide*. The following additional documents provide supplemental help:

- Dongarra, J.J., J.R. Bunch, C.B. Moler, and G.W. Stewart. *LINPACK Users' Guide*. Philadelphia, PA: SIAM Publications. 1979.
- Garbow, B.S., *et al* "Matrix Eigensystem Routines—EISPACK Guide Extension." *Lecture Notes in Computer Science*, Vol. 51. New York: Springer-Verlag. 1977.
- Smith, B.T., *et al* "Matrix Eigensystem Routines—EISPACK Guide." *Lecture Notes in Computer Science*, Vol. 6, 2nd edition. New York: Springer-Verlag. 1976.

Chapter Objectives

After reading this chapter you will:

- Know why there are two libraries and how to access them
- Understand how LAPACK works in a parallel computing environment
- Know how LAPACK interacts with the HP Performance Analyzer and other profilers
- Know LAPACK naming conventions
- Know the overall structure and contents of LAPACK
- Be able to use Fortran type declarations and compiler options
- Understand how LAPACK handles errors
- Know how to access the online *HP MLIB Man Pages*
- Know what to do if you are having trouble using LAPACK subprograms

What You Need to Know to Use LAPACK

You should be familiar with the following sections to make efficient use of LAPACK.

Standardization

LAPACK fully conforms with public domain version 2.0 of LAPACK in all user-visible usage conventions. ("User-visible" means all subprograms indicated in Tables 1-4 through 1-9 or documented in this manual.) However, even though the user interface is standardized, internal workings of some subprograms have been specialized for supported computers.

Two LAPACK Libraries

Often, it is desirable to run a single precision program in double precision. To support changing the precision without changing the code, HP Fortran Compilers provide several compilation options, namely, **+autodbl** and **+autodbl4**, that affect the size of Fortran data types. For compatibility with these compiler options, LAPACK provides two libraries, LAPACK and LAPACK8.

- The LAPACK library works with default-sized Fortran INTEGER, REAL, DOUBLE PRECISION, COMPLEX, and LOGICAL data types, that is, the sizes you get when you do not use the "***n**" size specifications or either of the above compiler options.
- The LAPACK8 library is a subset of the LAPACK library that is designed for use by programs that are compiled with one of the above compiler options. The LAPACK8 library is available only on computer systems with compilers that support the INTEGER*8 data type.

For more information about these options, refer to a Fortran language reference and the "Required Data Item Byte Lengths and How to Get Them" section in this chapter. To determine if a subprogram is included in LAPACK8, consult the LAPACK8 section under each subprogram specification in the following chapters.

Accessing LAPACK

The LAPACK and LAPACK8 libraries consist of compiled subprograms ready for you to incorporate into your programs with the linker. Simply include the appropriate declarations and CALL statements in your Fortran source program and specify that LAPACK or LAPACK8 be used as an object library at link time.

MLIB libraries are installed in the */opt/mlib/* directory. The entire path depends on your system type, as follows:

System type	CPU Type	Installation Directory
C-, D-, or K-Class	PA-8000	*/opt/mlib/lib/pa2.0*
S- or X-Class	PA-8000	*/opt/mlib/lib/pa2.0parallel*
C-, D-, J-, or K-Class	PA-7200	*/opt/mlib/lib/pa1.1*
SPP-1200 or SPP-1600	PA-7200	*/opt/mlib/lib/pa1.1parallel*

The file names of the LAPACK and LAPACK8 libraries are *liblapack.a* and *liblapack8.a*.

There are several ways to specify the linking of your program with LAPACK or LAPACK8:

- specify the entire path of the library file on the f77 or f90 command line that links your program. For example, with the f77 compiler on a C-Class PA-8000 system, use:

  f77 [*options*] *file* **/opt/mlib/lib/pa2.0/liblapack.a**

- use the **-l** option on the f77 or f90 command line that links your program, preceded by the option **-Wl,-L**<*path*>, where <*path*> is the appropriate one of the above installation directories. For example, the above f77 command line could be written as:

  f77 [*options*] *file* **-Wl, -L/opt/mlib/lib/pa2.0 -llapack**

- set the LDOPTS environment variable to include **-L**<*path*>, where <*path*> is the appropriate one of the above installation directories, and use the **-l** option on the f77 or f90 command line that links your program. For example, with the f90 compiler, use:

  f90 [*options*] *file* **-llapack**

  or

  f90 [*options*] *file* **-llapack8**

Do not try to use subprograms from both **-llapack** and **-llapack8** in the same program.

NOTE If you are running MLIB on an S- or X-Class machine, the LAPACK, VECLIB, and SCILIB libraries contain parallelized subprograms. See "Parallel Processing" for additional information about linking your program.

VECLIB is documented in the *HP MLIB VECLIB User's Guide*. If your program uses subprograms from both LAPACK and VECLIB, specify both **-llapack** and **-lveclib**, or both **-llapack8** and **-lveclib8**. For example, using the second method above to specify the location of the libraries, link with

f77 [*options*] *file* **-llapack -lveclib**

and

f90 [*options*] *file* **-llapack8 -lveclib8**

See "Interactions Between VECLIB, SCILIB, and LAPACK" for details about how to order the two **-l** options. Do not try to use subprograms from both **-llapack** and **-lveclib8** or both **-llapack8** and **-lveclib** in the same program.

SCILIB is documented in the *HP MLIB SCILIB User's Guide*. If you use subprograms from both LAPACK and SCILIB, specify both libraries when you

link your program. For example, using the second method above on an S-Class machine, link with

f90 [*options*] *file* **–Wl, –L/opt/mlib/lib/pa2.0parallel –llapack8 –lscilib**

Add the linker option **–lveclib8** if VECLIB subprograms are also used. See "Interactions Between VECLIB, SCILIB, and LAPACK" for details about the order of the –l options. Do not try to use subprograms from both **–llapack** and **–lscilib** in the same program.

Interactions Between VECLIB, SCILIB, and LAPACK

Each of the five library files in VECLIB, SCILIB, and LAPACK is complete in itself, meaning that you will not need to load one library merely because you have used subprograms from another. This is accomplished by including various subprograms in more than one library. For example, subroutine SGEMV is in all of these products, but with identical functionality. Thus, in general, you have to load only the libraries you need, and you may list them in any order on your load command line, as described in the previous section. However, there are a few differences between the libraries that may force you to put the libraries into a specific order to obtain the results you expect.

Differences between VECLIB8 and SCILIB

Five subprograms common to VECLIB8 and SCILIB differ slightly in functionality.

Subprograms ICAMAX, ISAMAX, ISAMIN, ISMAX, and ISMIN in VECLIB8 handle a negative **incx** argument by taking its absolute value and searching the **x** vector in forward order, while in SCILIB, a negative **incx** argument results in searching the array **x** in backward order. No VECLIB8 subprograms call any of these subprograms with a negative **incx** argument, so you may safely load SCILIB before VECLIB8 if you need the SCILIB functionality.

Two other subprograms in both VECLIB8 and SCILIB have the same functionality but different numbers of arguments.

Subroutines SGEMMS and CGEMMS from the two libraries implement Strassen's method for matrix multiplication, but the SCILIB versions have an extra argument, for working storage, that is not needed in the VECLIB8 versions. Be certain that your calls to these subprograms have 14 arguments if you load SCILIB before VECLIB8.

Differences between LAPACK8 and SCILIB

Two subprograms common to LAPACK8 and SCILIB differ slightly in functionality.

Subprograms ICAMAX and ISAMAX in LAPACK8 handle a negative **incx** argument by taking its absolute value and searching the **x** vector in forward order, while in SCILIB, a negative **incx** argument results in searching the array **x** in backward order. No LAPACK8 subprograms call either of these subprograms with a negative **incx** argument, so you may safely load SCILIB before LAPACK8 if you need the SCILIB functionality.

Optimization

LAPACK has been optimized by using a highly efficient implementation of the Basic Linear Algebra Subprograms (BLAS) and the Level 2 and Level 3 BLAS. In addition, certain algorithmic improvements have been made, and several tunable parameters have been adjusted for good execution performance.

Parallel Processing

This section applies only to Hewlett-Packard S- and X-Class computer systems.

Parallel processing is available on Hewlett-Packard S- and X-Class computer systems. These systems can divide a single computational process into small streams of execution, called *threads*. The result is that you can have more than one processor executing on behalf of the same process.

You can permit or disable parallel processing at link time or at run time. To permit parallel processing at link time, your link step must produce a multithreaded executable. The S-Class f77, C and C++ compilers always pass **+tm S2000** to the linker, so you always get a multithreaded executable from the Fortran 77 and C compilers. Similarly, the X-Class f77, C, and C++ compilers always pass **+tm X2000**. Fortran 90, on the other hand, does not pass the **+tm** string to the linker so you must include the **-Wl,+tm,S2000** or **-Wl,+tm,X2000** option on the f90 command line that links your program.

A multithreaded executable will go parallel when the **+parallel** flag is passed to the linker. The executable will go parallel without further ado if compiled with **+O3 +Oparallel**, or simply linked with **+Oparallel**:

f77 [*options* including **+O3 +Oparallel**] *file* **-llapack**

To disable MLIB's automatic parallelism at link time, you omit the **+Oparallel** option and include the following required runtime libraries:

f77 [*options*] *file* **-llapack -lpthread -lcps -lpthread -lail**

The f90 command lines corresponding to these f77 command lines are:

f90 [*options* including **-Wl,+tm,S2000,+parallel**] *file* **-llapack -lpthread -lcps -lpthread -lail**

and

f90 [*options* including **-Wl,+tm,S2000**] *file* **-lscilib -lpthread -lcps -lpthread -lail**

At run time, you can use the *mpa*(1) utility or the MP_NUMBER_OF_THREADS environment variable to control parallelism. Refer to the *mpa*(1) or *f77*(1) man page, respectively, for details.

If parallelism is permitted, each parallelized LAPACK subprogram determines at run time whether multiple processors are available. If so, it detects whether the program is already using multiple threads. It uses this information to automatically choose between a single- or parallel-processor algorithm.

If you are using an S- or X-Class system, you can realize the performance benefits of parallel processing in three ways. First, you can call any parallelized LAPACK subprogram and let it use parallelism internally if it determines that it is appropriate to do so, based on such factors as problem size, system configuration, and user environment. Alternatively, you can call LAPACK subprograms in a parallelized loop or region. To use this mechanism, you must be familiar with the techniques of parallel processing; refer to the *Exemplar Programming Guide*. The third mechanism is to use the MPI explicit parallel model. See the *MPI*(1) man page for details.

LAPACK subprograms are reentrant. This means that they may be called several times in parallel to do independent computations without one call interfering with another. You can use this feature to call LAPACK subprograms in a parallelized loop or region. The compiler does not automatically parallelize loops containing a function reference or subroutine call. You can force it to parallelize such a loop by inserting compiler directives before the loop.

For example, the following Fortran code makes parallel calls to subprogram SGETRS:

```
C$DIR LOOP_PRIVATE (J)
C$DIR LOOP_PARALLEL
      DO 10 J=1, N
         CALL SGETRS ('N', N, 1, A, LDA, IPIV, B(1,J), LDB, INFO(J))
   10 CONTINUE
```

While optimizing a parallel program, you might want to make parallel calls to a LAPACK subprogram to execute independent operations where the call statements are not in a loop. The Fortran compiler does not automatically parallelize code outside a loop, but you can use the BEGIN_TASKS, NEXT_TASK, and END_TASKS compiler directives to tell the compiler to parallelize such code.

If a parallelized LAPACK subprogram is called from a parallelized loop or region, the internal parallelism is disabled.

Profiling LAPACK Applications

The Hewlett-Packard Performance Analyzer, CXpa, is an interactive tool for Hewlett-Packard computer systems that gathers and analyzes program execution timing (profiling) data. CXpa provides the programmer with the means to study the timing behavior of a program for the purposes of optimizing, benchmarking, and debugging. To use the performance analyzer, you must first compile your Fortran program with the **+pa** compiler option. This option instruments the compiled program so that its performance can be measured.

LAPACK has been instrumented so that the performance of LAPACK subprograms can be included in the analysis. This instrumentation is nonintrusive, so it is not necessary to use a different version of LAPACK when you desire to profile your program. Also, the CXpa instrumentation does not interfere with the *prof* or *gprof* instrumentation in your program. However, you may not profile your program with both CXpa and *prof* or *gprof* at the same time.

Subprogram-level profiling produces summary information about the subprograms that are called during profiled execution of the program. This information includes:

- The number of times each subprogram is called
- The CPU time in each subprogram and the percentage of the program total, either including or excluding the cumulative time in called subprograms
- A dynamic call graph, listing the subprogram calls that take place within a computer program

CXpa is an optional product. For more information about CXpa, refer to the *CXpa Reference: Exemplar S-Class and X-Class Servers*, or contact your Hewlett-Packard sales representative.

Floating-Point Formats

Hewlett-Packard Exemplar and other computers with PA-RISC-based architectures operate only on floating-point data in the IEEE format. For further information on Hewlett-Packard floating-point formats, refer to the *Fortran User's Guide*.

Roundoff Effects

LAPACK subprograms may use a different arithmetic order of evaluation than other implementations. Different roundoff characteristics may result. Accuracy of results is usually about the same, so using LAPACK should not materially affect the accumulation of roundoff errors in a complete application program. If it does, you should examine the mathematical analysis of the

problem, which will likely show that the problem is ill-conditioned. Ill-conditioned means that the small roundoff errors that are inadvertently introduced into any computation are magnified out of proportion to the desired result. Similarly, if results with and without LAPACK differ materially, both sets of answers are probably inaccurate and you should investigate further. If the program correctly applies stable computational algorithms, the problem itself is probably ill-posed.

Working Storage

Many LAPACK subprograms require the user to supply one or more arrays to be used for work space. In some cases, the length of the required work space is not specified exactly in the subprogram documentation. In these subroutine descriptions, the work space length is described as follows, for example:

lwork	The length of array work. **lwork** ≥ max(1,**m**). For good performance, *lwork* must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1)

The performance of these subprograms can be improved, often dramatically, by providing at least the optimum amount of work space. This amount can be a complicated function of the problem size and "job" arguments, so you should make **lwork** amply large or compare it to the value returned in **work**(1).

LAPACK Organization and Naming Convention

Data Types and Precision

LAPACK provides the same range of functionality for both real and complex data. Matching pairs of subprograms, one for real data and one for complex data, are available for most computations, but there are a few exceptions. For example, subprograms for both complex Hermitian and complex symmetric systems of linear equations correspond to the subprograms for real symmetric indefinite systems, because both types of complex systems occur in practical applications. For another example, there is no complex analogue of the subprograms for finding selected eigenvalues of a real symmetric tridiagonal matrix, because a complex Hermitian matrix can always be reduced to a real symmetric tridiagonal matrix. Matching subprograms for real and complex data have been coded to maintain a close correspondence between the two, wherever possible; but in some areas (especially the nonsymmetric eigenproblem), the correspondence is necessarily weaker.

All subprograms in LAPACK are provided in both 32-bit and 64-bit precision versions. All LAPACK8 subprograms use only 64-bit precision.

LAPACK Naming Convention

The name of each LAPACK subprogram is a coded specification of its function, within the limits of standard FORTRAN 77 6-character names. All driver and computational subprograms, as well as most of the auxiliary subprograms, (see "Classes of Subprograms") have names of the form TXXYYY, although for some subprograms the sixth character is blank.

The first letter, T, shows the predominant data type according to Table 1-1:

Table 1-1 LAPACK Naming Convention—Data Type

T	Data Type	LAPACK	LAPACK8
S	Single Precision	REAL*4	REAL*8
D	Double Precision	REAL*8	—
C	Complex	COMPLEX*8	COMPLEX*16
Z	Double Complex	COMPLEX*16	—

To refer to a LAPACK subprogram generically, without regard to data type, you replace the first letter by "_". Thus, "_GBSV" refers to any or all of the subprograms SGBSV, CGBSV, DGBSV, and ZGBSV.

The next two letters, XX, designate either the form of the matrix or the most significant matrix. Most of these two-letter codes apply to both real and complex matrices; a few apply specifically to one or the other, according to Table 1-2.

Table 1-2 LAPACK Naming Convention—Matrix Form

XX	Matrix Form
BD	Bidiagonal
DI	Diagonal
GB	General band
GE	General full
GG	General full generalized
GT	General tridiagonal
HB	Complex Hermitian band
HE	Complex Hermitian
HG	Complex Hermitian generalized
HP	Complex Hermitian, packed storage
HS	Upper Hessenberg
OP	Real orthogonal, packed storage
OR	Real orthogonal
PB	Symmetric or Hermitian positive definite band
PO	Symmetric or Hermitian positive definite
PP	Symmetric or Hermitian positive definite, packed storage
PT	Symmetric or Hermitian positive definite tridiagonal
SB	Symmetric band
SP	Symmetric, packed storage
ST	Symmetric tridiagonal
SY	Symmetric
TB	Triangular band
TG	Triangular generalized
TP	Triangular, packed storage
TR	Triangular (or in some cases quasi-triangular)
TZ	Trapezoidal
UN	Complex unitary
UP	Complex unitary, packed storage

The last three letters YYY designate the computation performed. Their meanings are listed in Table 1-3.

Table 1-3 LAPACK Naming Convention—Computation

YYY	Computation
BAK	Back transformation of eigenvectors after balancing
BAL	Permute and balance to isolate eigenvalues
BRD	Reduce to bidiagonal form by orthogonal transformations
CON	Estimate condition number
EBZ	Compute selected eigenvalues by bisection
EDC	Compute eigenvalues and eigenvectors by divide-and-conquer method
EIN	Compute selected eigenvectors by inverse transformations
EQR	Compute eigenvalues and Schur Form using the *QR* algorithm
EQU	Equilibrate a matrix to reduce its condition number
EQZ	Compute eigenvalues and Schur Form using the *QZ* algorithm
ERF	Compute eigenvectors using the Pal-Walker-Kahan variant of the *QL* or *QR* algorithm
ES	Simple driver to compute all eigenvalues, Schur Form, and Schur vectors
ESX	Simple driver to compute all eigenvalues, Schur Form, and Schur vectors
EV	Simple driver to compute all eigenvalues and eigenvectors
EVC	Compute eigenvectors from Schur factorization
EVD	Simple driver to compute all eigenvalues and eigenvectors
EVX	Expert driver to compute selected eigenvalues and eigenvectors
EXC	Swap adjacent diagonal blocks in a quasi-upper-triangular matrix
GBR	Generate the orthogonal/unitary matrix from _GEBRD
GHR	Generate the orthogonal/unitary matrix from _GEHRD
GLM	Driver to solve generalized linear regression model problem
GLQ	Generate the orthogonal/unitary matrix from _GELQF
GQL	Generate the orthogonal/unitary matrix from _GEQLF
GQR	Generate the orthogonal/unitary matrix from _GEQRF
GRQ	Generate the orthogonal/unitary matrix from _GERQF
GS	Driver to compute generalized eigenvalues, Schur Form, and Schur vectors
GST	Reduce a symmetric definite generalized eigenvalue problem to standard form
GTR	Generate the orthogonal/unitary matrix from _XXTRD
GV	Driver to compute generalized eigenvalues and generalized eigenvectors
HRD	Reduce to upper Hessenberg form by orthogonal transformations
LQF	Compute an *LQ* factorization without pivoting

YYY	Computation
LS	Driver to solve over- or underdetermined linear system using orthogonal factorizations
LSE	Driver to solve linear equality constrained least squares problem
LSS	Driver to solve least squares problem using the singular value decomposition
LSX	Driver to compute minimum-norm solution using a complete orthogonal factorization
MBR	Multiply by the orthogonal/unitary matrix from _GEBRD
MHR	Multiply by the orthogonal/unitary matrix from _GEHRD
MLQ	Multiply by the orthogonal/unitary matrix from _GELQF
MQL	Multiply by the orthogonal/unitary matrix from _GEQLF
MQR	Multiply by the orthogonal/unitary matrix from _GEQRF
MRQ	Multiply by the orthogonal/unitary matrix from _GERQF
MTR	Multiply by the orthogonal/unitary matrix from _XXTRD
QLF	Compute a *QL* factorization without pivoting
QPF	Compute a *QR* factorization with column pivoting
QRF	Compute a *QR* factorization without pivoting
RFS	Refine initial solution returned by the TRS subprograms
RQF	Compute an *RQ* factorization without pivoting
SEN	Compute a basis and reciprocal condition number of an invariant subspace
SJA	Compute singular value decomposition
SNA	Estimate reciprocal condition numbers of eigenvalue/vector pairs
SQR	Compute singular values and singular vectors using the *QR* algorithm
STF	Compute a split Cholesky factorization
SV	Simple driver to solve a system of linear equations
SVD	Driver to compute the singular value decomposition
SVP	Preprocessing step for computing the singular value decomposition
SVX	Expert driver to solve a system of linear equations
SYL	Solve the Sylvester matrix equation
TRD	Reduce a symmetric matrix to real symmetric tridiagonal form
TRF	Compute a triangular factorization (*LU*, Cholesky, and so forth)
TRI	Compute inverse (based on triangular factorization)
TRS	Solve systems of linear equations (based on triangular factorization)

Classes of Subprograms

LAPACK contains several different classes of subprograms:

Driver subprograms, each of which solves a complete problem, such as solving a system of linear equations or computing the eigenvalues of a matrix. For some problems, there are both simple and expert driver subprograms. You should use a driver subprogram if one meets your requirements.

Computational subprograms, each of which does a distinct computational task, such as an LU factorization or the reduction of a real symmetric matrix to tridiagonal form. Driver subprograms typically call a sequence of computational subprograms, usually with computational and flow-control code sequences interspersed between the calls. Users may want to call computational subprograms directly to perform tasks, or task sequences, that cannot conveniently be performed by the driver subprograms.

Auxiliary subprograms, which, in turn, can be subclassified as follows:

- Subprograms to do subtasks of block algorithms—including subprograms that implement unblocked versions of the algorithms; this subclass has subprogram names of the form _XXYYY with YYY containing the digit "2".
- Subprograms to do some commonly-required low-level computations, such as scaling a matrix, computing a matrix norm, or generating an elementary Householder matrix; these subprograms have names of the form _LAYYY, where YYY designates the specific computation performed.
- Extensions to the BLAS, such as subprograms for applying complex plane rotations, or matrix-vector operations involving complex symmetric matrices; the names of these subprograms are BLAS-like.

Most auxiliary subprograms are not user-visible and, therefore, are not documented in this manual and are not guaranteed to be included in future releases of LAPACK.

LAPACK Contents

The driver subprograms provided in LAPACK are shown in Table 1-4. Table 1-5 identifies the computational subroutines for the solution of systems of linear equations. The computational subroutine names for the solution of least squares problems are given in Table 1-6. Table 1-7 lists the computational subroutines in LAPACK for finding the eigenvalues and eigenvectors of matrices. Table 1-8 shows the names of the LAPACK computational subprograms for the singular value decomposition. Finally, see Table 1-9 for a list of LAPACK auxiliary subprograms.

Following is the key for the table entries in Tables 1-4 to 1-8:

"√" — Subprogram name begins with S, D, C, and Z.
"S" — Subprogram name begins with S and D only.
"C" — Subprogram name begins with C and Z only.
"-" — There are no subprograms with that XXYYY combination.

Table 1-4 Driver Subprograms

Computation	Matrix Form (XX)														
(YYY)	GB	GE	GG	GT	HB	HE	HP	PB	PO	PP	PT	SB	SP	ST	SY
ES	-	√	-	-	-	-	-	-	-	-	-	-	-	-	-
ESX	-	√	-	-	-	-	-	-	-	-	-	-	-	-	-
EV	-	√	-	-	C	C	C	-	-	-	-	S	S	S	S
EVD	-	-	-	-	C	C	C	-	-	-	-	S	S	S	S
EVX	-	√	-	-	C	C	C	-	-	-	-	S	S	S	S
GLM	-	-	√	-	-	-	-	-	-	-	-	-	-	-	-
GS	-	√	-	-	-	-	-	-	-	-	-	-	-	-	-
GV	-	√	-	-	C	C	C	-	-	-	-	S	S	-	S
LS	-	√	-	-	-	-	-	-	-	-	-	-	-	-	-
LSE	-	-	√	-	-	-	-	-	-	-	-	-	-	-	-
LSS	-	√	-	-	-	-	-	-	-	-	-	-	-	-	-
LSX	-	√	-	-	-	-	-	-	-	-	-	-	-	-	-
SV	√	√	-	√	-	C	C	√	√	√	√	-	√	-	√
SVD	-	√	√	-	-	-	-	-	-	-	-	-	-	-	-
SVX	√	√	-	√	-	C	C	√	√	√	√	-	√	-	√

Table 1-5 Computational Subprograms for Linear Equations

Computation	Matrix Form (XX)												
(YYY)	GB	GE	GT	HE	HP	PB	PO	PP	PT	SP	SY	TB	TP	TR
CON	√	√	√	C	C	√	√	√	√	√	√	√	√	√
EQU	√	√	-	-	-	√	√	√	-	-	-	-	-	-
RFS	√	√	√	C	C	√	√	√	√	√	√	√	√	√
TRF	√	√	√	C	C	√	√	√	√	√	√	-	-	-
TRI	-	√	-	C	C	-	√	√	-	√	√	-	√	√
TRS	√	√	√	C	C	√	√	√	√	√	√	√	√	√

Table 1-6 Computational Subprograms for Least Squares

Computation (YYY)	Matrix Form (XX)				
	GE	GG	OR	TZ	UN
GLQ	-	-	S	-	C
GQL	-	-	S	-	C
GQR	-	-	S	-	C
GRQ	-	-	S	-	C
LQF	√	-	-	-	-
MLQ	-	-	S	-	C
MQL	-	-	S	-	C
MQR	-	-	S	-	C
MRQ	-	-	S	-	C
QLF	√	-	-	-	-
QPF	√	-	-	-	-
QRF	√	√	-	-	-
RQF	√	√	-	√	-

Table 1-7 Computational Subprograms for Eigenvalue Problems

Computation (YYY)	Matrix Form (XX)																			
	GE	GG	HB	HE	HG	HP	HS	OP	OR	PT	SB	SP	ST	SY	TG	TR	UN	UP	DI	PB
BAK	√	√	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
BAL	√	√	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
EBZ	-	-	-	-	-	-	-	-	-	-	-	-	S	-	-	-	-	-	-	-
EDC	-	-	-	-	-	-	-	-	-	-	-	-	√	-	-	-	-	-	-	-
EIN	-	-	-	-	-	-	√	-	-	-	-	-	√	-	-	-	-	-	-	-
EQR	-	-	-	-	-	-	√	-	-	√	-	-	√	-	-	-	-	-	-	-
EQZ	-	-	-	-	√	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
ERF	-	-	-	-	-	-	-	-	-	-	-	-	S	-	-	-	-	-	-	-
EVC	-	-	-	-	-	-	-	-	-	-	-	-	-	-	√	√	-	-	-	-
EXC	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	√	-	-	-	-
GHR	-	-	-	-	-	-	-	-	S	-	-	-	-	-	-	-	C	-	-	-
GST	-	-	C	C	-	C	-	-	-	-	S	S	-	S	-	-	-	-	-	-
GTR	-	-	-	-	-	-	-	S	S	-	-	-	-	-	-	-	C	C	-	-
HRD	√	√	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
MHR	-	-	-	-	-	-	-	-	S	-	-	-	-	-	-	-	C	-	-	-
MTR	-	-	-	-	-	-	-	S	S	-	-	-	-	-	-	-	C	C	-	-
SEN	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	√	-	-	-	-
SNA	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	√	-	-	S	-
STF	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	√
SYL	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	√	-	-	-	-
TRD	-	-	C	C	-	C	-	-	-	-	S	S	-	S	-	-	-	-	-	-

Table 1-8 Computational Subprograms for Singular Value Decomposition

Computation (YYY)	Matrix Form (XX)						
	BD	GB	GE	GG	OR	TG	UN
BRD	-	√	√	-	-	-	-
GBR	-	-	-	-	S	-	C
MBR	-	-	-	-	S	-	C
SJA	-	-	-	-	-	√	-
SQR	√	-	-	-	-	-	-
SVP	-	-	-	√	-	-	-

Most LAPACK auxiliary subprograms are internal implementation details and are not user-visible. In addition, their subprogram names do not follow the naming convention in Tables 1-1 to 1-3. Table 1-9 lists the names and operations or functions performed by those auxiliary subprograms that are user-visible. Following is the key for the first character of the subprogram names in Table 1-9:

"I"	—	Subprogram name begins with I only.
"_"	—	Subprogram name begins with S, D, C, and Z.
"C"	—	Subprogram name begins with C and Z only.
"S"	—	Subprogram name begins with S and D only.
"X"	—	Subprogram name begins with X only.

Table 1-9 LAPACK User-Visible Auxiliary Subprograms

Subprogram Name	Operation or Function Performed
ILAENV	Choose Problem-Dependent Parameters
SLAMCH	Choose Machine-Dependent Parameters
_LANGB	Compute a Norm of a General Band Matrix
_LANGE	Compute a Norm of a General Full Matrix
_LANGT	Compute a Norm of a General Tridiagonal Matrix
_LANSB	Compute a Norm of a Symmetric Band Matrix
CLANHB	Compute a Norm of a Hermitian Band Matrix
_LANSP	Compute a Norm of a Symmetric Matrix Stored in Packed Form
CLANHP	Compute a Norm of a Hermitian Matrix Stored in Packed Form
SLANST	Compute a Norm of a Symmetric Tridiagonal Matrix
CLANHT	Compute a Norm of a Hermitian Tridiagonal Matrix
_LANSY	Compute a Norm of a Symmetric Full Matrix
CLANHE	Compute a Norm of a Hermitian Full Matrix
XERBLA	LAPACK Error Handler

Required Data Item Byte Lengths and How to Get Them

Throughout LAPACK, there is a relationship between the data type of a subprogram, designated by the first character of its name, which is denoted by T in Table 1-1, and the byte lengths of its arguments. This relationship, which differs between the LAPACK and the LAPACK8 libraries, is shown in Table 1-10:

Table 1-10 Data Item Byte Length vs. Data Type and Library

T	LAPACK Argument Lengths			LAPACK8 Argument Lengths		
	INTEGER LOGICAL	REAL	COMPLEX	INTEGER LOGICAL	REAL	COMPLEX
S	4	4	†	8	8	†
D	4	8	†	‡	‡	‡
C	4	4	8	8	8	16
Z	4	8	16	‡	‡	‡

† - no user-visible LAPACK S and D subprograms have COMPLEX arguments.

‡ - the D and Z subprograms are not included in LAPACK8.

As mentioned in "Two LAPACK Libraries," you may want to run a 32-bit precision program with 64 bits of precision. To support changing the precision without changing the code, Hewlett-Packard Fortran 90 compilers provide two compilation options, namely, **+autodbl** and **+autodbl4**, that affect the size of Fortran data types. By taking care in your use of Fortran data type declarations, you can write a program that will compile with one set of compiler options and run correctly in 32-bit precision with the LAPACK library or compile with another set of compiler options and run correctly in 64-bit precision with LAPACK8. One constraint is that the program must not use any D or Z subprograms from LAPACK, because the D and Z subprograms are not included in LAPACK8. (Note that a program that calls D or Z LAPACK subprograms would not be a 32-bit program.)

Another scenario is that you might be porting a program from a computer with default 8-byte integer and real data items, and you want to use 4-byte integers while continuing to use 8-byte reals. A program change is required, since the original program would be using the S and C LAPACK subprograms, while the Hewlett-Packard version would have to use the D and Z subprograms from the LAPACK library because they are the only ones that combine 4-byte integers with 8-byte reals. The C preprocessor **#define** statement may be an appropriate conversion tool. Or, for example, the *f90* command line options **+cpp –DSGBSV=DGBSV –Dsgbsv=dgbsv** may be used to translate all SGBSV references to DGBSV. You can deal with constants by replacing them with variables or using the Fortran **PARAMETER** statement.

Table 1-11 shows how the lengths of data items depends on their declarations and the compiler options used.

Table 1-11 Data Item Byte Length vs. Declaration and Compiler Option

Fortran Declaration	Fortran Compiler Option		
	none	+autodbl	+autodbl4
INTEGER	4	8	8
INTEGER*4	4	4	4
INTEGER*8	8	8	8
Integer by default	4	8	8
REAL	4	8	8
REAL*4	4	4	4
REAL*8	8	8	8
Real by default	4	8	8
DOUBLE PRECISION	8	16	8
Double Precision constant	8	16	8
COMPLEX	8	16	16
COMPLEX*8	8	8	8
COMPLEX*16	16	16	16
Complex constant	8	16	16
DOUBLE COMPLEX	16	16	16
Double Complex constant	16	16	16
LOGICAL	4	8	8
LOGICAL*4	4	4	4
LOGICAL*8	8	8	8
Logical constant	4	8	8

By comparing Tables 1-10 and 1-11, you notice that if the Fortran data types are not given length specifiers (for example, **REAL** is used instead of **REAL*4**) and neither of the compiler options, **+autodbl** or **+autodbl4**, are used, the LAPACK library is type compatible for the I, S, C prefixes and also for D if the type is DOUBLE PRECISION. On the other hand, if no length specifiers are used and one of these compiler options is chosen, LAPACK8 is type-compatible for the I, S, and C prefixes. This provides the easiest interchangeability between 32-bit and 64-bit execution.

In cases of mixed data types, you must choose the correct LAPACK library and subprogram carefully. In particular, LAPACK8 accepts no INTEGER*4 arguments. For more information on Fortran data types and Fortran compiler options refer to a Fortran language reference.

Error Handling

Most documented subprograms have a diagnostic argument **info**, which reports the success or failure of the computation, as follows:

info = 0	Successful exit
info < 0	Invalid value of an argument—computation not completed
info > 0	Failure during the computation

All LAPACK driver and computational subprograms, and some auxiliary subprograms, check that numeric-valued input arguments such as **n** and **lda**, and character-valued option arguments such as **trans** and **uplo**, have permitted values. If the k-th argument is invalid, the subprogram sets **info** = $-k$ and calls the error handling subprogram XERBLA.

The standard version of XERBLA writes an error message onto the standard error file. If your main program is in Fortran, a call traceback is also written onto the standard error file. XERBLA then terminates execution with a nonzero exit status. Thus, using the standard version of XERBLA, no LAPACK subprogram would ever return to the calling program with **info** < 0. You may supply a version of XERBLA that alters this action.

The description of each high level subprogram defines the specific error code numbers and the related error conditions when **info** ≠ 0. Always check the output argument **info** after calling an LAPACK subprogram that has **info** as an argument and take appropriate action should the output argument suggest a problem.

HP MLIB Man Pages

The *HP MLIB Man Pages* contain online documentation that includes information from the *HP MLIB LAPACK User's Guide*. This reference contains an introduction to LAPACK and to each set of subprograms in LAPACK and reference entries for each subprogram.

This reference is provided for users to easily and efficiently obtain online information on LAPACK. Because of the limited number of fonts supported and the difficulty of presenting mathematical equations in the *man*(1) system, the *HP MLIB Man Pages* is not a substitute for the user's guides; the most detailed information on LAPACK is in the user's guide.

The *HP MLIB Man Pages* are installed in the directory */opt/mlib/share/man*. You must have this path in your MANPATH environment variable to access man pages for VECLIB, SCILIB, or LAPACK.

For further explanation and a table of contents of reference entries for LAPACK, refer to the *lapack*(3m) entry by typing

man lapack

after you have added */opt/mlib/share/man* to your MANPATH environment variable.

Support Services

Hewlett-Packard maintains a staff to provide technical help if you have difficulty. Located in the Hewlett-Packard Convex Technical Assistance Center (TAC), these people are the primary link between you and the company, and they stand ready to assist you with any difficulties. Note, though, that LAPACK has been tested extensively and is very reliable. Therefore, before contacting the TAC about a LAPACK problem, follow this procedure to isolate the cause of the trouble and to simplify the job of resolving it:

- Check any error response provided by the subprogram in question. The subprogram descriptions in this manual describe how to check an error response. If the answer is wrong because an error has been detected, correct the cause of the error and run the job again.
- Verify that the subprogram usage in the program matches the subprogram specifications in this manual. Pay special attention to the number of arguments in the **CALL** statement and to the declarations of arrays and integer constants or variables that describe them. If everything is in order, write out all the arguments immediately before and after the **CALL** statement.
- Make sure there really is a problem. For example, if an apparently incorrect answer is being computed, check to see if the answer does satisfy the problem as defined in the program. Also, for problems with more than one answer, LAPACK may produce a different answer or give the answers in a different order than expected. If the problem is ill-conditioned, LAPACK may not be able to compute a reliable answer at all. Again, error messages often suggest the cause of the problem.
- Isolate the problem. If possible, write a small test program that encounters the same difficulty. Perhaps data causing the problem may be written out from the original program and read into the small one. Try to remove the problem area from a large program and concentrate it in a small program. In this way, you eliminate extraneous code from suspicion. If the problem area is large, try to pare it to a manageable size. For example, if a 50-by-50 linear system fails, try to produce a 2-by-2 system that fails in the same way. Clearly, this is not always possible, but the process often leads to insight.

You will frequently discover a usage error and resolve the problem by following the steps above. If the trouble persists, contact the Technical Assistance Center for help. Providing a small test program and expected answers will help the TAC further analyze the problem.

2 Simple Drivers for Linear Equations

Overview

This chapter explains how to use LAPACK simple drivers to solve systems of linear equations for a variety of types of matrices, including:

- Real and complex general full matrices
- Real and complex general band matrices
- Real symmetric and complex Hermitian positive definite full matrices
- Real symmetric and complex Hermitian positive definite band matrices
- Real and complex general tridiagonal matrices
- Real symmetric and complex Hermitian positive definite tridiagonal matrices
- Real and complex symmetric and complex Hermitian indefinite matrices

The following documents provide supplemental material for this chapter:

- Forsythe, G. and C.B. Moler. *Computer Solution of Linear Algebraic Systems*. Englewood Cliffs, NJ: Prentice-Hall, Inc. 1967.
- Golub, G.H. and C.F. Van Loan. *Matrix Computations*, 2nd Edition. Baltimore, MD: The Johns Hopkins University Press. 1989.

Chapter Objectives

After reading this chapter you will:

- Know how to use the described subprograms
- Know when to use the expert drivers for linear equations described in Chapter 3 or the computational subprograms for linear equations, described in Chapter 4

What You Need to Know to Use These Subprograms

LAPACK simple drivers for linear equations are organized so that it is usually necessary to call only one subprogram to solve one or more systems of linear equations. All systems must use the same coefficient matrix, and the different right-hand sides must be given all at once. If these conditions do not hold, use the subprograms in Chapter 4.

Simple drivers for linear equations use a somewhat faster test for singularity than the expert drivers described in Chapter 3. The simple drivers simply look for a pivot element that is zero, while the expert driver test is based on an estimate of the condition number of the coefficient matrix. The condition number test is significantly more reliable, so if you are more concerned about singularity than short run time, use the expert driver subprograms in Chapter 3.

NAME

SGBSV/DGBSV/CGBSV/ZGBSV – Solve General Band Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is a band matrix of order n and X and B are n-by-$nrhs$ matrices. A band matrix is a matrix whose nonzero elements all lie near the principal diagonal. Specifically, $a_{ij} = 0$ if $i-j > kl$ or $j-i > ku$ for some integers kl and ku. The smallest such kl and ku for a given matrix are called the lower and upper bandwidths, respectively, and $k = kl+ku+1$ is the total bandwidth.

Tridiagonal matrices are the special case $kl = ku = 1$. They can be handled more efficiently by LAPACK subprograms SGTSV, DGTSV, CGTSV, or ZGTSV. For positive definite band matrices, use SPBSV, DPBSV, CPBSV, or ZPBSV. These subprograms are documented elsewhere in this chapter.

Gaussian elimination with partial pivoting and row interchanges is used to factor A as $A = PLU$, where P is a permutation matrix, L is unit lower triangular 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 $AX = B$.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, you need only provide the elements within the band of A. Compared to storing the entire matrix, this can save memory if $2kl+ku+1 < n$.

The following example illustrates the storage of general band matrices. Consider the following matrix A of order $n = 9$ and lower and upper bandwidths $kl = 2$ and $ku = 3$, respectively:

11	12	13	14	0	0	0	0	0
21	22	23	24	25	0	0	0	0
31	32	33	34	35	36	0	0	0
0	42	43	44	45	46	47	0	0
0	0	53	54	55	56	57	58	0
0	0	0	64	65	66	67	68	69
0	0	0	0	75	76	77	78	79
0	0	0	0	0	86	87	88	89
0	0	0	0	0	0	97	98	99

When Gaussian elimination is performed on a general band matrix, pivoting introduces nonzero elements above the band. L can be stored with a lower bandwidth of kl, but U requires an upper bandwidth of $kl+ku$. You must, therefore, provide storage for the extra kl diagonals. This is done by presenting the original matrix to the subprogram in an array large enough to satisfy the additional storage requirements. Thus, for the above matrix, A is given in an array **ab** with at least $2kl+ku+1 = 8$ rows and $n = 9$ columns as follows:

*	*	*	*	*	+	+	+	+
*	*	*	*	+	+	+	+	+
*	*	*	14	25	36	47	58	69
*	*	13	24	35	46	57	68	79
*	12	23	34	45	56	67	78	89
11	22	33	44	55	66	77	88	99
21	32	43	54	65	76	87	98	*
31	42	53	64	75	86	97	*	*

The asterisks in the $(kl+ku)$-by-$(kl+ku)$ triangle at the upper left corner and in the kl-by-kl triangle at the lower right corner represent elements of **ab** that are not referenced, and the plus signs in the first kl rows indicate elements that may be filled in during the factorization. Thus, if a_{ij} is an element within the band of A, then it is stored in **ab**$(kl+ku+1+i-j,j)$. Therefore, the columns of A are stored in the columns of **ab**, and the diagonals of A are stored in the rows of **ab**, such that the principal diagonal is stored in row $kl+ku+1$ of **ab**.

Usage

LAPACK:

```
INTEGER*4          info, kl, ku, ldab, ldb, n, nrhs
INTEGER*4          ipiv(n)
REAL*4             ab(ldab, n), b(ldb, nrhs)
CALL SGBSV(n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)

INTEGER*4          info, kl, ku, ldab, ldb, n, nrhs
INTEGER*4          ipiv(n)
REAL*8             ab(ldab, n), b(ldb, nrhs)
CALL DGBSV(n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)

INTEGER*4          info, kl, ku, ldab, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*8          ab(ldab, n), b(ldb, nrhs)
CALL CGBSV(n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)

INTEGER*4          info, kl, ku, ldab, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*16         ab(ldab, n), b(ldb, nrhs)
```

```
CALL ZGBSV(n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)
```

LAPACK8:

```
INTEGER*8          info, kl, ku, ldab, ldb, n, nrhs
INTEGER*8          ipiv(n)
REAL*8             ab(ldab, n), b(ldb, nrhs)
CALL SGBSV(n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)

INTEGER*8          info, kl, ku, ldab, ldb, n, nrhs
INTEGER*8          ipiv(n)
COMPLEX*16         ab(ldab, n), b(ldb, nrhs)
CALL CGBSV(n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)
```

Input

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

kl The number of subdiagonals within the band of A. **kl** ≥ 0.

ku The number of superdiagonals within the band of A. **ku** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ab The matrix A in band storage, in rows **kl**+1 to 2**kl**+**ku**+1; rows 1 to **kl** of the array need not be set. The j-th column of A is stored in the j-th column of the array **ab** as follows: **ab**(**kl**+**ku**+1+i–j,j) = $A(i,j)$ for max(1,j–**ku**) $\leq i \leq$ min(**n**,j+**kl**).

ldab The leading dimension of array **ab** in the calling program unit. **ldab** $\geq$ 2**kl**+**ku**+1.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** $\geq$ max(1,**n**).

Output

ab On successful exit, details of the factorization. U is an upper triangular band matrix with **kl**+**ku** superdiagonals, stored in rows 1 to **kl**+**ku**+1. The multipliers, L, used during the factorization, are stored in rows **kl**+**ku**+2 to 2**kl**+**ku**+1.

ipiv On successful exit, the pivot indices that define the permutation matrix P; row i of the matrix was interchanged with row **ipiv**(i).

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k, $U(k,k)$ is zero. The factorization has been completed, but the factor U is singular, and the solution has not been computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

n < 0,
kl < 0,
ku < 0,
nrhs < 0,
ldab < 2**kl**+**ku**+1, and
ldb < max(1,**n**).

NAME

SGESV/DGESV/CGESV/ZGESV – Solve General Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n matrix and X and B are n-by-$nrhs$ matrices.

Gaussian elimination with partial pivoting and row interchanges is used to factor A as $A = PLU$, 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 $AX = B$.

Usage

LAPACK:

```
INTEGER*4          info, lda, ldb, n, nrhs
INTEGER*4          ipiv(n)
REAL*4             a(lda, n), b(ldb, nrhs)
CALL SGESV(n, nrhs, a, lda, ipiv, b, ldb, info)

INTEGER*4          info, lda, ldb, n, nrhs
INTEGER*4          ipiv(n)
REAL*8             a(lda, n), b(ldb, nrhs)
CALL DGESV(n, nrhs, a, lda, ipiv, b, ldb, info)

INTEGER*4          info, lda, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*8          a(lda, n), b(ldb, nrhs)
CALL CGESV(n, nrhs, a, lda, ipiv, b, ldb, info)

INTEGER*4          info, lda, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*16         a(lda, n), b(ldb, nrhs)
CALL ZGESV(n, nrhs, a, lda, ipiv, b, ldb, info)
```

LAPACK8:

```
INTEGER*8          info, lda, ldb, n, nrhs
INTEGER*8          ipiv(n)
REAL*8             a(lda, n), b(ldb, nrhs)
CALL SGESV(n, nrhs, a, lda, ipiv, b, ldb, info)

INTEGER*8          info, lda, ldb, n, nrhs
INTEGER*8          ipiv(n)
COMPLEX*16         a(lda, n), b(ldb, nrhs)
CALL CGESV(n, nrhs, a, lda, ipiv, b, ldb, info)
```

Input

n	The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.
nrhs	The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.
a	The **n**-by-**n** matrix of coefficients A.
lda	The leading dimension of array **a** in the calling program unit. **lda** $\geq \max(1,\mathbf{n})$.
b	The **n**-by-**nrhs** matrix of right hand side vectors for the system of equations $AX = B$.
ldb	The leading dimension of array **b** in the calling program unit. **ldb** $\geq \max(1,\mathbf{n})$.

Output

a	On successful exit, the factors L and U from the factorization $A = PLU$; the unit diagonal elements of L are not stored.	
ipiv	On successful exit, the pivot indices that define the permutation matrix P; row i of the matrix was interchanged with row **ipiv**(i).	
b	On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k, $U(k,k)$ is zero. The factorization has been completed, but the factor U is singular, so the solution could not be computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

n < 0,
nrhs < 0,

lda < max(1,**n**), and
ldb < max(1,**n**).

NAME

SGTSV/DGTSV/.../ZGTSV – Solve General Tridiagonal Linear System

Purpose

These subprograms solve the equation $AX = B$, where A is an n-by-n tridiagonal matrix, by Gaussian elimination with partial pivoting. A tridiagonal matrix $A = (a_{ij})$ is a matrix whose nonzero elements lie only on the principal diagonal ($i = j$), the subdiagonal ($i = j+1$), and the superdiagonal ($i = j-1$) of the matrix.

Note that the equation $A^TX = B$ may be solved by interchanging the order of the arguments **du** and **dl**, where A^T is the transpose of A.

Matrix Storage

The following example illustrates the storage of general tridiagonal matrices. Consider the following tridiagonal matrix of order $n = 7$:

11	12	0	0	0	0	0
21	22	23	0	0	0	0
0	32	33	34	0	0	0
0	0	43	44	45	0	0
0	0	0	54	55	56	0
0	0	0	0	65	66	67
0	0	0	0	0	76	77

The subdiagonal is stored in array **dl**, the principal diagonal is stored in array **d**, and the superdiagonal is stored in array **du**, as follows:

i	**dl**(i)	**d**(i)	**du**(i)
1	21	11	12
2	32	22	23
3	43	33	34
4	54	44	45
5	65	55	56
6	76	66	67
7		77	

Usage

LAPACK:

```
INTEGER*4          info, ldb, n, nrhs
REAL*4             b(ldb, nrhs), d(n), dl(n–1), du(n–1)
CALL SGTSV(n, nrhs, dl, d, du, b, ldb, info)

INTEGER*4          info, ldb, n, nrhs
REAL*8             b(ldb, nrhs), d(n), dl(n–1), du(n–1)
CALL DGTSV(n, nrhs, dl, d, du, b, ldb, info)

INTEGER*4          info, ldb, n, nrhs
COMPLEX*8          b(ldb, nrhs), d(n), dl(n–1), du(n–1)
CALL CGTSV(n, nrhs, dl, d, du, b, ldb, info)

INTEGER*4          info, ldb, n, nrhs
COMPLEX*16         b(ldb, nrhs), d(n), dl(n–1), du(n–1)
CALL ZGTSV(n, nrhs, dl, d, du, b, ldb, info)
```

LAPACK8:

```
INTEGER*8          info, ldb, n, nrhs
REAL*8             b(ldb, nrhs), d(n), dl(n–1), du(n–1)
CALL SGTSV(n, nrhs, dl, d, du, b, ldb, info)

INTEGER*8          info, ldb, n, nrhs
COMPLEX*16         b(ldb, nrhs), d(n), dl(n–1), du(n–1)
CALL CGTSV(n, nrhs, dl, d, du, b, ldb, info)
```

Input

n	The order of the matrix A. **n** ≥ 0.
nrhs	The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.
dl	The **n**–1 subdiagonal elements of A.
d	The diagonal elements of A.
du	The **n**–1 superdiagonal elements of A.
b	The **n**-by-**nrhs** matrix of right hand side vectors for the system of equations $AX = B$.
ldb	The leading dimension of array **b** in the calling program unit. **ldb** $\geq \max(1,$**n**$)$.

Output

dl	On successful exit, overwritten by the **n**–2 elements of the second superdiagonal of the upper triangular matrix U from the LU factorization of A, in **dl**(1), ..., **dl**(**n**–2).
d	On successful exit, overwritten by the **n** diagonal elements of U.

du	On successful exit, overwritten by the **n**–1 elements of the first superdiagonal of U.	
b	On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k, $U(k,k)$ is zero, and the solution has not been computed. The factorization has not been completed unless **info** = **n**.

Notes

These subprograms have different functionality and usage than those with the same names in VECLIB. Be sure to load LAPACK before VECLIB if you want these subroutines and use both libraries.

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11) may be replaced with a user-supplied version to change the error procedure. Error conditions are

n < 0,
nrhs < 0, and
ldb < max(1,**n**).

NAME

SPBSV/DPBSV/.../ZPBSV – Solve Positive Definite Band Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n real symmetric or complex Hermitian positive definite band matrix and X and B are n-by-$nrhs$ matrices. A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x; a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

A positive definite band matrix is a positive definite matrix whose nonzero elements all lie fairly near the principal diagonal. Specifically, $a_{ij} = 0$ if $|i-j| > kd$ for some integer kd. The smallest such kd for a given matrix is called the half bandwidth, and $2kd+1$ is called the total bandwidth.

Tridiagonal matrices are the special case $kd = 1$. They can be handled more efficiently by the LAPACK subprograms SPTSV, DPTSV, CPTSV, and ZPTSV.

Cholesky decomposition is used to factor A as $A = U^*U$, if **uplo** = 'U' or 'u', or $A = LL^*$, if **uplo** = 'L' or '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 $AX = B$.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, and since either triangle of A may be obtained from the other, you need only provide the band within one triangle of A. Compared to storing the entire matrix, this can save memory in two ways: only the elements within the band are stored, and of them, only the upper or the lower triangle.

The following examples illustrate the storage of positive definite band matrices. Consider the following matrix A of order $n = 7$ and half bandwidth $kd = 2$:

11	12	13	0	0	0	0
12	22	23	24	0	0	0
13	23	33	34	35	0	0
0	24	34	44	45	46	0
0	0	35	45	55	56	57
0	0	0	46	56	66	67
0	0	0	0	57	67	77

Upper triangular storage. The upper triangle of A is stored in an array **ab** with at least $kd+1 = 3$ rows and 7 columns as follows:

*	*	13	24	35	46	57
*	12	23	34	45	56	67
11	22	33	44	55	66	77

The asterisks represent elements in the kd-by-kd triangle at the upper left corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the upper triangle of A, it is stored in **ab**$(kd+1+i-j,j)$. Therefore, the columns of the upper triangle of A are stored in the columns of **ab**, and the diagonals of the upper triangle of A are stored in the rows of **ab**.

Lower triangular storage. The lower triangle of A is stored in the array **ab** as follows:

11	22	33	44	55	66	77
12	23	34	45	56	67	*
13	24	35	46	57	*	*

The asterisks represent elements in the kd-by-kd triangle at the lower right corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the lower triangle of A, it is stored in **ab**$(1+i-j,j)$. Therefore, the columns of the lower triangle of A are stored in the columns of **ab**, and the diagonals of the lower triangle of A are stored in the rows of **ab**.

Usage

LAPACK:

```
CHARACTER*1          uplo
INTEGER*4            info, kd, ldab, ldb, n, nrhs
REAL*4               ab(ldab, n), b(ldb, nrhs)
CALL SPBSV(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, kd, ldab, ldb, n, nrhs
REAL*8               ab(ldab, n), b(ldb, nrhs)
CALL DPBSV(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, kd, ldab, ldb, n, nrhs
COMPLEX*8            ab(ldab, n), b(ldb, nrhs)
CALL CPBSV(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)
```

```
CHARACTER*1      uplo
INTEGER*4        info, kd, ldab, ldb, n, nrhs
COMPLEX*16       ab(ldab, n), b(ldb, nrhs)
CALL ZPBSV(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1      uplo
INTEGER*8        info, kd, ldab, ldb, n, nrhs
REAL*8           ab(ldab, n), b(ldb, nrhs)
CALL SPBSV(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)

CHARACTER*1      uplo
INTEGER*8        info, kd, ldab, ldb, n, nrhs
COMPLEX*16       ab(ldab, n), b(ldb, nrhs)
CALL CPBSV(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)
```

Input

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or '1': The lower triangular part of A is stored.

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

kd The number of superdiagonals of the matrix A if **uplo** = 'U' or 'u', or the number of subdiagonals if **uplo** = 'L' or '1'. **kd** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ab The upper or lower triangle of the symmetric or Hermitian band matrix A, stored in the first **kd**+1 rows of the array. The j-th column of A is stored in the j-th column of the array **ab** as follows:

If **uplo** = 'U' or 'u', **ab**(**kd**+1+i–j,j) = $A(i,j)$ for max(1,j–**kd**) $\leq i \leq j$;

If **uplo** = 'L' or '1', **ab**(1+i–j,j) = $A(i,j)$ for $j \leq i \leq$ min (**n**,j+**kd**).

ldab The leading dimension of array **ab** in the calling program unit. **ldab** $\geq$ **kd**+1.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

Output

ab On successful exit, 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.

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, the leading minor of order k of A is not positive definite, so the factorization could not be completed, and the solution has not been computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
kd < 0,
nrhs < 0,
ldab < **kd**+1, and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPOSV/DPOSV/CPOSV/ZPOSV – Solve Positive Definite Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n real symmetric or complex Hermitian positive definite matrix and X and B are n-by-$nrhs$ matrices. A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x; a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

Cholesky decomposition is used to factor A as $A = U^*U$ if **uplo** = 'U' or 'u', or $A = LL^*$ if **uplo** = 'L' or '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 $AX = B$.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A. You may supply either the upper or the lower triangle of A, in a two-dimensional array large enough to hold the entire array. The other triangle of the array is not referenced.

Usage

LAPACK:

```
CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
REAL*4             a(lda, n), b(ldb, nrhs)
CALL SPOSV(uplo, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
REAL*8             a(lda, n), b(ldb, nrhs)
CALL DPOSV(uplo, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
COMPLEX*8          a(lda, n), b(ldb, nrhs)
CALL CPOSV(uplo, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
COMPLEX*16         a(lda, n), b(ldb, nrhs)
CALL ZPOSV(uplo, n, nrhs, a, lda, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, lda, ldb, n, nrhs
REAL*8             a(lda, n), b(ldb, nrhs)
CALL SPOSV(uplo, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1        uplo
INTEGER*8          info, lda, ldb, n, nrhs
COMPLEX*16         a(lda, n), b(ldb, nrhs)
CALL CPOSV(uplo, n, nrhs, a, lda, b, ldb, info)
```

Input

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or 'l': The lower triangular part of A is stored.

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

a The upper or lower triangle of the symmetric or Hermitian matrix A.

If **uplo** = 'U' or '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' or '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 The leading dimension of array **a** in the calling program unit. **lda** $\geq \max(1,\mathbf{n})$.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** $\geq \max(1,\mathbf{n})$.

Output

a On successful exit, if **uplo** = 'U' or 'u', the upper triangular part of A has been overwritten by U, or if **uplo** = 'L' or 'l', the lower triangular part of A has been overwritten by L.

b	On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k, the leading minor of order k of A is not positive definite, so the factorization could not be completed, and the solution has not been computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
nrhs < 0,
lda < max(1,**n**), and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPPSV/DPPSV/.../ZPPSV – Solve Positive Definite Packed Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n real symmetric or complex Hermitian positive definite matrix stored in packed form and X and B are n-by-$nrhs$ matrices. A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x; a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

The Cholesky decomposition is used to factor A as $A = U^*U$ if **uplo** = 'U' or 'u', or $A = LL^*$ if **uplo** = 'L' or '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 $AX = B$.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A, either the upper or the lower triangle. Compared to storing the entire matrix, you save memory by supplying that triangle stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular storage. If the lower triangle of A is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**($i+(j-1)\times(2n-j)/2$).

Usage

LAPACK:

```
CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
REAL*4               ap((n*(n+1))/2), b(ldb, nrhs)
CALL SPPSV(uplo, n, nrhs, ap, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
REAL*8               ap((n*(n+1))/2), b(ldb, nrhs)
CALL DPPSV(uplo, n, nrhs, ap, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
COMPLEX*8            ap((n*(n+1))/2), b(ldb, nrhs)
CALL CPPSV(uplo, n, nrhs, ap, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
COMPLEX*16           ap((n*(n+1))/2), b(ldb, nrhs)
CALL ZPPSV(uplo, n, nrhs, ap, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1          uplo
INTEGER*8            info, ldb, n, nrhs
REAL*8               ap((n*(n+1))/2), b(ldb, nrhs)
CALL SPPSV(uplo, n, nrhs, ap, b, ldb, info)
```

```
CHARACTER*1     uplo
INTEGER*8       info, ldb, n, nrhs
COMPLEX*16      ap((n*(n+1))/2), b(ldb, nrhs)
CALL CPPSV(uplo, n, nrhs, ap, b, ldb, info)
```

Input

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or 'l': The lower triangular part of A is stored.

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ap The upper or lower triangle of the symmetric or Hermitian 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' or 'u', **ap**$(i + (j-1) \times j/2) = A(i,j)$ for $1 \leq i \leq j$;

If **uplo** = 'L' or 'l', **ap**$(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \leq i \leq \mathbf{n}$.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** $\geq \max(1,\mathbf{n})$.

Output

ap On successful exit, the factor U or L, from the Cholesky factorization $A = U^*U$ or $A = LL^*$, overwrites the input in the same storage format as A.

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info Status response:

- **info** = 0: Successful exit.
- **info** < 0: If **info** = $-k$, the k-th argument had an invalid value.

info > 0:	If **info** = k, the leading minor of order k of A is not positive definite, so the factorization could not be completed, and the solution has not been computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
nrhs < 0, and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPTSV/.../ZPTSV – Solve Positive Definite Tridiagonal Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n real symmetric or complex Hermitian positive definite tridiagonal matrix, and X and B are n-by-$nrhs$ matrices. A tridiagonal matrix $A = (a_{ij})$ is a matrix whose nonzero elements lie only on the principal diagonal ($i = j$), the subdiagonal ($i = j+1$), and the superdiagonal ($i = j-1$) of the matrix.

A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x; a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

Matrix Storage

The following example illustrates the storage of symmetric or Hermitian tridiagonal matrices. Consider the following symmetric tridiagonal matrix of order $n = 7$:

11	21	0	0	0	0	0
21	22	32	0	0	0	0
0	32	33	43	0	0	0
0	0	43	44	54	0	0
0	0	0	54	55	65	0
0	0	0	0	65	66	76
0	0	0	0	0	76	77

The subdiagonal is stored in array **e** and the principal diagonal is stored in array **d**, as follows:

i	**e**(i)	**d**(i)
1	21	11
2	32	22
3	43	33
4	54	44
5	65	55
6	76	66
7		77

Usage

LAPACK:

```
INTEGER*4          info, ldb, n, nrhs
REAL*4             b(ldb, nrhs), d(n), e(n–1)
CALL SPTSV(n, nrhs, d, e, b, ldb, info)

INTEGER*4          info, ldb, n, nrhs
REAL*8             b(ldb, nrhs), d(n), e(n–1)
CALL DPTSV(n, nrhs, d, e, b, ldb, info)

INTEGER*4          info, ldb, n, nrhs
REAL*4             d(n)
COMPLEX*8          b(ldb, nrhs), e(n–1)
CALL CPTSV(n, nrhs, d, e, b, ldb, info)

INTEGER*4          info, ldb, n, nrhs
REAL*8             d(n)
COMPLEX*16         b(ldb, nrhs), e(n–1)
CALL ZPTSV(n, nrhs, d, e, b, ldb, info)
```

LAPACK8:

```
INTEGER*8          info, ldb, n, nrhs
REAL*8             b(ldb, nrhs), d(n), e(n–1)
CALL SPTSV(n, nrhs, d, e, b, ldb, info)

INTEGER*8          info, ldb, n, nrhs
REAL*8             d(n)
COMPLEX*16         b(ldb, nrhs), e(n–1)
CALL CPTSV(n, nrhs, d, e, b, ldb, info)
```

Input

n	The order of the matrix A. $\mathbf{n} \geq 0$.
nrhs	The number of right hand sides, that is, the number of columns of the matrix B. $\mathbf{nrhs} \geq 0$.
d	The **n** diagonal elements of the tridiagonal matrix A.
e	The **n**–1 subdiagonal elements of the tridiagonal matrix A.
b	The **n**-by-**nrhs** matrix of right hand side vectors for the system of equations $AX = B$.
ldb	The leading dimension of array **b** in the calling program unit. $\mathbf{ldb} \geq \max(1,\mathbf{n})$.

Output

d	On successful exit, the **n** diagonal elements of the diagonal matrix D from the LDL^* factorization of A.

e	On successful exit, the **n**–1 subdiagonal elements of the unit bidiagonal factor L from the LDL^* factorization of A. **e** can also be regarded as the superdiagonal of the unit bidiagonal factor U from the U^*DU factorization of A.	
b	On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k, the leading minor of order k is not positive definite, and the solution has not been computed. The factorization has not been completed unless **info** = **n**.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

n < 0,
nrhs < 0, and
ldb < max(1,**n**).

NAME

SSPSV/.../ZSPSV – Solve Symmetric or Hermitian Packed Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n real or complex symmetric or complex Hermitian matrix stored in packed form and X and B are n-by-$nrhs$ matrices. If A is known to be positive definite, other subprograms in this chapter, specifically designed for positive definite matrices, are more efficient than these subprograms.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

The structure of A is indicated by the name of the subprogram used:

SSPSV or	DSPSV A is a real symmetric packed matrix.
CSPSV or	ZSPSV A is a complex symmetric packed matrix.
CHPSV or	ZHPSV A is a complex Hermitian packed matrix.

If A is real or complex symmetric, the factorization has the form $A = UDU^T$ or $A = LDL^T$ where U is a product of permutation and unit upper triangular matrices, $L$is a product of permutation and unit lower triangular matrices, and $D$is symmetric and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

If A is complex Hermitian, the factorization has the form $A = UDU^*$ or $A = LDL^*$ where U and L are as above, 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 $AX = B$.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A, either the upper or the lower triangle. Compared to storing the entire matrix, you save memory by supplying that triangle stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular storage. If the lower triangle of A is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**(i+(j–1)×(2n–j)/2).

Usage

LAPACK:

```
CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
INTEGER*4            ipiv(n)
REAL*4               ap((n*(n+1))/2), b(ldb, nrhs)
CALL SSPSV(uplo, n, nrhs, ap, ipiv, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
INTEGER*4            ipiv(n)
REAL*8               ap((n*(n+1))/2), b(ldb, nrhs)
CALL DSPSV(uplo, n, nrhs, ap, ipiv, b, ldb, info)
```

```
CHARACTER*1        uplo
INTEGER*4          info, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*8          ap((n*(n+1))/2), b(ldb, nrhs)
CALL CHPSV(uplo, n, nrhs, ap, ipiv, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*8          ap((n*(n+1))/2), b(ldb, nrhs)
CALL CSPSV(uplo, n, nrhs, ap, ipiv, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2), b(ldb, nrhs)
CALL ZHPSV(uplo, n, nrhs, ap, ipiv, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2), b(ldb, nrhs)
CALL ZSPSV(uplo, n, nrhs, ap, ipiv, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, ldb, n, nrhs
INTEGER*8          ipiv(n)
REAL*8             ap((n*(n+1))/2), b(ldb, nrhs)
CALL SSPSV(uplo, n, nrhs, ap, ipiv, b, ldb, info)

CHARACTER*1        uplo
INTEGER*8          info, ldb, n, nrhs
INTEGER*8          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2), b(ldb, nrhs)
CALL CHPSV(uplo, n, nrhs, ap, ipiv, b, ldb, info)

CHARACTER*1        uplo
INTEGER*8          info, ldb, n, nrhs
INTEGER*8          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2), b(ldb, nrhs)
CALL CSPSV(uplo, n, nrhs, ap, ipiv, b, ldb, info)
```

Input

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or 'l': The lower triangular part of A is stored.

n The number of linear equations, that is, the order of the matrix A. $\mathbf{n} \geq 0$.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. $\mathbf{nrhs} \geq 0$.

ap The upper or lower triangle as part of the symmetric 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' or 'u', $\mathbf{ap}(i + (j-1) \times j/2) = A(i,j)$ for $1 \leq i \leq j$;

If **uplo** = 'L' or 'l', $\mathbf{ap}(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \leq i \leq \mathbf{n}$.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. $\mathbf{ldb} \geq \max(1,\mathbf{n})$.

Output

ap On successful exit, the block diagonal matrix D and the multipliers used to obtain the factor U or L from the factorization $A = U^T DU$ or $A = LDL^T$, stored as a packed triangular matrix in the same storage format as A.

ipiv On successful exit, details of the interchanges and the block structure of D:

If $\mathbf{ipiv}(k) > 0$, then rows and columns k and $\mathbf{ipiv}(k)$ were interchanged, and $D(k,k)$ is a 1-by-1 diagonal block.

If **uplo** = 'U' or 'u' and $\mathbf{ipiv}(k) = \mathbf{ipiv}(k-1) < 0$, then rows and columns $k-1$ and $-\mathbf{ipiv}(k)$ were interchanged and $D(k-1{:}k,k-1{:}k)$ is a 2-by-2 diagonal block.

If **uplo** = 'L' or 'l' and $\mathbf{ipiv}(k) = \mathbf{ipiv}(k+1) < 0$, then rows and columns $k+1$ and $-\mathbf{ipiv}(k)$ were interchanged and $D(k{:}k+1,k{:}k+1)$ is a 2-by-2 diagonal block.

b	On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k, D (k,k) is zero. The factorization has been completed, but the block diagonal matrix D is singular, so the solution could not be computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
nrhs < 0, and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SSYSV/.../ZHESV/ZSYSV – Solve Symmetric or Hermitian Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n real or complex symmetric or complex Hermitian matrix and X and B are n-by-$nrhs$ matrices. If A is known to be positive definite, other subprograms in this chapter, specifically designed for positive definite matrices, are more efficient than these subprograms.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

The structure of A is indicated by the name of the subprogram used:

SSYSV	or	DSYSV	A is a real symmetric matrix.
CSYSV	or	ZSYSV	A is a complex symmetric matrix.
CHESV	or	ZHESV	A is a complex Hermitian matrix.

If A is real or complex symmetric, the factorization has the form $A = UDU^T$ or $A = LDL^T$ where U is a product of permutation and unit upper triangular matrices, L is a product of permutation and unit lower triangular matrices, and $D$is symmetric and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

If A is complex Hermitian, the factorization has the form $A = UDU^*$ or $A = LDL^*$ where U and L are as above, 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 $AX = B$.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A. You may supply either the upper or the lower triangle of A, in a two-dimensional array large enough to hold the entire matrix. The other triangle of the array is not referenced.

Usage

LAPACK:

```
CHARACTER*1     uplo
INTEGER*4       info, lda, ldb, lwork, n, nrhs
INTEGER*4       ipiv(n)
REAL*4          a(lda, n), b(ldb, nrhs), work(lwork)
CALL SSYSV(uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info)
```

```
CHARACTER*1     uplo
INTEGER*4       info, lda, ldb, lwork, n, nrhs
INTEGER*4       ipiv(n)
REAL*8          a(lda, n), b(ldb, nrhs), work(lwork)
CALL DSYSV(uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info)

CHARACTER*1     uplo
INTEGER*4       info, lda, ldb, lwork, n, nrhs
INTEGER*4       ipiv(n)
COMPLEX*8       a(lda, n), b(ldb, nrhs), work(lwork)
CALL CHESV(uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info)

CHARACTER*1     uplo
INTEGER*4       info, lda, ldb, lwork, n, nrhs
INTEGER*4       ipiv(n)
COMPLEX*8       a(lda, n), b(ldb, nrhs), work(lwork)
CALL CSYSV(uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info)

CHARACTER*1     uplo
INTEGER*4       info, lda, ldb, lwork, n, nrhs
INTEGER*4       ipiv(n)
COMPLEX*16      a(lda, n), b(ldb, nrhs), work(lwork)
CALL ZHESV(uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info)

CHARACTER*1     uplo
INTEGER*4       info, lda, ldb, lwork, n, nrhs
INTEGER*4       ipiv(n)
COMPLEX*16      a(lda, n), b(ldb, nrhs), work(lwork)
CALL ZSYSV(uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info)
```

LAPACK8:

```
CHARACTER*1     uplo
INTEGER*8       info, lda, ldb, lwork, n, nrhs
INTEGER*8       ipiv(n)
REAL*8          a(lda, n), b(ldb, nrhs), work(lwork)
CALL SSYSV(uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info)

CHARACTER*1     uplo
INTEGER*8       info, lda, ldb, lwork, n, nrhs
INTEGER*8       ipiv(n)
COMPLEX*16      a(lda, n), b(ldb, nrhs), work(lwork)
CALL CHESV(uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info)

CHARACTER*1     uplo
INTEGER*8       info, lda, ldb, lwork, n, nrhs
INTEGER*8       ipiv(n)
COMPLEX*16      a(lda, n), b(ldb, nrhs), work(lwork)
CALL CSYSV(uplo, n, nrhs, a, lda, ipiv, b, ldb, work, lwork, info)
```

Input

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or 'l': The lower triangular part of A is stored.

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

a The upper or lower triangle part of the symmetric matrix A.

If **uplo** = 'U' or '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' or '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 The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

lwork The length of array **work**. **lwork** ≥ max(1,**n**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the block diagonal matrix D and the multipliers used to obtain the factor U or L from the factorization $A = UDU^*$ or $A = LDL^*$.

ipiv On successful exit, details of the interchanges and the block structure of D:

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' or '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' or '1' 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.

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = –k, the k-th argument had an invalid value.
info > 0:	If **info** = k, $D(k,k)$ is zero. The factorization has been completed, but the block diagonal matrix D is singular, so the solution could not be computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or '1' or 'U' or 'u',
n < 0,
nrhs < 0,
lda < max(1,**n**),
ldb < max(1,**n**), and
lwork < 1.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

3 Expert Drivers for Linear Equations

Overview

This chapter explains how to use LAPACK expert driver subprograms to solve systems of linear equations.

This operation is performed for a variety of types of matrices including:

- Real and complex general full matrices
- Real and complex general band matrices
- Real symmetric and complex Hermitian positive definite full matrices
- Real symmetric and complex Hermitian positive definite band matrices
- Real and complex general tridiagonal matrices
- Real symmetric and complex Hermitian positive definite tridiagonal matrices
- Real and complex symmetric and complex Hermitian indefinite matrices

The following documents provide supplemental material for this chapter:

- Anderson, E. *et al. LAPACK Users' Guide*, Second Edition. Philadelphia, PA: Society for Industrial and Applied Mathematics. 1995.
- Forsythe, G. and C.B. Moler. *Computer Solution of Linear Algebraic Systems*. Englewood Cliffs, NJ: Prentice-Hall, Inc. 1967.
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Chapter Objectives

After you read this chapter you will:

- Understand the role of the condition number in solving linear equations
- Know how to compute the inverse of a matrix
- Know when not to compute the inverse of a matrix
- Know how to use the described subprograms

What You Need to Know to Use These Subprograms

LAPACK expert drivers for linear equations are organized so that it is usually necessary to call only one subprogram to solve one or more systems of linear equations. All systems must use the same coefficient matrix, and the different right hand sides must be given all at once. If these conditions do not hold, use the subprograms in Chapter 4.

The expert drivers for linear equations use a significantly more reliable test for singularity than do the simple drivers described in Chapter 2. The expert driver test is based on an estimate of the condition number of the coefficient matrix, while the simple drivers merely look for a pivot element that is zero. The condition number test is slower, so if you are more concerned about run time than singularity, use the simple driver subprograms in Chapter 2.

Condition Number

The standard method for solving a linear system $Ax = b$ is to use Gaussian elimination, usually with some pivoting strategy, to factor a permuted A, for example $PA = LU$, and then to solve the two triangular systems $Ly = Pb$ and $Ux = y$.

Under reasonable assumptions on the floating-point arithmetic and with reasonable assumptions about the matrix A, useful bounds on the errors in the factoring and solution phases can be proven. Ignoring the permutation for now (although some pivoting strategy is necessary to make the bounds valid, unless the matrix has some special property such as positive definiteness) and letting the primed symbols represent computed quantities, some classical error bounds are:

- The computed factorization is the exact factorization of a slightly perturbed A, that is,

$$\|A - L'U'\|_\infty \leq \varepsilon\ p_2(n)\ r(n)\ \|A\|_\infty$$

- The computed solution x' nearly satisfies the specified equations, meaning that the residual is small, that is,

$$\|b - Ax'\|_\infty \leq \varepsilon\ p_3(n)\ r(n)\ \|A\|_\infty\ \|x'\|_\infty$$

- A *backward* error bound: the computed solution x' is an exact solution to a perturbed problem $(A+\delta A)x' = b$, where δA is the perturbation in A and

$$\|\delta A\|_\infty \leq \varepsilon\ p_3(n)\ r(n)\ \|A\|_\infty$$

- A *forward* error bound: the error in x' itself is small if A is not too badly conditioned, that is,

$$\|x' - x\|_\infty \leq \varepsilon\ p_3(n)\ r(n)\ \kappa(A)\ \|x'\|_\infty.$$

In the above, $\|\ \|_\infty$ represents the ∞ vector norm and its subordinate matrix norm, ϵ is the machine precision (the distance from 1.0 to the next greater floating-point number), p_2 and p_3 are polynomials of degree two and three, respectively, with moderate lead coefficients, $r(n)$ is the maximal growth factor of elements of U in the factorization process, and $\kappa(A)$ is the condition number of A, defined as $\|A\|_\infty\ \|A^{-1}\|_\infty$.

The rigorous bounds on $r(n)$ for partial pivoting are pessimistic: $r(n) = O(2^n)$. Such growth in $r(n)$ is never seen in practice. By the consensus of the numerical analysis community, $r(n)$ safely can be replaced by a modestly growing function such as $0.15n$ or even by a constant such as 20. Applying these bounds to a particular problem requires a combination of theoretical knowledge and experience with the problem.

The condition number, $\kappa(A)$, appears frequently in error analysis. Large condition numbers are associated with numerical instability, and infinite or overflowing condition numbers are usually taken to suggest *numerical singularity*. The LAPACK expert drivers for linear equations return an estimate of the condition number. Since $1 < \kappa(A) \leq \infty$, it is more convenient to compute the reciprocal condition number, $1/\kappa(A)$, than $\kappa(A)$ itself. Roughly speaking, the reciprocal condition number has the interpretation that if $1/\kappa(A)$ is about 10^{-d}, elements of x' can be expected to have about d fewer significant digits of accuracy than the elements of A or b. Consequently, if uncertainty in the elements of the coefficient matrix and right hand side exceeds $1/\kappa(A)$, or if $1/\kappa(A)$ is on the order of ϵ, then x' may have no significant digits at all.

Equilibration

Transforming the problem in an attempt to reduce the condition number is a common technique. The expert drivers offer the option of transforming the problem using an operation called *equilibration*. The basic idea is straightforward: letting R and C denote diagonal matrices (standing for "row" and "column" scaling), the problem is transformed from $Ax = b$ to $(RAC)y = Rb$, where $Cy = x$. The goal is to choose R and C to make $\kappa(RAC)$ small, and, in turn, to put an error bound on $\|y' - y\|$ that uses a smaller condition number. This technique often works well in practice. The theoretical justification for this procedure is not air-tight, however, and there are cases where equilibration can lead to larger errors. The following points should be kept in mind:

- The equilibration is not guaranteed to reduce the condition number. In practice, $\kappa(RAC)$ will generally be less than $\kappa(A)$, but that is a heuristically plausible statement that is generally corroborated by experience, not a theorem.
- Reducing the condition number does not guarantee a reduced error bound. It is possible that the maximal growth factor $r(n)$ for matrix RAC could be larger than that for the matrix A.
- Reducing the error bound does not guarantee a reduced error. For example, even if $error_1 \leq bound_1$, $error_2 \leq bound_2$, and $bound_1 < bound_2$, it can still happen that $error_1 > error_2$.
- The error bound for the transformed system is on the y vector. Equivalently, the error bound on the error in x is in a different norm, the C-norm defined by $\|z\|_C = \|C^{-1}z\|$.The appropriateness of the C-norm to the application at hand needs to be considered.

These points in no way deny the usefulness of equilibration. Used with judgment, equilibration is an effective technique that can improve accuracy and broaden the class of solvable problems. But it should not be viewed as a black box guaranteed to eliminate all problems stemming from machine arithmetic and numerical instability.

Iterative Refinement

The classical bounds are unsatisfying in the sense that nothing is known about the relative errors in the individual components of, say, the residual. That is, the error bounds are bounds for the relative errors in vector and matrix norms rather than bounds for the relative error of individual elements. Given knowledge about the structure of A, it might be possible to place stricter bounds on some elements of the residual than on other elements.

Except in pathological cases, the method of iterative refinement used by the expert drivers attains such componentwise bounds and gives estimates for the bounds.

Iterative refinement is motivated by an optimistic but naive idea: if x' is the computed solution and $x'+\delta x$ is the exact solution, then $A(x'+\delta x) = b$, so $A\delta x = b - Ax'$, the residual. Thus, you can compute a correction term for the cost of a matrix-vector multiplication and two triangular solves. Unless the residual is computed in double precision, a cursory analysis leads to pessimism about reducing the error in x'. Somewhat surprisingly, though, recent results have shown that iterative refinement, even without the higher precision residual calculation, can improve the computed solution in certain senses described below.

If M is a matrix or vector, let $|M|$ denote the matrix or vector whose elements are the absolute values of the elements of M. The i-th component of the residual $b - Ax'$ is made small compared to the i-th component of $|A|\ |x| + |b|$, that is, compared to a quantity depending only on the i-th equation. The computed solution is the exact solution of a perturbed system $(A+\delta A)x' = b+\delta b$ where the elements of δA and δb are small compared to their corresponding elements in A and b.

That is the solution is *backward stable in a componentwise relative sense.* Although the componentwise relative error in the computed solution cannot be bounded, the standard condition number $\|A\|\ \|A^{-1}\|$is replaced by a *componentwise condition number*, $\||A^{-1}|\ (|A|\ |x'|+|b|)\|$, that depends on b and x' and takes more advantage of any special structure A and A^{-1} may have. Furthermore, although some terms in the error bounds may not be known (for example $\|A^{-1}\|$), the expert drivers estimate various condition numbers and compute *a posteriori* estimates for the backward and forward error.

The overall situation with equilibration, iterative refinement, and condition number estimation is complicated. See the LAPACK references and the vast literature on error analysis for more details. See (Forsythe and Moler) for an early and easily accessible account of the basic principles. A more recent and more complete account, together with an extensive bibliography, can be found in (Golub and Van Loan). But it should be emphasized that:

- These bounds vary depending on the matrix type. The literature for the particular matrix type should be consulted.
- These bounds depend on reasonable assumptions about the floating point arithmetic.
- Some of the error bounds depend on reasonable hypotheses that seldom appear in bold type, such as $n\,\varepsilon < 0.05$ or $n\,\varepsilon\,\kappa(A) < 1$.
- There are many other potential sources of error in addition to the LAPACK subroutines, such as experimental error, errors in the mathematical model, and truncation errors when the problem is stored in floating-point representation.

Matrix Inversion

Subprograms for computing the inverse of a matrix are provided, although it is almost never necessary to compute one.

While papers and reference books extensively use the notation "$A^{-1}b$" to mean "the solution x of the system of linear equations $Ax = b$," it is more efficient and accurate to compute the solution directly than to invert the coefficient matrix and multiply the inverse times the right hand side vector. This is true even if there are many systems of equations, all using the same coefficient matrix; the matrix may be factored once and the systems may be solved from the factors usually just as efficiently—and more accurately—than by matrix multiplication by the inverse.

NAME

SGBSVX/DGBSVX/.../ZGBSVX – Solve General Band Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is a band matrix of order n with kl subdiagonals and ku superdiagonals, and X and B are n-by-$nrhs$ matrices. You may supply either a new matrix A or an A that was used in a previous call, together with its previously computed scaling matrices, if any, and its L and U factors.

These subroutines perform the following:

1. If you provide a new A matrix and request equilibration (**fact** = 'E' or 'e'), A is analyzed to determine whether or not to do row equilibration, and, independently, whether or not to do column equilibration. If both equilibrations are done, real diagonal scaling matrices, R and C, are computed to equilibrate the system. If row equilibration is not done, R is the identity; if column equilibration is not done, C is the identity. Output argument **equed** indicates which equilibrations were done.

   If you supply a previously factored A matrix (**fact** = 'F' or 'f') and it was equilibrated (**equed** = 'R' or 'r' or 'C' or 'c' or 'B' or 'b'), then the previously computed scaling matrices are used in the solution phase.

   In either case, if equilibration is done, the system actually solved depends upon the **trans** argument as follows:

   If **trans** = 'N' or 'n', equilibrate the system as $(RAC)(C^{-1}X) = RB$.

   If **trans** = 'T' or 't', equilibrate the system as $(RAC)^T(R^{-1}X) = CB$.

   If **trans** = 'C' or 'c', equilibrate the system as $(RAC)^*(R^{-1}X) = CB$.

   If equilibration is done, A is overwritten by RAC.

   If equilibration is done, or if A was factored in a previous call where equilibration was done, then B may be overwritten. Specifically, if **trans** = 'N' or 'n' and **equed** is 'R' or 'r' or 'B' or 'b', then B is overwritten by RB. If **trans** = 'T' or 't' or 'C' or 'c' and **equed** is 'C' or 'c' or 'B' or 'b', then B is overwritten by CB.

2. If **fact** = 'N' or 'n' or 'E' or 'e', A is copied from array **ab** to array **afb** (after equilibration, if performed), where it is factored as $A = PLU$, where P is a permutation matrix, L is a unit lower triangular matrix with kl subdiagonals, and U is upper triangular with as many as $kl+ku$ superdiagonals due to fill-in.

3. 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 the machine precision, steps 4 through 6 are skipped.

4. The system of equations $AX = B$ is solved for X using the factored form of A.
5. Iterative refinement is applied to improve the computed solution vectors and calculate error bounds and backward error estimates.
6. If equilibration was used before factoring the A matrix, X is scaled, if necessary, so as to solve the original system. Specifically, if **trans** = 'N' or 'n' and the final value of **equed** is 'C' or 'c' or 'B' or 'b', then X is premultiplied by C. If **trans** = 'T' or 't' or 'C' or 'c' and the final value of **equed** is 'R' or 'r' or 'B' or 'b', then X is premultiplied by R.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, you need only provide the elements within the band of A. Compared to the expert driver for general full matrices, this expert driver can save memory if $3kl/2+ku+1 < n$.

The following example illustrates the storage of general band matrices. Consider the following matrix A of order $n = 9$ and lower and upper bandwidths $kl = 2$ and $ku = 3$, respectively:

11	12	13	14	0	0	0	0	0
21	22	23	24	25	0	0	0	0
31	32	33	34	35	36	0	0	0
0	42	43	44	45	46	47	0	0
0	0	53	54	55	56	57	58	0
0	0	0	64	65	66	67	68	69
0	0	0	0	75	76	77	78	79
0	0	0	0	0	86	87	88	89
0	0	0	0	0	0	97	98	99

A is given in an array **ab** with at least $kl+ku+1 = 6$ rows and $n = 9$ columns as follows:

*	*	*	14	25	36	47	58	69
*	*	13	24	35	46	57	68	79
*	12	23	34	45	56	67	78	89
11	22	33	44	55	66	77	88	99
21	32	43	54	65	76	87	98	*
31	42	53	64	75	86	97	*	*

The asterisks in the *ku*-by-*ku* triangle at the upper left corner and in the *kl*-by-*kl* triangle at the lower right corner represent elements of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of A, then it is stored in **ab**(*ku*+1+*i*–*j*,*j*). Therefore, the columns of A are stored in the columns of **ab**, and the diagonals of A are stored in the rows of **ab**, such that the principal diagonal is stored in row *ku*+1 of **ab**.

Note that this storage format omits the first *kl* rows reserved for fill-in in the general band storage for _GBSV and _GBTRF.

Usage

LAPACK:

```
CHARACTER*1        equed, fact, trans
INTEGER*4          info, kl, ku, ldab, ldafb, ldb, ldx, n, nrhs
REAL*4             rcond
INTEGER*4          ipiv(n), iwork(n)
REAL*4             ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), berr(nrhs),
                   c(n), ferr(nrhs), r(n), work(3*n), x(ldx, nrhs)
CALL SGBSVX(fact, trans, n, kl, ku, nrhs, ab, ldab, afb, ldafb, ipiv, equed,
  r, c, b, ldb, x, ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1        equed, fact, trans
INTEGER*4          info, kl, ku, ldab, ldafb, ldb, ldx, n, nrhs
REAL*8             rcond
INTEGER*4          ipiv(n), iwork(n)
REAL*8             ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), berr(nrhs),
                   c(n), ferr(nrhs), r(n), work(3*n), x(ldx, nrhs)
CALL DGBSVX(fact, trans, n, kl, ku, nrhs, ab, ldab, afb, ldafb, ipiv, equed,
  r, c, b, ldb, x, ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1        equed, fact, trans
INTEGER*4          info, kl, ku, ldab, ldafb, ldb, ldx, n, nrhs
REAL*4             rcond
INTEGER*4          ipiv(n)
REAL*4             berr(nrhs), c(n), ferr(nrhs), r(n), rwork(n)
COMPLEX*8          ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), work(2*n),
                   x(ldx, nrhs)
CALL CGBSVX(fact, trans, n, kl, ku, nrhs, ab, ldab, afb, ldafb, ipiv, equed,
  r, c, b, ldb, x, ldx, rcond, ferr, berr, work, rwork, info)
```

```
CHARACTER*1        equed, fact, trans
INTEGER*4          info, kl, ku, ldab, ldafb, ldb, ldx, n, nrhs
REAL*8             rcond
INTEGER*4          ipiv(n)
REAL*8             berr(nrhs), c(n), ferr(nrhs), r(n), rwork(n)
COMPLEX*16         ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), work(2*n),
                   x(ldx, nrhs)
CALL ZGBSVX(fact, trans, n, kl, ku, nrhs, ab, ldab, afb, ldafb, ipiv, equed,
  r, c, b, ldb, x, ldx, rcond, ferr, berr, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1        equed, fact, trans
INTEGER*8          info, kl, ku, ldab, ldafb, ldb, ldx, n, nrhs
REAL*8             rcond
INTEGER*8          ipiv(n), iwork(n)
REAL*8             ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), berr(nrhs),
                   c(n), ferr(nrhs), r(n), work(3*n), x(ldx, nrhs)
CALL SGBSVX(fact, trans, n, kl, ku, nrhs, ab, ldab, afb, ldafb, ipiv, equed,
  r, c, b, ldb, x, ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1        equed, fact, trans
INTEGER*8          info, kl, ku, ldab, ldafb, ldb, ldx, n, nrhs
REAL*8             rcond
INTEGER*8          ipiv(n)
REAL*8             berr(nrhs), c(n), ferr(nrhs), r(n), rwork(n)
COMPLEX*16         ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), work(2*n),
                   x(ldx, nrhs)
CALL CGBSVX(fact, trans, n, kl, ku, nrhs, ab, ldab, afb, ldafb, ipiv, equed,
  r, c, b, ldb, x, ldx, rcond, ferr, berr, work, rwork, info)
```

Input

fact 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, as follows:

- **fact** = 'F' or 'f': **afb** and **ipiv** contain the factored form of A. If **equed** = 'R' or 'r' or 'C' or 'c' or 'B' or 'b', A was equilibrated before factoring and the scaling matrices are provided in one or both of **r** and **c**.
- **fact** = 'N' or 'n': The matrix A is copied to **afb** and factored.
- **fact** = 'E' or 'e': The matrix A is equilibrated, if necessary, then copied to **afb** and factored.

trans Specifies the form of the system of equations, as follows:

trans = 'N' or 'n': Solve $AX = B$.

trans = 'T' or 't': Solve $A^TX = B$.

trans = 'C' or 'c': Solve $A^*X = B$.

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

kl The number of subdiagonals within the band of A. **kl** ≥ 0.

ku The number of superdiagonals within the band of A. **ku** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ab The matrix A in band storage, in the first **kl+ku+1** rows. The j-th column of A is stored in the j-th column of the array **ab** as follows:

ab(**ku**+1+i–j,j) = $A(i,j)$ for max(1,j–**ku**) ≤ i ≤ min(**n**,j+**kl**)

ldab The leading dimension of array **ab** in the calling program unit. **ldab** ≥ **kl+ku+1**.

afb If **fact** = 'F' or 'f', the details of the LU factorization of the band matrix A, as computed by a previous call. U, an upper triangular band matrix with **kl+ku** superdiagonals, is stored in the first **kl+ku+1** rows. The multipliers, L, used during the factorization, are stored in rows **kl+ku+2** to **2kl+ku+1**.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

ldafb The leading dimension of array **afb** in the calling program unit. **ldafb** ≥ **2kl+ku+1**.

ipiv If **fact** = 'F' or 'f', the pivot indices from the factorization $A = PLU$ as computed by a previous call; row i of the matrix was interchanged with row **ipiv**(i).

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

equed If **fact** = 'F' or 'f', the type of equilibration, if any, that was done before factoring A on a previous call, as follows:

equed = 'N' or 'n': No equilibration was done.

equed = 'R' or 'r': Only row equilibration was done.

equed = 'C' or 'c': Only column equilibration was done.

equed = 'B' or 'b': Both row and column equilibration were done.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

r The diagonal elements of the diagonal row scaling matrix R if the matrix A was factored during a previous call (**fact** = 'F' or 'f'), and if row equilibration was done during that call (**equed** = 'R' or 'r' or 'B' or 'b'). $\mathbf{r}(i) > 0$, $i = 1, 2, ..., \mathbf{n}$.

Otherwise, not used as input.

c The diagonal elements of the diagonal column scaling matrix C if the matrix A was factored during a previous call (**fact** = 'F' or 'f'), and if column equilibration was done during that call (**equed** = 'C' or 'c' or 'B' or 'b'). $\mathbf{c}(i) > 0$, $i = 1, 2, ..., \mathbf{n}$.

Otherwise, not used as input.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(**1**,**n**).

ldx The leading dimension of array **x** in the calling program unit. **ldx** ≥ max(**1**,**n**).

Working Storage

work, iwork, rwork Arrays used for work space.

On successful exit from SGBSVX or DGBSVX, **work**(1) contains the reciprocal growth factor, $\|A\|_\Delta / \|U\|_\Delta = (\max_{ij} |a_{ij}|) / (\max_{ij} |u_{ij}|)$.

On successful exit from CGBSVX or ZGBSVX, **rwork**(1) contains the reciprocal growth factor, $\|A\|_\Delta / \|U\|_\Delta = (\max_{ij} |a_{ij}|) / (\max_{ij} |u_{ij}|)$.

If $\|A\|_\Delta / \|U\|_\Delta \ll 1$, then the stability of the LU factorization of the (equilibrated) A matrix could be poor. This also means that the solution vector X, reciprocal condition number estimate **rcond**, and forward error bound **ferr** could be unreliable.

If the factorization fails with 0 < **info** ≤ **n**, then **work**(1) or **rwork**(1) contains the reciprocal growth factor for the leading **info** columns of A.

Output

ab

If **fact** = 'E' or 'e' and **equed** = 'R', then A was overwritten by RA.

If **fact** = 'E' or 'e' and **equed** = 'C', then A was overwritten by AC.

If **fact** = 'E' or 'e' and **equed** = 'B', then A was overwritten by RAC.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n', or if **fact** = 'E' or 'e' and **equed** = 'N' on exit.

afb

If **fact** = 'N' or 'n' or 'E' or 'e', then **afb** returns details of the LU factorization of A, after equilibration, if performed. U, an upper triangular band matrix with **kl+ku** superdiagonals, is stored in the first **kl+ku**+1 rows. The multipliers, L, used during the factorization, are stored in rows **kl+ku**+2 to 2**kl+ku**+1.

Not used as output if **fact** = 'F' or 'f'.

ipiv

If **fact** = 'N' or 'n', then **ipiv** contains the pivot indices from the factorization $A = PLU$ of the original matrix A.

If **fact** = 'E' or 'e', then **ipiv** contains the pivot indices from the factorization $A = PLU$ of the equilibrated matrix A.

Not used as output if **fact** = 'F' or 'f'.

equed

If **fact** = 'E' or 'e', specifies the form of equilibration that was done, as follows:

equed = 'N':	No equilibration.
equed = 'R':	Row equilibration; A was premultiplied by R.
equed = 'C':	Column equilibration; A was postmultiplied by C.
equed = 'B':	Both row and column equilibration; A was replaced with RAC.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n'.

r

If **fact** = 'E' or 'e' and **equed** = 'R' or 'B' on exit, the diagonal elements of the diagonal row scaling matrix R.

Destroyed if **fact** = 'E' or 'e' and **equed** = 'N' or 'C' on exit.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n'.

c If **fact** = 'E' or 'e' and **equed** = 'C' or 'B' on exit, the diagonal elements of the diagonal column scaling matrix C.

Destroyed if **fact** = 'E' or 'e' and **equed** = 'N' or 'R' on exit.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n'.

b If **equed** = 'N' or 'n', **b** is not modified.

If **trans** = 'N' or 'n' and **equed** = 'R' or 'r' or 'B' or 'b', $B$is overwritten by RB.

If **trans** = 'T' or 't' or 'C' or 'c' and **equed** = 'C' or 'c' or 'B' or 'b', B was overwritten by CB.

x On successful exit, the solution vectors X to the original system of equations $AX = B$.

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, after equilibration, if performed. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. This condition is indicated by a return code of **info** > 0, and the solution and error bounds are not computed.

ferr On successful exit, estimated forward error bounds for each solution vector. Let x_{true} and x represent column j of the true and computed solutions, respectively. Then **ferr**(j) is intended to bound $||x-x_{true}||_\infty/||x||_\infty$. The quality of the error bound depends on the quality of the computed estimate of $||A^{-1}||$ computed in the code; if the estimate is accurate, the error bound is valid.

berr On successful exit, **berr**(j) is the componentwise relative backward error of solution vector j (that is, the smallest relative change in any entry of A or column j of B that makes column j of X an exact solution).

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

info > 0: If **info** = $k \le$ **n**, $U(k,k)$ is zero. If **info** = **n**+1, the factor U is nonsingular, but **rcond** is less than the machine precision. The factorization has been completed, but the matrix A is singular to working precision, and the solution and error bounds have not been computed.

Notes

If you provide a previously factored matrix, the following output arguments from the **fact** = 'N' or 'n' or 'E' or 'e' call are input arguments to the **fact** = 'F' or 'f' call: **afb, ipiv, equed,** and possibly **r** and **c**, depending on the value of **equed.**

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

fact ≠ 'E' or 'e' or 'F' or 'f' or 'N' or 'n',
trans ≠ 'N' or 'n' or 'T' or 't' or 'C' or 'c',
n < 0,
kl < 0,
ku < 0,
nrhs < 0,
ldab < **kl**+**ku**+1,
ldafb < 2**kl**+**ku**+1,
fact = 'F' or 'f' and **equed** ≠ 'N', 'n', 'B', 'b', 'R', 'r', 'C' or 'c',
r is an input argument but contains a non-positive value,
c is an input argument but contains a non-positive value,
ldb < max(1,**n**), and
ldx < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **fact** argument as 'Factored' for 'F', 'NoEquilibration' for 'N', or 'Equilibration' for 'E'.

NAME

SGESVX/DGESVX/CGESVX/ZGESVX – Solve General Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n matrix and X and B are n-by-$nrhs$ matrices. You may supply either a new matrix A or an A that was used in a previous call, together with its previously computed scaling matrices, if any, and its L and U factors.

These subroutines perform the following:

1. If you provide a new A matrix and request equilibration (**fact** = 'E' or 'e'), A is analyzed to determine whether or not to do row equilibration, and, independently, whether or not to do column equilibration. If both equilibrations are done, real diagonal scaling matrices, R and C, are computed to equilibrate the system. If row equilibration is not done, R is the identity; if column equilibration is not done, C is the identity. Output argument **equed** indicates which equilibrations were done.

   If you supply a previously factored A matrix (**fact** = 'F' or 'f') and it was equilibrated (**equed** = 'R' or 'r' or 'C' or 'c' or 'B' or 'b'), then the previously computed scaling matrices are used in the solution phase.

   In either case, if equilibration is done, the system actually solved depends upon the **trans** argument as follows:

   If **trans** = 'N' or 'n', equilibrate the system as $(RAC)(C^{-1}X) = RB$.

   If **trans** = 'T' or 't', equilibrate the system as $(RAC)^T(R^{-1}X) = CB$.

   If **trans** = 'C' or 'c', equilibrate the system as $(RAC)^*(R^{-1}X) = CB$.

   If equilibration is done, A is overwritten by RAC.

   If equilibration is done, or if A was factored on a previous call where equilibration was done, then B may be overwritten. Specifically, if **trans** = 'N' or 'n' and **equed** is 'R' or 'r' or 'B' or 'b', then B is overwritten by RB. If **trans** = 'T' or 't' or 'C' or 'c' and **equed** is 'C' or 'c' or 'B' or 'b', then B is overwritten by CB.

2. If **fact** = 'N' or 'n' or 'E' or 'e', A is copied from array **a** to array **af** (after equilibration, if performed), where it is factored as $A = PLU$, where P is a permutation matrix, L is a unit lower triangular matrix, and U is upper triangular.

3. 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 the machine precision, steps 4 through 6 are skipped.

4. The system of equations $AX = B$ is solved for X using the factored form of A.

5. Iterative refinement is applied to improve the computed solution vectors and calculate error bounds and backward error estimates.
6. If equilibration was used before factoring the A matrix, X is scaled, if necessary, so as to solve the original system. Specifically, if **trans** = 'N' or 'n' and the final value of **equed** is 'C' or 'c' or 'B' or 'b', then X is premultiplied by C. If **trans** = 'T' or 't' or 'C' or 'c' and the final value of **equed** is 'R' or 'r' or 'B' or 'b', then X is premultiplied by R.

Usage

LAPACK:

```
CHARACTER*1        equed, fact, trans
INTEGER*4          info, lda, ldaf, ldb, ldx, n, nrhs
REAL*4             rcond
INTEGER*4          ipiv(n), iwork(n)
REAL*4             a(lda, n), af(ldaf, n), b(ldb, nrhs), berr(nrhs), c(n),
                   ferr(nrhs), r(n), work(3*n), x(ldx, n)
CALL SGESVX(fact, trans, n, nrhs, a, lda, af, ldaf, ipiv, equed, r, c, b, ldb,
  x, ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1        equed, fact, trans
INTEGER*4          info, lda, ldaf, ldb, ldx, n, nrhs
REAL*8             rcond
INTEGER*4          ipiv(n), iwork(n)
REAL*8             a(lda, n), af(ldaf, n), b(ldb, nrhs), berr(nrhs), c(n),
                   ferr(nrhs), r(n), work(3*n), x(ldx, n)
CALL DGESVX(fact, trans, n, nrhs, a, lda, af, ldaf, ipiv, equed, r, c, b, ldb,
  x, ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1        equed, fact, trans
INTEGER*4          info, lda, ldaf, ldb, ldx, n, nrhs
REAL*4             rcond
INTEGER*4          ipiv(n)
REAL*4             berr(nrhs), c(n), ferr(nrhs), r(n), rwork(n)
COMPLEX*8          a(lda, n), af(ldaf, n), b(ldb, nrhs), work(2*n), x(ldx,
                   nrhs)
CALL CGESVX(fact, trans, n, nrhs, a, lda, af, ldaf, ipiv, equed, r, c, b, ldb,
  x, ldx, rcond, ferr, berr, work, rwork, info)

CHARACTER*1        equed, fact, trans
INTEGER*4          info, lda, ldaf, ldb, ldx, n, nrhs
REAL*8             rcond
INTEGER*4          ipiv(n)
REAL*8             berr(nrhs), c(n), ferr(nrhs), r(n), rwork(n)
COMPLEX*16         a(lda, n), af(ldaf, n), b(ldb, nrhs), work(2*n), x(ldx,
                   nrhs)
CALL ZGESVX(fact, trans, n, nrhs, a, lda, af, ldaf, ipiv, equed, r, c, b, ldb,
  x, ldx, rcond, ferr, berr, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1     equed, fact, trans
INTEGER*8       info, lda, ldaf, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*8       ipiv(n), iwork(n)
REAL*8          a(lda, n), af(ldaf, n), b(ldb, nrhs), berr(nrhs), c(n),
                ferr(nrhs), r(n), work(3*n), x(ldx, n)
CALL SGESVX(fact, trans, n, nrhs, a, lda, af, ldaf, ipiv, equed, r, c, b, ldb,
  x, ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1     equed, fact, trans
INTEGER*8       info, lda, ldaf, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*8       ipiv(n)
REAL*8          berr(nrhs), c(n), ferr(nrhs), r(n), rwork(n)
COMPLEX*16      a(lda, n), af(ldaf, n), b(ldb, nrhs), work(2*n), x(ldx,
                nrhs)
CALL CGESVX(fact, trans, n, nrhs, a, lda, af, ldaf, ipiv, equed, r, c, b, ldb,
  x, ldx, rcond, ferr, berr, work, rwork, info)
```

Input

fact 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, as follows:

- **fact** = 'F' or 'f': **af** and **ipiv** contain the factored form of A. If **equed** = 'R' or 'r' or 'C' or 'c' or 'B' or 'b', A was equilibrated before factoring and the scaling matrices are provided in one or both of **r** and **c**.
- **fact** = 'N' or 'n': The matrix A is copied to **af** and factored.
- **fact** = 'E' or 'e': The matrix A is equilibrated, if necessary, then copied to **af** and factored.

trans Specifies the form of the system of equations, as follows:

- **trans** = 'N' or 'n': Solve $AX = B$.
- **trans** = 'T' or 't': Solve $A^TX = B$.
- **trans** = 'C' or 'c': Solve $A^*X = B$.

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

a The **n**-by-**n** matrix A.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

af If **fact** = 'F' or 'f', the factors L and U from the factorization $A = PLU$ as computed by a previous call.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

ldaf The leading dimension of array **af** in the calling program unit. **ldaf** ≥ max(1,**n**).

ipiv If **fact** = 'F' or 'f', the pivot indices from the factorization $A = PLU$ as computed by a previous call; row i of the matrix was interchanged with row **ipiv**(i).

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

equed If **fact** = 'F' or 'f', the type of equilibration, if any, that was done before factoring A on a previous call, as follows:

equed = 'N' or 'n':	No equilibration was done.
equed = 'R' or 'r':	Only row equilibration was done.
equed = 'C' or 'c':	Only column equilibration was done.
equed = 'B' or 'b':	Both row and column equilibration were done.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

r The diagonal elements of the diagonal row scaling matrix R if the matrix A was factored during a previous call (**fact** = 'F' or 'f'), and if row equilibration was done during that call (**equed** = 'R' or 'r' or 'B' or 'b'). **r**(i) > 0, i = 1, 2, ..., **n**.

Otherwise, not used as input.

c The diagonal elements of the diagonal column scaling matrix C if the matrix A was factored during a previous call (**fact** = 'F' or 'f'), and if column equilibration was done during that call (**equed** = 'C' or 'c' or 'B' or 'b'). **c**(i) > 0, i = 1, 2, ..., **n**.

Otherwise, not used as input.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

ldx The leading dimension of array **x** in the calling program unit. **ldx** ≥ max(1,**n**).

Working Storage

work, iwork, rwork — Arrays used for work space.

On successful exit from SGESVX or DGESVX, **work**(1) contains the reciprocal growth factor, $\|A\|_\Delta / \|U\|_\Delta = (\max_{ij} |a_{ij}|) / (\max_{ij} |u_{ij}|)$.

On successful exit from CGESVX or ZGESVX, **rwork**(1) contains the reciprocal growth factor, $\|A\|_\Delta / \|U\|_\Delta = (\max_{ij} |a_{ij}|) / (\max_{ij} |u_{ij}|)$.

If $\|A\|_\Delta / \|U\|_\Delta \ll 1$, then the stability of the LU factorization of the (equilibrated) A matrix could be poor. This also means that the solution vector X, reciprocal condition number estimate **rcond**, and forward error bound **ferr** could be unreliable.

If the factorization fails with $0 <$ **info** $\le$ **n**, then **work**(1) or **rwork**(1) contains the reciprocal growth factor for the leading **info** columns of A.

Output

a — If **fact** = 'E' or 'e' and **equed** = 'R', then A was overwritten by RA.

If **fact** = 'E' or 'e' and **equed** = 'C', then A was overwritten by AC.

If **fact** = 'E' or 'e' and **equed** = 'B', then A was overwritten by RAC.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n', or if **fact** = 'E' or 'e' and **equed** = 'N' on exit.

af — If **fact** = 'N' or 'n' or 'E' or 'e', then **af** returns the factors L and U from the factorization $A = PLU$ of the matrix A, after equilibration, if performed.

Not used as output if **fact** = 'F' or 'f'.

ipiv — If **fact** = 'N' or 'n', then **ipiv** contains the pivot indices from the factorization $A = PLU$ of the original matrix A.

If **fact** = 'E' or 'e', then **ipiv** contains the pivot indices from the factorization $A = PLU$ of the equilibrated matrix A.

Not used as output if **fact** = 'F' or 'f'.

equed If **fact** = 'E' or 'e', specifies the form of equilibration that was done, as follows:

equed = 'N':	No equilibration.
equed = 'R':	Row equilibration; A was premultiplied by R.
equed = 'C':	Column equilibration; A was postmultiplied by C.
equed = 'B':	Both row and column equilibration; A was replaced with RAC.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n'.

r If **fact** = 'E' or 'e' and **equed** = 'R' or 'B' on exit, the diagonal elements of the diagonal row scaling matrix R.

Destroyed if **fact** = 'E' or 'e' and **equed** = 'N' or 'C' on exit.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n'.

c If **fact** = 'E' or 'e' and **equed** = 'C' or 'B' on exit, the diagonal elements of the diagonal column scaling matrix C.

Destroyed if **fact** = 'E' or 'e' and **equed** = 'N' or 'R' on exit.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n'.

b If **equed** = 'N' or 'n', **b** is not modified.

If **trans** = 'N' or 'n' and **equed** = 'R' or 'r' or 'B' or 'b', $B$is overwritten by RB.

If **trans** = 'T' or 't' or 'C' or 'c' and **equed** = 'C' or 'c' or 'B' or 'b', B was overwritten by CB.

x On successful exit, the solution vectors X to the original system of equations $AX = B$.

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, after equilibration, if performed. If **rcond** is small enough so that the logical expression

$$1.0 + \textbf{rcond} \text{ .EQ. } 1.0$$

is true, then A can be regarded as singular to working precision. This condition is indicated by a return code of **info** > 0, and the solution and error bounds are not computed.

ferr On successful exit, estimated forward error bounds for each solution vector. Let x_{true} and x represent column j of the true and computed solutions, respectively. Then **ferr**(j) is intended to bound $\|x-x_{true}\|_\infty/\|x\|_\infty$. The quality of the error bound depends on the quality of the computed estimate of $\|A^{-1}\|$ computed in the code; if the estimate is accurate, the error bound is valid.

berr On successful exit, **berr**(j) is the componentwise relative backward error of solution vector j (that is, the smallest relative change in any entry of A or column j of B that makes column j of X an exact solution).

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = $k \le$ **n**, $U(k,k)$ is zero. If **info** = **n**+1, the factor U is nonsingular, but **rcond** is less than the machine precision. The factorization has been completed, but the matrix A is singular to working precision, and the solution and error bounds have not been computed.

Notes

If you provide a previously factored matrix, the following output arguments from the **fact** = 'N' or 'n' or 'E' or 'e' call are input arguments to the **fact** = 'F' or 'f' call: **af, ipiv, equed,** and possibly **r** and **c,** depending on the value of **equed.**

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

fact ≠ 'E' or 'e' or 'F' or 'f' or 'N' or 'n',
trans ≠ 'N' or 'n' or 'T' or 't' or 'C' or 'c',
n < 0,
nrhs < 0,
lda < max(1,**n**),
ldaf < max(1,**n**),
fact = 'F' or 'f' and **equed** ≠ 'N', 'n', 'B', 'b', 'R', 'r', 'C' or 'c',
r is an input argument but contains a non-positive value,
c is an input argument but contains a non-positive value,
ldb < max(1,**n**), and
ldx < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **fact** argument as 'Factored' for 'F', 'NoEquilibration' for 'N', or 'Equilibration' for 'E'.

NAME

SGTSVX/DGTSVX/.../ZGTSVX – Solve General Tridiagonal Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is a tridiagonal matrix of order n and X and B are n-by-$nrhs$ matrices. A tridiagonal matrix $A = (a_{ij})$ is a matrix whose nonzero elements lie only on the principal diagonal ($i = j$), the subdiagonal ($i = j+1$), and the superdiagonal ($i = j-1$) of the matrix.

These subroutines perform the following:

1. If **fact** = 'N' or 'n', the matrix A is copied from arrays **dl**, **d**, and **du** to arrays **dlf**, **df**, and **duf**, where it is factored as $A = LU$, where L is a product of permutation and unit lower bidiagonal matrices and U is upper triangular with nonzeros in only the main diagonal and first two superdiagonals.
2. 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 the machine precision, steps 3 and 4 are skipped.
3. The system of equations $AX = B$ is solved for X using the factored form of A.
4. Iterative refinement is applied to improve the computed solution vectors and calculate error bounds and backward error estimates.

Matrix Storage

The following example illustrates the storage of general tridiagonal matrices. Consider the following tridiagonal matrix of order $n = 7$:

$$\begin{matrix} 11 & 12 & 0 & 0 & 0 & 0 & 0 \\ 21 & 22 & 23 & 0 & 0 & 0 & 0 \\ 0 & 32 & 33 & 34 & 0 & 0 & 0 \\ 0 & 0 & 43 & 44 & 45 & 0 & 0 \\ 0 & 0 & 0 & 54 & 55 & 56 & 0 \\ 0 & 0 & 0 & 0 & 65 & 66 & 67 \\ 0 & 0 & 0 & 0 & 0 & 76 & 77 \end{matrix}$$

The subdiagonal is stored in array **dl**, the principal diagonal is stored in array **d**, and the superdiagonal is stored in array **du**, as follows:

i	dl(i)	d(i)	du(i)
1	21	11	12
2	32	22	23
3	43	33	34
4	54	44	45
5	65	55	56
6	76	66	67
7		77	

Usage

LAPACK:

CHARACTER*1 fact, trans
INTEGER*4 info, ldb, ldx, n, nrhs
REAL*4 rcond
INTEGER*4 ipiv(n), iwork(n)
REAL*4 b(ldb, nrhs), berr(nrhs), d(n), df(n), dl(n–1), dlf(n–1), du(n–1), du2(n–2), duf(n–1), ferr(nrhs), work(3*n), x(ldx, nrhs)

CALL SGTSVX(fact, trans, n, nrhs, dl, d, du, dlf, df, duf, du2, ipiv, b, ldb, x, ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1 fact, trans
INTEGER*4 info, ldb, ldx, n, nrhs
REAL*8 rcond
INTEGER*4 ipiv(n), iwork(n)
REAL*8 b(ldb, nrhs), berr(nrhs), d(n), df(n), dl(n–1), dlf(n–1), du(n–1), du2(n–2), duf(n–1), ferr(nrhs), work(3*n), x(ldx, nrhs)

CALL DGTSVX(fact, trans, n, nrhs, dl, d, du, dlf, df, duf, du2, ipiv, b, ldb, x, ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1 fact, trans
INTEGER*4 info, ldb, ldx, n, nrhs
REAL*4 rcond
INTEGER*4 ipiv(n)
REAL*4 berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*8 b(ldb, nrhs), d(n), df(n), dl(n–1), dlf(n–1), du(n–1), du2(n–2), duf(n–1), work(2*n), x(ldx, nrhs)

CALL CGTSVX(fact, trans, n, nrhs, dl, d, du, dlf, df, duf, du2, ipiv, b, ldb, x, ldx, rcond, ferr, berr, work, rwork, info)

CHARACTER*1 fact, trans
INTEGER*4 info, ldb, ldx, n, nrhs

```
REAL*8          rcond
INTEGER*4       ipiv(n)
REAL*8          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*16      b(ldb, nrhs), d(n), df(n), dl(n–1), dlf(n–1), du(n–1),
                du2(n–2), duf(n–1), work(2*n), x(ldx, nrhs)
CALL ZGTSVX(fact, trans, n, nrhs, dl, d, du, dlf, df, duf, du2, ipiv, b, ldb, x,
  ldx, rcond, ferr, berr, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1     fact, trans
INTEGER*8       info, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*8       ipiv(n), iwork(n)
REAL*8          b(ldb, nrhs), berr(nrhs), d(n), df(n), dl(n–1),
                dlf(n–1), du(n–1), du2(n–2), duf(n–1), ferr(nrhs),
                work(3*n), x(ldx, nrhs)
CALL SGTSVX(fact, trans, n, nrhs, dl, d, du, dlf, df, duf, du2, ipiv, b, ldb, x,
  ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1     fact, trans
INTEGER*8       info, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*8       ipiv(n)
REAL*8          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*16      b(ldb, nrhs), d(n), df(n), dl(n–1), dlf(n–1), du(n–1),
                du2(n–2), duf(n–1), work(2*n), x(ldx, nrhs)
CALL CGTSVX(fact, trans, n, nrhs, dl, d, du, dlf, df, duf, du2, ipiv, b, ldb,
  x, ldx, rcond, ferr, berr, work, rwork, info)
```

Input

fact Specifies whether or not the factored form of A has been supplied on entry, as follows:

- **fact** = 'F' or 'f': **dlf**, **df**, **duf**, **du2**, and **ipiv2** contain the factored form of A.
- **fact** = 'N' or 'n': The matrix is copied to **dlf**, **df**, **duf**, and **du2** and factored.

trans Specifies the form of the system of equations, as follows:

- **trans** = 'N' or 'n': Solve $AX = B$.
- **trans** = 'T' or 't': Solve $A^T = B$.
- **trans** = 'C' or 'c': Solve $A^*X = B$.

n The order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

dl The **n**–1 subdiagonal elements of A.

d The **n** diagonal elements of A.

du The **n**–1 superdiagonal elements of A.

dlf If **fact** = 'F' or 'f', the **n**–1 multipliers that define the matrix L from the LU factorization of A as computed by a previous call.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

df If **fact** = 'F' or 'f', the **n** diagonal elements of the upper triangular matrix U from the LU factorization of A.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

duf If **fact** = 'F' or 'f', the **n**–1 elements of the first superdiagonal of U.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

du2 If **fact** = 'F' or 'f', the **n**–2 elements of the second superdiagonal of U.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

ipiv If **fact** = 'F' or 'f', the pivot indices from the LU factorization of A as computed by a previous call.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

ldx The leading dimension of array **x** in the calling program unit. **ldx** ≥ max(1,**n**).

Working Storage

work, iwork, rwork Arrays used for work space.

Output

dlf If **fact** = 'N' or 'n', the **n**–1 multipliers that define the matrix L from the LU factorization of A.

Not used as output if **fact** = 'F' or 'f'.

df If **fact** = 'N' or 'n', the **n** diagonal elements of the upper triangular matrix U from the LU factorization of A.

Not used as output if **fact** = 'F' or 'f'.

duf If **fact** = 'N' or 'n', the **n**–1 elements of the first superdiagonal of U.

Not used as output if **fact** = 'F' or 'f'.

du2 If **fact** = 'N' or 'n', the **n**–2 elements of the second superdiagonal of U.

Not used as output if **fact** = 'F' or 'f'.

ipiv If **fact** = 'N' or 'n', the pivot indices from the LU factorization of A; row i of the matrix was interchanged with row **ipiv**(i). **ipiv**(i) will always be either i or i+1; **ipiv**(i) = $i$indicates a row interchange was not required.

x On successful exit, the **n**-by-**nrhs** matrix of solution vectors $X$for the system of equations $AX = B$.

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. This condition is indicated by a return code of **info** > 0, and the solution and error bounds are not computed.

ferr On successful exit, estimated forward error bounds for each solution vector. Let x_{true} and x represent column j of the true and computed solutions, respectively. Then **ferr**(j) is intended to bound $\|x-x_{true}\|_\infty/\|x\|_\infty$. The quality of the error bound depends on the quality of the computed estimate of $\||A^{-1}|\|$ computed in the code; if the estimate is accurate, the error bound is valid.

berr On successful exit, **berr**(j) is the componentwise relative backward error of solution vector j (that is, the smallest relative change in any entry of A or column j of B that makes column j of X an exact solution).

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

info > 0: If **info** = $k \leq$ **n**, $U(k,k)$ is zero. The factorization has not been completed unless k = **n**, but the factor U is exactly singular, so the solution and error bounds could not be computed.

If **info** = **n**+1, **rcond** is less than the machine precision. The factorization has been completed, but the matrix A is singular to working precision, and the solution and error bounds have not been computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

fact ≠ 'F' or 'f' or 'N' or 'n',
trans ≠ 'T' or 't' or 'C' or 'c',
n < 0,
nrhs < 0,
ldb < max(1,**n**), and
ldx < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **fact** argument as 'Factored' for 'F', 'NoEquilibration' for 'N', or 'Equilibration' for 'E'.

NAME

SPBSVX/.../ZPBSVX – Solve Positive Definite Band Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n real symmetric or complex Hermitian positive definite band matrix and X and B are n-by-$nrhs$ matrices. You may supply either a new matrix A or an A that was used in a previous call, together with its previously computed scaling matrix, if any, and its L or U factor.

A real matrix is symmetric if $A = A^T$, its transpose, and a real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x. A complex matrix is Hermitian if $A = A^*$, its conjugate transpose, and a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

A positive definite band matrix is a positive definite matrix whose nonzero elements all lie fairly near the principal diagonal. Specifically, $a_{ij} = 0$ if $|i-j| > kd$ for some integer kd. The smallest such kd for a given matrix is called the half bandwidth, and $2kd+1$ is called the total bandwidth.

Tridiagonal matrices are the special case $kd = 1$. They can be handled more efficiently by the LAPACK subprograms SPTSVX, DPTSVX, CPTSVX, and ZPTSVX.

These subroutines perform the following:

1. If you provide a new A matrix and request equilibration (**fact** = 'E' or 'e'), A is analyzed to determine whether or not to do equilibration. If equilibration is done, a real diagonal scaling matrix, S, is computed to equilibrate the system. If equilibration is not done, S is the identity.

   If you supply a previously factored A matrix (**fact** = 'F' or 'f') and it was equilibrated (**equed** = 'Y' or 'y'), then the previously computed scaling matrix is used in the solution phase.

   In either case, if equilibration is done, the system actually solved is

   $$(SAS)(S^{-1}X) = SB.$$

   If equilibration is done, A is overwritten by SAS.

   If equilibration is done, or if A was factored in a previous call where equilibration was done, then B is overwritten by SB.

2. If **fact** = 'N' or 'n' or 'E' or 'e', the matrix A is copied from array **ab** to array **afb** (after equilibration if **fact** = 'E' or 'e') where the Cholesky decomposition is used to factor A as

   $A = U^*U$, if **uplo** = 'U' or 'u', or

   $A = LL^*$, if **uplo** = 'L' or 'l',

   where U is an upper triangular matrix, L is a lower triangular matrix, and * indicates conjugate transpose.

3. 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 the machine precision, steps 4 through 6 are skipped.
4. The system of equations $AX = B$ is solved for X using the factored form of A.
5. Iterative refinement is applied to improve the computed solution vectors and calculate error bounds and backward error estimates.
6. If equilibration was used before factoring the A matrix, X is scaled so as to solve the original system.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, and since either triangle of A may be obtained from the other, you need only provide the band within one triangle of A. Compared to storing the entire matrix, this can save memory in two ways: only the elements within the band are stored, and of them, only the upper or the lower triangle.

The following examples illustrate the storage of positive definite band matrices. Consider the following matrix A of order $n = 7$ and half bandwidth $kd = 2$:

$$\begin{bmatrix} 11 & 12 & 13 & 0 & 0 & 0 & 0 \\ 12 & 22 & 23 & 24 & 0 & 0 & 0 \\ 13 & 23 & 33 & 34 & 35 & 0 & 0 \\ 0 & 24 & 34 & 44 & 45 & 46 & 0 \\ 0 & 0 & 35 & 45 & 55 & 56 & 57 \\ 0 & 0 & 0 & 46 & 56 & 66 & 67 \\ 0 & 0 & 0 & 0 & 57 & 67 & 77 \end{bmatrix}$$

Upper triangular storage. The upper triangle of A is stored in an array **ab** with at least $kd+1 = 3$ rows and 7 columns as follows:

*	*	13	24	35	46	57
*	12	23	34	45	56	67
11	22	33	44	55	66	77

The asterisks represent elements in the kd-by-kd triangle at the upper left corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the upper triangle of A, it is stored in **ab**($kd+1+i-j,j$). Therefore, the columns of the upper triangle of A are stored in the columns of **ab**, and the diagonals of the upper triangle of A are stored in the rows of **ab**.

Lower triangular storage. The lower triangle of A is stored in the array **ab** as follows:

11	22	33	44	55	66	77
12	23	34	45	56	67	*
13	24	35	46	57	*	*

The asterisks represent elements in the kd-by-kd triangle at the lower right corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the lower triangle of A, it is stored in **ab**($1+i-j,j$). Therefore, the columns of the lower triangle of A are stored in the columns of **ab**, and the diagonals of the lower triangle of A are stored in the rows of **ab**.

Usage

LAPACK:

CHARACTER*1	**equed, fact, uplo**
INTEGER*4	**info, kd, ldab, ldafb, ldb, ldx, n, nrhs**
REAL*4	**rcond**
INTEGER*4	**iwork(n)**
REAL*4	**ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), berr(nrhs), ferr(nrhs), s(n), work(3*n), x(ldx, nrhs)**

CALL SPBSVX(fact, uplo, n, kd, nrhs, ab, ldab, afb, ldafb, equed, s, b, ldb, x, ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1	**equed, fact, uplo**
INTEGER*4	**info, kd, ldab, ldafb, ldb, ldx, n, nrhs**
REAL*8	**rcond**
INTEGER*4	**iwork(n)**
REAL*8	**ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), berr(nrhs), ferr(nrhs), s(n), work(3*n), x(ldx, nrhs)**

```
CALL DPBSVX(fact, uplo, n, kd, nrhs, ab, ldab, afb, ldafb, equed, s, b, ldb,
  x, ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1        equed, fact, uplo
INTEGER*4          info, kd, ldab, ldafb, ldb, ldx, n, nrhs
REAL*4             rcond
REAL*4             berr(nrhs), ferr(nrhs), s(n), rwork(n)
COMPLEX*8          ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), work(2*n),
                   x(ldx, nrhs)
CALL CPBSVX(fact, uplo, n, kd, nrhs, ab, ldab, afb, ldafb, equed, s, b, ldb,
  x, ldx, rcond, ferr, berr, work, rwork, info)

CHARACTER*1        equed, fact, uplo
INTEGER*4          info, kd, ldab, ldafb, ldb, ldx, n, nrhs
REAL*8             rcond
REAL*8             berr(nrhs), ferr(nrhs), s(n), rwork(n)
COMPLEX*16         ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), work(2*n),
                   x(ldx, nrhs)
CALL ZPBSVX(fact, uplo, n, kd, nrhs, ab, ldab, afb, ldafb, equed, s, b, ldb,
  x, ldx, rcond, ferr, berr, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1        equed, fact, uplo
INTEGER*8          info, kd, ldab, ldafb, ldb, ldx, n, nrhs
REAL*8             rcond
INTEGER*8          iwork(n)
REAL*8             ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), berr(nrhs),
                   ferr(nrhs), s(n), work(3*n), x(ldx, nrhs)
CALL SPBSVX(fact, uplo, n, kd, nrhs, ab, ldab, afb, ldafb, equed, s, b, ldb,
  x, ldx, rcond, ferr, berr, work, iwork, info)

CHARACTER*1        equed, fact, uplo
INTEGER*8          info, kd, ldab, ldafb, ldb, ldx, n, nrhs
REAL*8             rcond
REAL*8             berr(nrhs), ferr(nrhs), s(n), rwork(n)
COMPLEX*16         ab(ldab, n), afb(ldafb, n), b(ldb, nrhs), work(2*n),
                   x(ldx, nrhs)
CALL CPBSVX(fact, uplo, n, kd, nrhs, ab, ldab, afb, ldafb, equed, s, b, ldb,
  x, ldx, rcond, ferr, berr, work, rwork, info)
```

Input

fact 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, as follows:

fact = 'F' or 'f': **afb** contains the factored form of A. If **equed** = 'Y' or 'y', A was equilibrated before factoring and the scaling matrix is provided in **s**.

fact = 'N' or 'n': The matrix A is copied to **afb** and factored.

fact = 'E' or 'e': The matrix A is equilibrated, if necessary, then copied to **afb** and factored.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

uplo = 'U' or 'u': The upper triangular part of A is stored.

uplo = 'L' or '1': The lower triangular part of A is stored.

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

kd The number of super-diagonals of the matrix A if **uplo** = 'U' or 'u', or the number of sub-diagonals if **uplo** = 'L' or '1'. **kd** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ab The upper or lower triangle of the real symmetric or complex Hermitian band matrix A, stored in the first **kd**+1 rows of the array. The j-th column of A is stored in the j-th column of the array **ab** as follows:

If **uplo** = 'U' or 'u', **ab**(**kd**+1+i–j,j) = $A(i,j)$ for $max(1,j-\mathbf{kd}) \le i \le j$.

If **uplo** = 'L' or '1', **ab**(1+i–j,j) = $A(i,j)$ for $j \le i \le min(\mathbf{n},j+\mathbf{kd})$.

ldab The leading dimension of array **ab** in the calling program unit. **ldab** ≥ **kd**+1.

afb If **fact** = 'F' or 'f', 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 (see **ab**).

ldafb The leading dimension of array **afb** in the calling program unit. **ldafb** ≥ **kd**+1.

equed If **fact** = 'F' or 'f', the type of equilibration, if any, that was done before factoring A on a previous call, as follows:

equed = 'N' or 'n': No equilibration was done.

equed = 'Y' or 'y': Equilibration was done.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

s The diagonal elements of the diagonal scaling matrix S if the matrix A was factored during a previous call (**fact** = 'F' or 'f'), and if equilibration was done during that call (**equed** = 'Y' or 'y'). **s**(i) > 0, i = 1, 2, ..., **n**.

Otherwise, not used as input.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

ldx The leading dimension of array **x** in the calling program unit. **ldx** ≥ max(1,**n**).

Working Storage

work, iwork, rwork Arrays used for work space.

Output

ab If **fact** = 'E' or 'e' and **equed** = 'Y', then A was overwritten by SAS.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n', or if **fact** = 'E' or 'e' and **equed** = 'N' on exit.

afb If **fact** = 'N' or 'n' or 'E' or 'e', the triangular factor U or $L$from the Cholesky factorization $A = U^*U$ or $A = LL^*$ of the matrix A, after equilibration, if performed.

Not used as output if **fact** = 'F' or 'f'.

equed If **fact** = 'E' or 'e', specifies the form of equilibration that was done, as follows:

equed = 'N':	No equilibration.
equed = 'Y':	Equilibration was done; A was replaced with SAS.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n'.

s If **fact** = 'E' or 'e' and **equed** = 'Y' on exit, the diagonal elements of the diagonal scaling matrix S.

Destroyed if **fact** = 'E' or 'e' and **equed** = 'N' on exit.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n'.

b If **equed** = 'N' or 'n', **b** is not modified.

If **equed** = 'Y' or 'y', B was overwritten by SB.

x On successful exit, the solution vectors X to the original system of equations $AX = B$.

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, after equilibration, if performed. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. This condition is indicated by a return code of **info** > 0, and the solution and error bounds are not computed.

ferr On successful exit, estimated forward error bounds for each solution vector. Let x_{true} and x represent column j of the true and computed solutions, respectively. Then **ferr**(j) is intended to bound $\|x-x_{true}\|_\infty/\|x\|_\infty$. The quality of the error bound depends on the quality of the computed estimate of $\|A^{-1}\|$ computed in the code; if the estimate is accurate, the error bound is valid.

berr On successful exit, **berr**(j) is the componentwise relative backward error of solution vector j (that is, the smallest relative change in any entry of A or column j of B that makes column j of X an exact solution).

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = $k \le$ **n**, the leading minor of order k of A is not positive definite, so the factorization could not be completed, and the solution has not been computed.
	If **info** = **n**+1, **rcond** is less than the machine precision. The factorization has been completed, but the matrix A is singular to working precision, and the solution and error bounds have not been computed.

Notes

If you provide a previously factored matrix, the following output arguments from the **fact** = 'N' or 'n' or 'E' or 'e' call are input arguments to the **fact** = 'F' or 'f' call: **afb**, **equed**, and possibly **s**, depending on the value of **equed**.

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

fact ≠ 'E' or 'e' or 'F' or 'f' or 'N' or 'n',
uplo ≠ 'U' or 'u' or 'L' or 'l',
n < 0,
kd < 0,
nrhs < 0,
ldab < **kd**+1,
ldafb < **kd**+1,
fact = 'F' or 'f' and **equed** ≠ 'N' or 'n' or 'Y' or 'y',
s is an input argument but contains a non-positive value,
ldb < max(1,**n**), and
ldx < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPOSVX/DPOSVX/.../ZPOSVX – Solve Positive Definite Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n real symmetric or complex Hermitian positive definite matrix and X and B are n-by-$nrhs$ matrices. You may supply either a new matrix A or an A that was used in a previous call, together with its previously computed scaling matrix, if any, and its L or U factor.

A real matrix is symmetric if $A = A^T$, its transpose. A real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x. A complex matrix is Hermitian if $A = A^*$, its conjugate transpose, and a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

These subroutines perform the following:

1. If you provide a new A matrix and request equilibration (**fact** = 'E' or 'e'), A is analyzed to determine whether or not to do equilibration. If equilibration is done, a real diagonal scaling matrix, S, is computed to equilibrate the system. If equilibration is not done, S is the identity.

   If you supply a previously factored A matrix (**fact** = 'F' or 'f') and it was equilibrated (**equed** = 'Y' or 'y'), then the previously computed scaling matrix is used in the solution phase.

   In either case, if equilibration is done, the system actually solved is

   $$(SAS)(S^{-1}X) = SB.$$

   If equilibration is done, A is overwritten by SAS.

   If equilibration is done, or if A was factored in a previous call where equilibration was done, then B is overwritten by SB.

2. If **fact** = 'N' or 'n' or 'E' or 'e', the matrix A is copied from array **a** to array **af** (after equilibration if **fact** = 'E' or 'e') where the Cholesky decomposition is used to factor A as

   $A = U^*U$, if **uplo** = 'U' or 'u', or

   $A = LL^*$, if **uplo** = 'L' or 'l',

   where U is an upper triangular matrix, L is a lower triangular matrix, and * indicates conjugate transpose.

3. 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 the machine precision, steps 4 through 6 are skipped.

4. The system of equations $AX = B$ is solved for X using the factored form of A.
5. Iterative refinement is applied to improve the computed solution vectors and calculate error bounds and backward error estimates.
6. If equilibration was used before factoring the A matrix, X is scaled so as to solve the original system.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A. You may supply either the upper or the lower triangle of A, in a two-dimensional array large enough to hold the entire matrix. The other triangle of the array is not referenced.

Usage

LAPACK:

```
CHARACTER*1     equed, fact, uplo
INTEGER*4       info, lda, ldaf, ldb, ldx, n, nrhs
REAL*4          rcond
INTEGER*4       iwork(n)
REAL*4          a(lda, n), af(ldaf, n), b(ldb, nrhs), berr(nrhs),
                ferr(nrhs), s(n), work(3*n), x(ldx, nrhs)
CALL SPOSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, equed, s, b, ldb, x, ldx,
  rcond, ferr, berr, work, iwork, info)

CHARACTER*1     equed, fact, uplo
INTEGER*4       info, lda, ldaf, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*4       iwork(n)
REAL*8          a(lda, n), af(ldaf, n), b(ldb, nrhs), berr(nrhs),
                ferr(nrhs), s(n), work(3*n), x(ldx, nrhs)
CALL DPOSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, equed, s, b, ldb, x, ldx,
  rcond, ferr, berr, work, iwork, info)

CHARACTER*1     equed, fact, uplo
INTEGER*4       info, lda, ldaf, ldb, ldx, n, nrhs
REAL*4          rcond
REAL*4          berr(nrhs), ferr(nrhs), rwork(n), s(n)
COMPLEX*8       a(lda, n), af(ldaf, n), b(ldb, nrhs), x(ldx, nrhs),
                work(2*n)
CALL CPOSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, equed, s, b, ldb, x, ldx,
  rcond, ferr, berr, work, rwork, info)
```

```
CHARACTER*1        equed, fact, uplo
INTEGER*4          info, lda, ldaf, ldb, ldx, n, nrhs
REAL*8 . rcond
REAL*8 . berr(nrhs), ferr(nrhs), rwork(n), s(n)
COMPLEX*16. a(lda, n), af(ldaf, n), b(ldb, nrhs), x(ldx, nrhs), work(2*n)
CALL ZPOSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, equed, s, b, ldb, x, ldx,
   rcond, ferr, berr, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1        equed, fact, uplo
INTEGER*8          info, lda, ldaf, ldb, ldx, n, nrhs
REAL*8             rcond
INTEGER*8          iwork(n)
REAL*8             a(lda, n), af(ldaf, n), b(ldb, nrhs), berr(nrhs),
                   ferr(nrhs), s(n), work(3*n), x(ldx, nrhs)
CALL SPOSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, equed, s, b, ldb, x, ldx,
   rcond, ferr, berr, work, iwork, info)

CHARACTER*1        equed, fact, uplo
INTEGER*4          info, lda, ldaf, ldb, ldx, n, nrhs
REAL*8             rcond
REAL*8             berr(nrhs), ferr(nrhs), rwork(n), s(n)
COMPLEX*16         a(lda, n), af(ldaf, n), b(ldb, nrhs), x(ldx, nrhs),
                   work(2*n)
CALL CPOSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, equed, s, b, ldb, x, ldx,
   rcond, ferr, berr, work, rwork, info)
```

Input

fact 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, as follows:

- **fact** = 'F' or 'f': **af** contains the factored form of A. If **equed** = 'Y' or 'y', A was equilibrated before factoring and the scaling matrix is provided in **s**.
- **fact** = 'N' or 'n': The matrix A is copied to **af** and factored.
- **fact** = 'E' or 'e': The matrix A is equilibrated, if necessary, then copied to **af** and factored.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

uplo = 'U' or 'u': The upper triangular part of A is stored.

uplo = 'L' or 'l': The lower triangular part of A is stored.

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

a The symmetric matrix A.

If **uplo** = 'U' or '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' or '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 The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

af If **fact** = 'F' or 'f', the triangular factor U or L from the Cholesky factorization $A = U^*U$ or $A = LL^*$, in the same storage format as A.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

ldaf The leading dimension of array **af** in the calling program unit. **ldaf** ≥ max(1,**n**).

equed If **fact** = 'F' or 'f', the type of equilibration, if any, that was done before factoring A on a previous call, as follows:

equed = 'N' or 'n': No equilibration was done.

equed = 'Y' or 'y': Equilibration was done.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

s The diagonal elements of the diagonal scaling matrix S if the matrix A was factored during a previous call (**fact** = 'F' or 'f'), and if equilibration was done during that call (**equed** = 'Y' or 'y'). $\mathbf{s}(i) > 0$, $i = 1, 2, ..., \mathbf{n}$.

Otherwise, not used as input.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

ldx The leading dimension of array **x** in the calling program unit. **ldx** ≥ max(1,**n**).

Working Storage

work, iwork, rwork Arrays used for work space.

Output

a If **fact** = 'E' or 'e' and **equed** = 'Y', then A was overwritten by SAS.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n', or if **fact** = 'E' or 'e' and **equed** = 'N' on exit.

af If **fact** = 'N' or 'n' or 'E' or 'e', then **af** returns the triangular factor U or L from the Cholesky factorization $A = U^*U$ or $A = LL^*$ of the matrix A, after equilibration, if performed.

Not used as output if **fact** = 'F' or 'f'.

equed If **fact** = 'E' or 'e', specifies the form of equilibration that was done, as follows:

equed = 'N':	No equilibration.
equed = 'Y':	Equilibration was done; A was replaced with SAS.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n'.

s If **fact** = 'E' or 'e' and **equed** = 'Y' on exit, the diagonal elements of the diagonal scaling matrix S.

Destroyed if **fact** = 'E' or 'e' and **equed** = 'N' on exit.

Not used as output if **fact** = 'F' or 'f' or 'N' or'n'.

b If **equed** = 'N' or 'n', **b** is not modified.

If **equed** = 'Y' or 'y', B was overwritten by SB.

x On successful exit, the solution vectors X to the original system of equations $AX = B$.

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, after equilibration, if performed. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. This condition is indicated by a return code of **info** > 0, and the solution and error bounds are not computed.

ferr On successful exit, estimated forward error bounds for each solution vector. Let x_{true} and x represent column j of the true and computed solutions, respectively. Then **ferr**(j) is intended to bound $\|x-x_{true}\|_\infty/\|x\|_\infty$. The quality of the error bound depends on the quality of the computed estimate of $\|A^{-1}\|$ computed in the code; if the estimate is accurate, the error bound is valid.

berr On successful exit, **berr**(j) is the componentwise relative backward error of solution vector j (that is, the smallest relative change in any entry of A or column j of B that makes column j of X an exact solution).

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = $k \le$ **n**, the leading minor of order k of A is not positive definite, so the factorization could not be completed, and the solution has not been computed.
	If **info** = **n**+1, **rcond** is less than the machine precision. The factorization has been completed, but the matrix A is singular to working precision, and the solution and error bounds have not been computed.

Notes

If you provide a previously factored matrix, the following output arguments from the **fact** = 'N' or 'n' or 'E' or 'e' call are input arguments to the **fact** = 'F' or 'f' call: **af**, **equed**, and possibly **s**, depending on the value of **equed**.

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

fact ≠ 'E' or 'e' or 'F' or 'f' or 'N' or 'n',
uplo ≠ 'U' or 'u' or 'L' or 'l',
n < 0,
nrhs < 0,
lda < max(1,**n**),
ldaf < max(1,**n**),
fact = 'F' or 'f' and **equed** ≠ 'N' or 'n' or 'Y' or 'y',
s is an input argument but contains a non-positive value,
ldb < max(1,**n**), and
ldx < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPPSVX/.../ZPPSVX – Solve Positive Definite Packed Linear System

Purpose

These subprograms to solve a system of linear equations $AX = B$, where A is an n-by-n real symmetric or complex Hermitian positive definite matrix stored in packed form and X and B are n-by-$nrhs$matrices. You may supply either a new matrix A or an A that was used in a previous call, together with its previously computed scaling matrix, if any, and its L or U factor.

A real matrix is symmetric if $A = A^T$, its transpose, and a real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x. a complex matrix is Hermitian if $A = A^*$, its conjugate transpose. a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

These subroutines perform the following:

1. If you provide a new A matrix and request equilibration (**fact** = 'E' or 'e'), A is analyzed to determine whether or not to do equilibration. If equilibration is done, a real diagonal scaling matrix, S, is computed to equilibrate the system. If equilibration is not done, S is the identity.

   If you supply a previously factored A matrix (**fact** = 'F' or 'f') and it was equilibrated (**equed** = 'Y' or 'y'), then the previously computed scaling matrix is used in the solution phase.

   In either case, if equilibration is done, the system actually solved is

   $$(SAS)(S^{-1}X) = SB.$$

   If equilibration is done, A is overwritten by SAS.

   If equilibration is done, or if A was factored in a previous call where equilibration was done, then B is overwritten by SB.

2. If **fact** = 'N' or 'n' or 'E' or 'e', the matrix A is copied from array **ap** to array **afp** (after equilibration if **fact** = 'E' or 'e') where the Cholesky decomposition is used to factor A as

   $A=U^*U$, if **uplo** = 'U' or 'u', or

   $A=LL^*$, if **uplo** = 'L' or 'l',

   where U is an upper triangular matrix, L is a lower triangular matrix, and * indicates conjugate transpose.

3. 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 the machine precision, steps 4 through 6 are skipped.

4. The system of equations $AX = B$ is solved for X using the factored form of A.
5. Iterative refinement is applied to improve the computed solution vectors and calculate error bounds and backward error estimates.
6. If equilibration was used before factoring the A matrix, X is scaled so as to solve the original system.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A, either the upper or the lower triangle. Compared to storing the entire matrix, you save memory by supplying that triangle stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular storage. If the lower triangle of A is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**($i+(j-1)\times(2n-j)/2$).

Usage

LAPACK:

```
CHARACTER*1        equed, fact, uplo
INTEGER*4          info, ldb, ldx, n, nrhs
REAL*4             rcond
INTEGER*4          iwork(n)
REAL*4             afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                   berr(nrhs), ferr(nrhs), s(n), work(3*n), x(ldx, nrhs)
CALL SPPSVX(fact, uplo, n, nrhs, ap, afp, equed, s, b, ldb, x, ldx, rcond,
  ferr, berr, work, iwork, info)

CHARACTER*1        equed, fact, uplo
INTEGER*4          info, ldb, ldx, n, nrhs
REAL*8             rcond
INTEGER*4          iwork(n)
REAL*8             afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                   berr(nrhs), ferr(nrhs), s(n), work(3*n), x(ldx, nrhs)
CALL DPPSVX(fact, uplo, n, nrhs, ap, afp, equed, s, b, ldb, x, ldx, rcond,
  ferr, berr, work, iwork, info)

CHARACTER*1        equed, fact, uplo
INTEGER*4          info, ldb, ldx, n, nrhs
REAL*4             rcond
REAL*4             berr(nrhs), ferr(nrhs), rwork(n), s(n)
COMPLEX*8          afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                   work(2*n), x(ldx, nrhs)
CALL CPPSVX(fact, uplo, n, nrhs, ap, afp, equed, s, b, ldb, x, ldx, rcond,
  ferr, berr, work, rwork, info)

CHARACTER*1        equed, fact, uplo
INTEGER*4          info, ldb, ldx, n, nrhs
```

```
REAL*8          rcond
REAL*8          berr(nrhs), ferr(nrhs), rwork(n), s(n)
COMPLEX*16      afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                work(2*n), x(ldx, nrhs)
CALL ZPPSVX(fact, uplo, n, nrhs, ap, afp, equed, s, b, ldb, x, ldx, rcond,
  ferr, berr, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1     equed, fact, uplo
INTEGER*8       info, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*8       iwork(n)
REAL*8          afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                berr(nrhs), ferr(nrhs), s(n), work(3*n), x(ldx, nrhs)
CALL SPPSVX(fact, uplo, n, nrhs, ap, afp, equed, s, b, ldb, x, ldx, rcond,
  ferr, berr, work, iwork, info)
```

```
CHARACTER*1     equed, fact, uplo
INTEGER*4       info, ldb, ldx, n, nrhs
REAL*8          rcond
REAL*8          berr(nrhs), ferr(nrhs), rwork(n), s(n)
COMPLEX*16      afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                work(2*n), x(ldx, nrhs)
CALL CPPSVX(fact, uplo, n, nrhs, ap, afp, equed, s, b, ldb, x, ldx, rcond,
  ferr, berr, work, rwork, info)
```

Input

fact 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, as follows:

- **fact** = 'F' or 'f': **afp** contains the factored form of A. If **equed** = 'Y' or 'y', A was equilibrated before factoring and the scaling matrix is provided in **s**.
- **fact** = 'N' or 'n': The matrix A is copied to **afp** and factored.
- **fact** = 'E' or 'e': The matrix A is equilibrated, if necessary, then copied to **afp** and factored.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.

uplo = 'L' or '1': The lower triangular part of A is stored.

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ap The upper or lower triangle of the symmetric 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' or 'u', **ap**$(i + (j-1) \times j/2) = A(i,j)$ for $1 \le i \le j$.

If **uplo** = 'L' or '1', **ap**$(i + (j-1) \times (2n-j)/2) = A(i,j)$ for $j \le i \le$ **n**.

afp If **fact** = 'F' or 'f', the triangular factor U or L from the Cholesky factorization $A = U^*U$ or $A = LL^*$, in the same storage format as A.

equed If **fact** = 'F' or 'f', the type of equilibration, if any, that was done before factoring A on a previous call, as follows:

equed = 'N' or 'n': No equilibration was done.

equed = 'Y' or 'y': Equilibration was done.

Not used as input if **fact** = 'N' or 'n' or 'E' or 'e'.

s The diagonal elements of the diagonal scaling matrix S if the matrix A was factored during a previous call (**fact** = 'F' or 'f'), and if equilibration was done during that call (**equed** = 'Y' or 'y'). **s**$(i) > 0$, $i = 1, 2, ...,$ **n**.

Otherwise, not used as input.

b The right hand side vectors **b** for the system of linear equations.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

ldx The leading dimension of array **x** in the calling program unit. **ldx** ≥ max(1,**n**).

Working Storage

work, iwork, rwork Arrays used for work space.

Output

ap If **equed** = 'Y', then A was overwritten by SAS.

Not modified if **fact** = 'F' or 'f' or 'N' or 'n', or if **fact** = 'E' or 'e' and **equed** = 'N' or 'n' on exit.

afp If **fact** = 'N' or 'n' or 'E' or 'e', the triangular factor U or $L$from the Cholesky factorization $A = U^*U$ or $A = LL^*$ of the matrix A, after equilibration, if performed.

equed If **fact** = 'E' or 'e', specifies the form of equilibration that was done, as follows:

equed = 'N':	No equilibration.
equed = 'Y':	Equilibration was done; A was replaced with SAS.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n'.

s If **fact** = 'F' or 'f' and **equed** = 'Y' on exit, the diagonal elements of the diagonal scaling matrix S.

Destroyed if **fact** = 'F' or 'f' and **equed** = 'N' on exit.

Not used as output if **fact** = 'F' or 'f' or 'N' or 'n'.

b If **equed** = 'N', **b** is not modified; if **equed** = 'Y', B was overwritten by SB.

x On successful exit, the solution vectors X to the system of equations $AX = B$.

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, after equilibration, if performed. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. This condition is indicated by a return code of **info** > 0, and the solution and error bounds are not computed.

ferr On successful exit, estimated forward error bounds for each solution vector. Let x_{true} and x represent column j of the true and computed solutions, respectively. Then **ferr**(j) is intended to bound $\|x-x_{true}\|_\infty/\|x\|_\infty$. The quality of the error bound depends on the quality of the computed estimate of $\|A^{-1}\|$ computed in the code; if the estimate is accurate, the error bound is valid.

berr On successful exit, **berr**(j) is the componentwise relative backward error of solution vector j (that is, the smallest relative change in any entry of A or column j of B that makes column j of X an exact solution).

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = $k \le$ **n**, the leading minor of order k of A is not positive definite, so the factorization could not be completed, and the solution has not been computed.
	If **info** = **n**+1, **rcond** is less than the machine precision. The factorization has been completed, but the matrix A is singular to working precision, and the solution and error bounds have not been computed.

Notes

If you provide a previously factored matrix, the following output arguments from the **fact** = 'N' or 'n' or 'E' or 'e' call are input arguments to the **fact** = 'F' or 'f' call: **afp**, **equed**, and possibly **s**, depending on the value of **equed**.

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

fact ≠ 'E' or 'e' or 'F' or 'f' or 'N' or 'n',
uplo ≠ 'U' or 'u' or 'L' or 'l',
n < 0,
nrhs < 0,
fact = 'F' or 'f' and **equed** ≠ 'N' or 'n' or 'Y' or 'y',
s is an input argument but contains a non-positive value,
ldb < max(1,**n**), and
ldx < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPTSVX/.../ZPTSVX – Solve Positive Definite Tridiagonal Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n real symmetric or complex Hermitian positive definite tridiagonal matrix and X and B are n-by-$nrhs$ matrices. A tridiagonal matrix $A = (a_{ij})$ is a matrix whose nonzero elements lie only on the principal diagonal ($i = j$), the subdiagonal ($i = j+1$), and the superdiagonal ($i = j-1$) of the matrix.

A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x; a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

These subroutines perform the following:

1. If **fact** = 'N' or 'n', the matrix A is copied from arrays **d** and **e** to arrays **df** and **ef**, where it is factored as $A = LDL^*$, where L is a unit lower bidiagonal matrix and $D$is diagonal. The factorization can also be regarded as having the form $A = U^*DU$.
2. 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 the machine precision, steps 3 and 4 are skipped.
3. The system of equations $AX = B$ is solved for X using the factored form of A.
4. Iterative refinement is applied to improve the computed solution vectors and calculate error bounds and backward error estimates.

Matrix Storage

The following example illustrates the storage of symmetric or Hermitian tridiagonal matrices. Consider the following symmetric tridiagonal matrix of order $n = 7$:

11	21	0	0	0	0	0
21	22	32	0	0	0	0
0	32	33	43	0	0	0
0	0	43	44	54	0	0
0	0	0	54	55	65	0
0	0	0	0	65	66	76
0	0	0	0	0	76	77

The subdiagonal is stored in array **e** and the principal diagonal is stored in array **d**, as follows:

i	**e**(i)	**d**(i)
1	21	11
2	32	22
3	43	33
4	54	44
5	65	55
6	76	66
7		77

Usage

LAPACK:

CHARACTER*1 **fact**
INTEGER*4 **info, ldb, ldx, n, nrhs**
REAL*4 **rcond**
REAL*4 **b(ldb, nrhs), berr(nrhs), d(n), df(n), e(n–1), ef(n–1), ferr(nrhs), work(2*n), x(ldx, nrhs)**

CALL SPTSVX(fact, n, nrhs, d, e, df, ef, b, ldb, x, ldx, rcond, ferr, berr, work, info)

CHARACTER*1 **fact**
INTEGER*4 **info, ldb, ldx, n, nrhs**
REAL*8 **rcond**
REAL*8 **b(ldb, nrhs), berr(nrhs), d(n), df(n), e(n–1), ef(n–1), ferr(nrhs), work(2*n), x(ldx, nrhs)**

```
CALL DPTSVX(fact, n, nrhs, d, e, df, ef, b, ldb, x, ldx, rcond, ferr, berr,
  work, info)
CHARACTER*1        fact
INTEGER*4          info, ldb, ldx, n, nrhs
REAL*4             rcond
REAL*4             berr(nrhs), d(n), df(n), ferr(nrhs), rwork(n)
COMPLEX*8          b(ldb, nrhs), e(n–1), ef(n–1), work(n), x(ldx, nrhs)
CALL CPTSVX(fact, n, nrhs, d, e, df, ef, b, ldb, x, ldx, rcond, ferr, berr,
  work, rwork, info)
CHARACTER*1        fact
INTEGER*4          info, ldb, ldx, n, nrhs
REAL*8             rcond
REAL*8             berr(nrhs), d(n), df(n), ferr(nrhs), rwork(n)
COMPLEX*16         b(ldb, nrhs), e(n–1), ef(n–1), work(n), x(ldx, nrhs)
CALL ZPTSVX(fact, n, nrhs, d, e, df, ef, b, ldb, x, ldx, rcond, ferr, berr,
  work, rwork, info)
```

LAPACK8:

```
CHARACTER*1        fact
INTEGER*8          info, ldb, ldx, n, nrhs
REAL*8             rcond
REAL*8             b(ldb, nrhs), berr(nrhs), d(n), df(n), e(n–1), ef(n–1),
                   ferr(nrhs), work(2*n), x(ldx, nrhs)
CALL SPTSVX(fact, n, nrhs, d, e, df, ef, b, ldb, x, ldx, rcond, ferr, berr,
  work, info)
CHARACTER*1        fact
INTEGER*4          info, ldb, ldx, n, nrhs
REAL*8             rcond
REAL*8             berr(nrhs), d(n), df(n), ferr(nrhs), rwork(n)
COMPLEX*16         b(ldb, nrhs), e(n–1), ef(n–1), work(n), x(ldx, nrhs)
CALL CPTSVX(fact, n, nrhs, d, e, df, ef, b, ldb, x, ldx, rcond, ferr, berr,
  work, rwork, info)
```

Input

fact Specifies whether or not the factored form of A has been supplied on entry, as follows:

- **fact** = 'F' or 'f': **ef** and **df** contain the factored form of A.
- **fact** = 'N' or 'n': The matrix is copied to **ef** and **df** and factored.

n The order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

d The **n** diagonal elements of the tridiagonal matrix A.

e The **n**–1 subdiagonal elements of the tridiagonal matrix A.

df If **fact** = 'F' or 'f', the **n** diagonal elements of the diagonal matrix D from the LDL^* factorization of A.

Not used as input if **fact** = 'N' or 'n'.

ef If **fact** = 'F' or 'f', the **n**–1 subdiagonal elements of the unit bidiagonal factor L from the LDL^* factorization of A.

Not used as input if **fact** = 'N' or 'n'.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

ldx The leading dimension of array **x** in the calling program unit. **ldx** ≥ max(1,**n**).

Working Storage

work, rwork Arrays used for work space.

Output

df If **fact** = 'N' or 'n', the **n** diagonal elements of the diagonal matrix D from the LDL^* factorization of A. Not modified if **fact** = 'F' or 'f'.

ef If **fact** = 'N' or 'n', the **n**–1 subdiagonal elements of the unit bidiagonal factor L from the LDL^* factorization of A. Not modified if **fact** = 'F' or 'f'.

x On successful exit, the **n**-by-**nrhs** matrix of solution vectors for the system of equations $AX = B$.

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. This condition is indicated by a return code of **info** > 0, and the solution and error bounds are not computed.

ferr On successful exit, estimated forward error bounds for each solution vector. Let x_{true} and x represent column j of the true and computed solutions, respectively. Then **ferr**(j) is intended to bound $\|x-x_{true}\|_\infty/\|x\|_\infty$. The quality of the error bound depends on the quality of the computed estimate of $\|A^{-1}\|$ computed in the code; if the estimate is accurate, the error bound is valid.

berr On successful exit, **berr**(j) is the componentwise relative backward error of solution vector j (that is, the smallest relative change in any entry of A or column j of B that makes column j of X an exact solution).

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value
info > 0:	If **info** = $k \le$ **n**, the leading minor of order k of A is not positive definite, so the factorization could not be completed unless **info** = **n**, and the solution has not been computed.
	If **info** = **n**+1, **rcond** is less than the machine precision. The factorization has been completed, but the matrix A is singular to working precision, and the solution and error bounds have not been computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

fact ≠ 'F' or 'f' or 'N' or 'n',
n < 0,
nrhs < 0,
ldb < max(1,**n**), and
ldx < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **fact** argument as 'Factored' for 'F' or 'Not Factored' for 'N'.

NAME

SSPSVX/... – Solve Symmetric or Hermitian Packed Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n real or complex symmetric or complex Hermitian matrix stored in packed form and X and B are n-by-$nrhs$ matrices. If A is known to be positive definite, other subprograms in this chapter, specifically designed for positive definite matrices, are more efficient than these subprograms.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

The structure of A is indicated by the name of the subprogram used:

SSPSVX	or	DSPSVX	A is a real symmetric matrix.
CSPSVX	or	ZSPSVX	A is a complex symmetric matrix.
CHPSVX	or	ZHPSVX	A is a complex Hermitian matrix.

These subroutines perform the following:

1. If **fact** = 'N' or 'n', the matrix A is copied from array **ap** to array **afp**, where the diagonal pivoting method is used to factor A as

   $A=UDU^T$, if **uplo** = 'U' or 'u', or

   $A=LDL^T$, if **uplo** = 'L' or 'l',

   where U or L is a product of permutation and unit upper triangular or unit lower triangular matrices. D is symmetric and block diagonal with 1-by-1 and 2-by-2 diagonal blocks, and ^{T} indicates transpose.
2. 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 epsilon, steps 3 and 4 are skipped.
3. The system of equations $AX = B$ is solved for X using the factored form of A.
4. Iterative refinement is applied to improve the computed solution vectors and calculate error bounds and backward error estimates.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A, either the upper or the lower triangle. Compared to storing the entire matrix, you save memory by supplying that triangle stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular storage. If the lower triangle of A is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**(i+(j–1)×(2n–j)/2).

Usage

LAPACK:

```
CHARACTER*1     fact, uplo
INTEGER*4       info, ldb, ldx, n, nrhs
REAL*4          rcond
INTEGER*4       ipiv(n), iwork(n)
REAL*4          afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                berr(nrhs), ferr(nrhs), work(3*n), x(ldx, nrhs)
CALL SSPSVX(fact, uplo, n, nrhs, ap, afp, ipiv, b, ldb, x, ldx, rcond, ferr,
  berr, work, iwork, info)

CHARACTER*1     fact, uplo
INTEGER*4       info, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*4       ipiv(n), iwork(n)
REAL*8          afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                berr(nrhs), ferr(nrhs), work(3*n), x(ldx, nrhs)
CALL DSPSVX(fact, uplo, n, nrhs, ap, afp, ipiv, b, ldb, x, ldx, rcond, ferr,
  berr, work, iwork, info)

CHARACTER*1     fact, uplo
INTEGER*4       info, ldb, ldx, n, nrhs
REAL*4          rcond
INTEGER*4       ipiv(n)
REAL*4          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*8       afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                work(2*n), x(ldx, nrhs)
CALL CHPSVX(fact, uplo, n, nrhs, ap, afp, ipiv, b, ldb, x, ldx, rcond, ferr,
  berr, work, rwork, info)

CHARACTER*1     fact, uplo
INTEGER*4       info, ldb, ldx, n, nrhs
REAL*4          rcond
INTEGER*4       ipiv(n)
REAL*4          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*8       afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                work(2*n), x(ldx, nrhs)
CALL CSPSVX(fact, uplo, n, nrhs, ap, afp, ipiv, b, ldb, x, ldx, rcond, ferr,
  berr, work, rwork, info)

CHARACTER*1     fact, uplo
INTEGER*4       info, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*4       ipiv(n)
REAL*8          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*16      afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                work(2*n), x(ldx, nrhs)
CALL ZHPSVX(fact, uplo, n, nrhs, ap, afp, ipiv, b, ldb, x, ldx, rcond, ferr,
  berr, work, rwork, info)
```

```
CHARACTER*1     fact, uplo
INTEGER*4       info, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*4       ipiv(n)
REAL*8          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*16      afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                work(2*n), x(ldx, nrhs)
CALL ZSPSVX(fact, uplo, n, nrhs, ap, afp, ipiv, b, ldb, x, ldx, rcond, ferr,
  berr, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1     fact, uplo
INTEGER*8       info, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*8       ipiv(n), iwork(n)
REAL*8          afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                berr(nrhs), ferr(nrhs), work(3*n), x(ldx, nrhs)
CALL SSPSVX(fact, uplo, n, nrhs, ap, afp, ipiv, b, ldb, x, ldx,  rcond, ferr,
  berr, work, iwork, info)
```

```
CHARACTER*1     fact, uplo
INTEGER*8       info, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*8       ipiv(n)
REAL*8          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*16      afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                work(2*n), x(ldx, nrhs)
CALL CHPSVX(fact, uplo, n, nrhs, ap, afp, ipiv, b, ldb, x, ldx, rcond, ferr,
  berr, work, rwork, info)
```

```
CHARACTER*1     fact, uplo
INTEGER*8       info, ldb, ldx, n, nrhs
REAL*8          rcond
INTEGER*8       ipiv(n)
REAL*8          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*16      afp((n*(n+1))/2), ap((n*(n+1))/2), b(ldb, nrhs),
                work(2*n), x(ldx, nrhs)
CALL CSPSVX(fact, uplo, n, nrhs, ap, afp, ipiv, b, ldb, x, ldx, rcond, ferr,
  berr, work, rwork, info)
```

Input

fact Specifies whether or not the factored form of *A* has been supplied on entry, as follows:

fact = 'F' or 'f':	**afp** and **ipiv** contain the factored form of *A*.
fact = 'N' or 'n':	The matrix *A* is copied to **afp** and factored.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or '1': The lower triangular part of A is stored.

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ap The upper or lower triangle of the symmetric 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' or 'u', **ap**$(i + (j-1) \times j/2) = A(i,j)$ for $1 \leq i \leq j$.

If **uplo** = 'L' or '1', **ap**$(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \leq i \leq \mathbf{n}$.

afp If **fact** = 'F' or 'f', 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 a previous call, stored as a packed triangular matrix in the same storage format as A.

ipiv If **fact** = 'F' or 'f', the details of the interchanges and the block structure of D, as computed by a previous call.

b The **n**-by-**nrhs** matrix of right hand side vectors **b** for the system of equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** $\geq \max(1,\mathbf{n})$.

ldx The leading dimension of array **x** in the calling program unit. **ldx** $\geq \max(1,\mathbf{n})$.

Working Storage

work, iwork, rwork Arrays used for work space.

Output

afp If **fact** = 'N' or 'n', the block diagonal matrix D and the multipliers used to obtain the factor U or L from the factorization $A = UDU^T$ or $A = LDL^T$, stored as a packed triangular matrix in the same storage format as A.

ipiv If **fact** = 'N' or 'n', the details of the interchanges and the block structure of D.

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' or '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' or '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.

x On successful exit, the **n**-by-**nrhs** matrix of solution vectors for the system of equations $AX = B$.

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. This condition is indicated by a return code of **info** > 0, and the solution and error bounds are not computed.

ferr On successful exit, estimated forward error bounds for each solution vector. Let x_{true} and x represent column j of the true and computed solutions, respectively. Then **ferr**(j) is intended to bound $\|x-x_{true}\|_\infty/\|x\|_\infty$. The quality of the error bound depends on the quality of the computed estimate of $\|A^{-1}\|$ computed in the code; if the estimate is accurate, the error bound is valid.

berr On successful exit, **berr**(j) is the componentwise relative backward error of solution vector j (that is, the smallest relative change in any entry of A or column j of B that makes column j of X an exact solution).

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = –k, the k-th argument had an invalid value.

info > 0:	If **info** = k, D(k,k) is zero. The factorization has been completed, but the block diagonal matrix D is singular, so the solution and error bounds could not be computed. If **info** = **n**+1, The block diagonal matrix D is nonsingular, but **rcond** is less than machine epsilon. The factorization has been completed, but the matrix is singular to working precision, so the solution and error bounds have not been computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

fact ≠ 'F' or 'f' or 'N' or 'n',
uplo ≠ 'U' or 'u' or 'L' or 'l',
n < 0,
nrhs < 0,
ldb < max(1,**n**), and
ldx < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SSYSVX/DSYSVX/.../ZSYSVX – Solve Symmetric Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, where A is an n-by-n real or complex symmetric or complex Hermitian matrix stored in packed form and X and B are n-by-$nrhs$ matrices. If A is known to be positive definite, other subprograms in this chapter, specifically designed for positive definite matrices, are more efficient than these subprograms.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

The structure of A is indicated by the name of the subprogram used:

SSYSVX	or	DSYSVX	A is a real symmetric matrix.
CSYSVX	or	ZSYSVX	A is a complex symmetric matrix.
CHESVX	or	ZHESVX	A is a complex Hermitian matrix.

These subprograms perform the following:

1. If **fact** = 'N' or 'n', the matrix A is copied from array **a** to array **af**, where the diagonal pivoting method is used to factor A as

   $A = UDU^*$, if **uplo** = 'U' or 'u', or

   $A = LDL^*$, if **uplo** = 'L' or 'l',

   where U or L is a product of permutation and unit upper triangular or unit lower triangular matrices, D is symmetric and block diagonal with 1-by-1 and 2-by-2 diagonal blocks, and * indicates transpose in the symmetric cases and conjugate transpose in the Hermitian cases.
2. 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 epsilon, steps 3 and 4 are skipped.
3. The system of equations $AX = B$ is solved for X using the factored form of A.
4. Iterative refinement is applied to improve the computed solution vectors and calculate error bounds and backward error estimates.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A. You may supply either the upper or the lower triangle of A, in a two-dimensional array large enough to hold the entire matrix. The other triangle of the array is not referenced.

Usage

LAPACK:

```
CHARACTER*1     fact, uplo
INTEGER*4       info, lda, ldaf, ldb, ldx, lwork, n, nrhs
REAL*4          rcond
INTEGER*4       ipiv(n), iwork(n)
REAL*4          a(lda, n), af(ldaf, n), b(ldb, nrhs), berr(nrhs),
                ferr(nrhs), work(lwork), x(ldx, nrhs)
CALL SSYSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, ipiv, b, ldb, x, ldx, rcond,
  ferr, berr, work, lwork, iwork, info)

CHARACTER*1     fact, uplo
INTEGER*4       info, lda, ldaf, ldb, ldx, lwork, n, nrhs
REAL*8          rcond
INTEGER*4       ipiv(n), iwork(n)
REAL*8          a(lda, n), af(ldaf, n), b(ldb, nrhs), berr(nrhs),
                ferr(nrhs), work(lwork), x(ldx, nrhs)
CALL DSYSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, ipiv, b, ldb, x, ldx, rcond,
  ferr, berr, work, lwork, iwork, info)

CHARACTER*1     fact, uplo
INTEGER*4       info, lda, ldaf, ldb, ldx, lwork, n, nrhs
REAL*4          rcond
INTEGER*4       ipiv(n)
REAL*4          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*8       a(lda, n), af(ldaf, n), b(ldb, nrhs), work(lwork),
                x(ldx, nrhs)
CALL CHESVX(fact, uplo, n, nrhs, a, lda, af, ldaf, ipiv, b, ldb, x, ldx, rcond,
  ferr, berr, work, lwork, rwork, info)

CHARACTER*1     fact, uplo
INTEGER*4       info, lda, ldaf, ldb, ldx, lwork, n, nrhs
REAL*4          rcond
INTEGER*4       ipiv(n)
REAL*4          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*8       a(lda, n), af(ldaf, n), b(ldb, nrhs), work(lwork),
                x(ldx, nrhs)
CALL CSYSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, ipiv, b, ldb, x, ldx, rcond,
  ferr, berr, work, lwork, rwork, info)

CHARACTER*1     fact, uplo
INTEGER*4       info, lda, ldaf, ldb, ldx, lwork, n, nrhs
REAL*8          rcond
INTEGER*4       ipiv(n)
REAL*8          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*16      a(lda, n), af(ldaf, n), b(ldb, nrhs), work(lwork),
                x(ldx, nrhs)
CALL ZHESVX(fact, uplo, n, nrhs, a, lda, af, ldaf, ipiv, b, ldb, x, ldx, rcond,
  ferr, berr, work, lwork, rwork, info)
```

```
CHARACTER*1     fact, uplo
INTEGER*4       info, lda, ldaf, ldb, ldx, lwork, n, nrhs
REAL*8          rcond
INTEGER*4       ipiv(n)
REAL*8          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*16      a(lda, n), af(ldaf, n), b(ldb, nrhs), work(lwork),
                x(ldx, nrhs)
CALL ZSYSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, ipiv, b, ldb, x, ldx, rcond,
  ferr, berr, work, lwork, rwork, info)
```

LAPACK8:

```
CHARACTER*1     fact, uplo
INTEGER*8       info, lda, ldaf, ldb, ldx, lwork, n, nrhs
REAL*8          rcond
INTEGER*8       ipiv(n), iwork(n)
REAL*8          a(lda, n), af(ldaf, n), b(ldb, nrhs), berr(nrhs),
                ferr(nrhs), work(lwork), x(ldx, nrhs)
CALL SSYSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, ipiv, b, ldb, x, ldx, rcond,
  ferr, berr, work, lwork, iwork, info)
```

```
CHARACTER*1     fact, uplo
INTEGER*8       info, lda, ldaf, ldb, ldx, lwork, n, nrhs
REAL*8          rcond
INTEGER*8       ipiv(n)
REAL*8          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*16      a(lda, n), af(ldaf, n), b(ldb, nrhs), work(lwork),
                x(ldx, nrhs)
CALL CHESVX(fact, uplo, n, nrhs, a, lda, af, ldaf, ipiv, b, ldb, x, ldx, rcond,
  ferr, berr, work, lwork, rwork, info)
```

```
CHARACTER*1     fact, uplo
INTEGER*8       info, lda, ldaf, ldb, ldx, lwork, n, nrhs
REAL*8          rcond
INTEGER*8       ipiv(n)
REAL*8          berr(nrhs), ferr(nrhs), rwork(n)
COMPLEX*16      a(lda, n), af(ldaf, n), b(ldb, nrhs), work(lwork),
                x(ldx, nrhs)
CALL CSYSVX(fact, uplo, n, nrhs, a, lda, af, ldaf, ipiv, b, ldb, x, ldx, rcond,
  ferr, berr, work, lwork, rwork, info)
```

Input

fact Specifies whether or not the factored form of A has been supplied on entry, as follows:

fact = 'F' or 'f':	**af** and **ipiv** contain the factored form of A.
fact = 'N' or 'n':	The matrix A is copied to **af** and factored.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

uplo = 'U' or 'u':	The upper triangular part of A is stored.
uplo = 'L' or 'l':	The lower triangular part of A is stored.

n The number of linear equations, that is, the order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

a The symmetric or Hermitian matrix **a**.

If **uplo** = 'U' or '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' or '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 The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

af If **fact** = 'F' or 'f', the block diagonal matrix D and the multipliers used to obtain the factor U or L from the factorization $A=UDU^*$ or $A=LDL^*$.

Not used as input if **fact** = 'N' or 'n'.

ldaf The leading dimension of array **af** in the calling program unit. **ldaf** ≥ max(1,**n**).

ipiv If **fact** = 'F' or 'f', the details of the interchanges and the block structure of D.

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' or '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' or '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.

Not used as input if **fact** = 'N' or 'n'.

b	The **n**-by-**nrhs** matrix of right hand side vectors **b** for the system of equations $AX = B$.
ldb	The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).
ldx	The leading dimension of array **x** in the calling program unit. **ldx** ≥ max(1,**n**).
lwork	The length of array **work**. **lwork** ≥ max(1,3**n**) for SSYSVX and DSYSVX; **lwork** ≥ max(1,2**n**) for CHESVX, CSYSVX, ZHESVX, and DSYSVX. For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work, iwork, rwork	Arrays used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

af	If **fact** = 'N' or 'n', the block diagonal matrix D and the multipliers used to obtain the factor U or L from the factorization $A = UDU^*$ or $A = LDL^*$. Not used as output if **fact** = 'F' or 'f'.
ipiv	If **fact** = 'N' or 'n', the details of the interchanges and the block structure of D. 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' or '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' or '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. Not used as output if **fact** = 'F' or 'f'.
x	On successful exit, the **n**-by-**nrhs** matrix of solution vectors for the system of equations $AX = B$.

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. This condition is indicated by a return code of **info** > 0, and the solution and error bounds are not computed.

ferr On successful exit, estimated forward error bounds for each solution vector. Let x_{true} and x represent column j of the true and computed solutions, respectively. Then **ferr**(j) is intended to bound $\|x-x_{true}\|_\infty/\|x\|_\infty$. The quality of the error bound depends on the quality of the computed estimate of $\|A^{-1}\|$ computed in the code; if the estimate is accurate, the error bound is valid.

berr On successful exit, **berr**(j) is the componentwise relative backward error of solution vector j (that is, the smallest relative change in any entry of A or column j of B that makes column j of X an exact solution).

info Status response

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** ≤ **n**, $D(k,k)$ is zero. The factorization has been completed, but the block diagonal matrix D is singular, so the solution and error bounds could not be computed. If **info** = n+1 the block diagonal matrix D is nonsingular, but **rcond** is less than machine epsilon. The factorization has been completed, but the matrix is singular to working precision, so the solution and error bounds have not been computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

fact ≠ 'F' or 'f' or 'N' or 'n',
uplo ≠ 'U' or 'u' or 'L' or 'l',
n < 0,
nrhs < 0,
lda < max(1,**n**),
ldaf < max(1,**n**),
ldb < max(1,**n**),
ldx < max(1,**n**), and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

4 Computational Subprograms for Linear Equations

Overview

This chapter describes some of the computational subprograms to solve systems of linear equations. Although software is included for all LAPACK computational subprograms for linear equations, not all of them are described in this chapter.

This chapter explains how to use LAPACK subprograms to solve systems of linear equations or calculate the inverse of a matrix.

These operations are performed for a variety of types of matrices, including:

- Real and complex general full matrices
- Real and complex general band matrices
- Real symmetric and complex Hermitian positive definite full matrices
- Real symmetric and complex Hermitian positive definite band matrices
- Real and complex general tridiagonal matrices
- Real symmetric and complex Hermitian positive definite tridiagonal matrices
- Real and complex symmetric and complex Hermitian indefinite matrices

The following documents provide supplemental material for this chapter:

- Anderson, E. *et al. LAPACK Users' Guide*, Second Edition. Philadelphia, PA: Society for Industrial and Applied Mathematics. 1995.
- Forsythe, G. and C.B. Moler. *Computer Solution of Linear Algebraic Systems*. Englewood Cliffs, NJ: Prentice-Hall, Inc. 1967.
- Golub, G.H. and C.F. Van Loan. *Matrix Computations*, 2nd Edition. Baltimore, MD: The Johns Hopkins University Press. 1989.

Chapter Objectives

After you read this chapter you will:

- Understand the role of the condition number in solving linear equations
- Know how to compute the inverse of a matrix
- know when not to compute the inverse of a matrix
- know how to use the described subprograms

What You Need to Know to Use These Subprograms

The LAPACK subprograms in this chapter are organized so that it is usually necessary to call two or more subprograms to perform the above operations. This division of labor significantly enhances the number of processing options such as matrix factoring, condition number estimation, solving, and computing an inverse matrix that you may apply to a specific problem to obtain a suitable solution. It also allows you the flexibility to choose between subprograms that are fast but use a less reliable, elementary test for singularity and subprograms that are slightly slower but use a significantly more reliable test involving an estimate of the condition number of the coefficient matrix.

Condition Number

The condition number, $\kappa(A)$, of the coefficient matrix A measures the sensitivity of the solution x of the system of linear equations $Ax = b$ to errors in the matrix A and the right hand side b. Under reasonable assumptions, if δA and δb represent the errors in A and b, respectively, and if $\| \ \|$ represents any vector norm and its subordinate matrix norm, the error δx in x that results from solving $(A+\delta A)(x+\delta x) = b+\delta b$ instead of $Ax = b$ is bounded by

$$\frac{\|\delta x\|}{\|x\|} \leq \frac{\kappa(A)}{1 - \|A^{-1}\| \ \|\delta A\|} \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|} \right).$$

A standard result of numerical analysis shows that the roundoff error introduced by the solution process may be modeled by taking $\|\delta A\|/\|A\|$ and $\|\delta b\|/\|b\|$ to be small multiples of the computer's machine epsilon.Computational singularity of A results in $\kappa(A) = \infty$. A more common situation occurs when A is not numerically singular but is ill-conditioned. When a matrix is ill-conditioned, $\kappa(A)$ is large, so small errors in the matrix and right hand side and small roundoff errors introduced during the solution process itself may be magnified greatly in the solution.

Since $1 < \kappa(A) \leq \infty$, it is more convenient to compute the reciprocal condition number, $1/\kappa(A)$, than $\kappa(A)$ itself. Roughly speaking, the reciprocal condition number has the interpretation that if $1/\kappa(A)$ is about 10^{-d}, elements of x can be expected to have about d fewer significant digits of accuracy than the elements of A or b. Consequently, if errors in the coefficient matrix and right hand side exceed $1/\kappa(A)$, or if $1/\kappa(A)$ is negligible compared to 1.0, then x may have no significant digits at all.

Matrix Inversion

Subprograms for computing the inverse of a matrix are provided, although it is almost never necessary to compute one.

While papers and reference books extensively use the notation "$A^{-1}b$" to mean "the solution x of the system of linear equations $Ax = b$," it is almost always more efficient and more accurate to compute the solution directly than to invert the coefficient matrix and multiply the inverse times the right hand side vector. This is true even if there are many systems of equations, all using the same coefficient matrix; the matrix may be factored once and the systems may be solved from the factors about as efficiently—and more accurately—than by matrix multiplication by the inverse.

Combining Computational Subprograms

When you use the computational subprograms instead of calling the simple or expert drivers, you usually must put two or more of them together to carry out your entire computation. This section shows several ways to assemble an algorithm from several computational subprograms. In these examples, assume your matrix is a 5-by-5 real general matrix stored in a single precision array big enough to handle a 10-by-10 problem. The examples do not show how the matrix, or the right hand side, if needed, is generated. The examples generalize for other matrix formats, when the appropriate subprograms exist. However, since the inverse of a band matrix A generally is a full matrix, and therefore would not fit in the band storage for A, no direct provision is made for computing A^{-1} for band matrices. Thus, these examples do not generalize to computing the inverse of a band matrix.

Solving Linear Equations with a Simple Singularity Test

The following code segment shows how to solve a system of linear equations $Ax = b$, basing the test for matrix singularity on the generation of an exact zero pivot during matrix factorization. SGETRF computes the LU factorization of the coefficient matrix A. If no exact zero pivots occurred, then SGETRS computes the solution vector x, overwriting the right hand side vector B with it; otherwise, the matrix is singular.

```
INTEGER*4 INFO, LDA, LDB, N, NMAX, NRHS
PARAMETER ( NMAX  = 10 )
PARAMETER ( LDA   = NMAX )
PARAMETER ( LDB   = NMAX )
INTEGER*4 IPIV(NMAX)
REAL*4    A(LDA,NMAX), B(LDB)

N     = 5
NRHS  = 1
CALL SGETRF (N, N, A, LDA, IPIV, INFO)
IF ( INFO .EQ. 0 ) THEN
    CALL SGETRS ('NotTransposed', N, NRHS, A, LDA, IPIV, B, LDB, INFO)
ELSE
    handle singular matrix
ENDIF
```

Solving Linear Equations with a Condition Number Singularity Test

The following code segment shows how to solve a system of linear equations, basing the test for matrix singularity on the condition number of the matrix. SLANGE is used to compute $\|A\|_\infty$. SGETRF computes the LU factorization of A. If SGETRF indicates that an exact zero pivot occurred, then RCOND is set to zero; otherwise, SGECON is called to estimate the condition number. Finally, if RCOND is significant compared to 1.0, SGETRS is called to compute the solution; otherwise, the matrix is computationally singular.

```
INTEGER*4 INFO, LDA, LDB, N, NMAX, NRHS
REAL*4    ANORM, RCOND, SLANGE
PARAMETER ( NMAX  = 10 )
PARAMETER ( LDA   = NMAX )
PARAMETER ( LDB   = NMAX )
INTEGER*4 IPIV(NMAX), IWORK(NMAX)
REAL*4    A(LDA,NMAX), B(LDB), WORK(4*NMAX)

N     = 5
NRHS  = 1
ANORM = SLANGE ('InfinityNorm', N, N, A, LDA, WORK)
CALL SGETRF (N, N, A, LDA, IPIV, INFO)
IF ( INFO .NE. 0 ) THEN
    RCOND = 0.0
ELSE
    CALL SGECON ('InfinityNorm', N, A, LDA, ANORM, RCOND, WORK,
&                IWORK, INFO)
ENDIF
IF ( RCOND + 1.0 .NE. 1.0 ) THEN
    CALL SGETRS ('NotTransposed', N, NRHS, A, LDA, IPIV, B, LDB, INFO)
ELSE
    handle singular matrix
ENDIF
```

Inverting a Matrix with a Simple Singularity Test

Notwithstanding the previous advice not to invert your matrix, here is one way to do it in those unusual situations where the inverse really is required. SGETRF computes the *LU* factorization of *A*. If no zeros occurred on the diagonal of *U*, then SGETRI computes the inverse matrix, overwriting the *LU* factorization with it. If either SGETRF or SGETRI returns a nonzero status response, the matrix is singular.

```
INTEGER*4 INFO, LDA, LWORK, N, NMAX
PARAMETER ( NMAX  = 10 )
PARAMETER ( LDA   = NMAX )
PARAMETER ( LWORK = 5 * NMAX )
INTEGER*4 IPIV(LDA)
REAL*4    A(LDA,NMAX), WORK(LWORK)

N = 5
CALL SGETRF (N, N, A, LDA, IPIV, INFO)
IF ( INFO .EQ. 0 ) THEN
    CALL SGETRI (N, A, LDA, IPIV, WORK, LWORK, INFO)
ENDIF
IF ( INFO .NE. 0 ) THEN
    handle singular matrix
ENDIF
```

Inverting a Matrix with a Condition Number Singularity Test

Here is another way to compute the inverse of a matrix in those unusual situations where the inverse really is required, this time basing the singularity test on an estimate of the condition number. SLANGE is used to compute $\|A\|_\infty$. SGETRF computes the LU factorization of A. If SGETRF indicates that an exact zero pivot occurred, then RCOND is set to zero; otherwise, SGECON is called to estimate the condition number. Finally, if RCOND is significant compared to 1.0, then SGETRI computes the inverse matrix, overwriting the LU factorization with it; otherwise, the matrix is computationally singular.

```
INTEGER*4 INFO, LDA, LWORK, N, NMAX
REAL*4    ANORM, RCOND, SLANGE
PARAMETER ( NMAX  = 10 )
PARAMETER ( LDA   = NMAX )
PARAMETER ( LWORK = 5 * NMAX )
INTEGER*4 IPIV(LDA), IWORK(NMAX)
REAL*4    A(LDA,NMAX), WORK(LWORK)

N = 5
ANORM = SLANGE ('InfinityNorm', N, N, A, LDA, WORK)
CALL SGETRF (N, N, A, LDA, IPIV, INFO)
IF ( INFO .NE. 0 ) THEN
    RCOND = 0.0
ELSE
    CALL SGECON ('InfinityNorm', N, A, LDA, ANORM, RCOND, WORK,
&                IWORK, INFO)
ENDIF
IF ( RCOND + 1.0 .NE. 1.0 ) THEN
    CALL SGETRI (N, A, LDA, IPIV, WORK, LWORK, INFO)
ELSE
    handle singular matrix
ENDIF
```

NAME

SGBCON/.../ZGBCON – Condition Number of General Band Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a general band matrix A, in either the 1-norm or the ∞-norm, using the LU factorization computed by _GBTRF.

An estimate is obtained for $||A^{-1}||$, and the reciprocal of the condition number is computed as **rcond** = $(||A||\ ||A^{-1}||)^{-1}$.

Usage

LAPACK:

```
CHARACTER*1          norm
INTEGER*4            info, kl, ku, ldab, n
REAL*4               anorm, rcond
INTEGER*4            ipiv(n), iwork(n)
REAL*4               ab(ldab, n), work(3*n)
CALL SGBCON(norm, n, kl, ku, ab, ldab, ipiv, anorm, rcond, work, iwork,
  info)

CHARACTER*1          norm
INTEGER*4            info, kl, ku, ldab, n
REAL*8               anorm, rcond
INTEGER*4            ipiv(n), iwork(n)
REAL*8               ab(ldab, n), work(3*n)
CALL DGBCON(norm, n, kl, ku, ab, ldab, ipiv, anorm, rcond, work, iwork,
  info)

CHARACTER*1          norm
INTEGER*4            info, kl, ku, ldab, n
REAL*4               anorm, rcond
INTEGER*4            ipiv(n)
REAL*4               rwork(n)
COMPLEX*8            ab(ldab, n), work(2*n)
CALL CGBCON(norm, n, kl, ku, ab, ldab, ipiv, anorm, rcond, work,
  rwork, info)

CHARACTER*1          norm
INTEGER*4            info, kl, ku, ldab, n
REAL*8               anorm, rcond
INTEGER*4            ipiv(n)
REAL*8               rwork(n)
COMPLEX*16           ab(ldab, n), work(2*n)
CALL ZGBCON(norm, n, kl, ku, ab, ldab, ipiv, anorm, rcond, work, rwork,
  info)
```

LAPACK8:

```
CHARACTER*1        norm
INTEGER*8          info, kl, ku, ldab, n
REAL*8             anorm, rcond
INTEGER*8          ipiv(n), iwork(n)
REAL*8             ab(ldab, n), work(3*n)
CALL SGBCON(norm, n, kl, ku, ab, ldab, ipiv, anorm, rcond, work, iwork,
  info)

CHARACTER*1        norm
INTEGER*8          info, kl, ku, ldab, n
REAL*8             anorm, rcond
INTEGER*8          ipiv(n)
REAL*8             rwork(n)
COMPLEX*16         ab(ldab, n), work(2*n)
CALL CGBCON(norm, n, kl, ku, ab, ldab, ipiv, anorm, rcond, work,
  rwork, info)
```

Input

norm Specifies whether to use the 1-norm or the ∞-norm to estimate the condition number, as follows, as follows:

norm = '1', 'O', or 'o': Use $\| \ \|_1$.

norm = 'I' or 'i': Use $\| \ \|_\infty$.

n The order of the matrix A. **n** ≥ 0.

kl The number of subdiagonals within the band of A. **kl** ≥ 0.

ku The number of superdiagonals within the band of A. **ku** ≥ 0.

ab Details of the LU factorization of the band matrix A, as computed by _GBTRF. U is an upper triangular band matrix with **kl+ku** superdiagonals, stored in the first **kl+ku**+1 rows. The multipliers, L, used during the factorization, are stored in rows **kl+ku**+2 to 2**kl+ku**+1.

ldab The leading dimension of array **ab** in the calling program unit. **ldab** ≥ 2**kl+ku**+1.

ipiv The pivot indices; for $1 \le i \le$ **n**, row i of the matrix was interchanged with row **ipiv**(i).

anorm If **norm** = '1' or 'O' or 'o', $\|A\|_1$ of the original matrix A.

If **norm** = 'I' or 'i', $\|A\|_\infty$ of the original matrix A.

Working Storage

work, iwork, rwork — Arrays used for work space.

Output

rcond — On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as

rcond = $(\|A\| \, \|A^{-1}\|)^{-1}$, using the norm specified by **norm**. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info — Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11) may be replaced with a user-supplied version to change the error procedure. Error conditions are

norm ≠ '1' or 'O' or 'o' or 'I' or 'i',
n < 0,
kl < 0,
ku < 0,
ldab < 2**kl**+**ku**+1, and
anorm < 0.0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **norm** argument as 'One-norm' for 'O' or 'Infinity-norm' for 'I'.

NAME

SGBTRF/DGBTRF/.../ZGBTRF – Factor General Band Matrix

Purpose

These subprograms compute an LU factorization of an m-by-n general band matrix A using partial pivoting with row interchanges. A band matrix is a matrix whose nonzero elements all lie near the principal diagonal. Specifically, $a_{ij} = 0$ if $i-j > kl$ or $j-i > ku$ for some integers kl and ku. The smallest such kl and ku for a given matrix are called the lower and upper bandwidths, respectively, and $k = kl+ku+1$ is the total bandwidth.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, you need only provide the elements within the band of A. Compared to storing the entire matrix, this can save memory if $2kl+ku+1 < n$.

The following example illustrates the storage of general band matrices. Consider the following matrix A of order $n = 9$ and lower and upper bandwidths $kl = 2$ and $ku = 3$, respectively:

11	12	13	14	0	0	0	0	0
21	22	23	24	25	0	0	0	0
31	32	33	34	35	36	0	0	0
0	42	43	44	45	46	47	0	0
0	0	53	54	55	56	57	58	0
0	0	0	64	65	66	67	68	69
0	0	0	0	75	76	77	78	79
0	0	0	0	0	86	87	88	89
0	0	0	0	0	0	97	98	99

When Gaussian elimination is performed on a general band matrix, pivoting introduces nonzero elements above the band. L can be stored with a lower bandwidth of kl, but U requires an upper bandwidth of $kl+ku$. You must, therefore, provide storage for the extra kl diagonals. This is done by presenting the original matrix to the subprogram in an array large enough to satisfy the additional storage requirements. Thus, for the above matrix, A is given in an array **ab** with at least $2kl+ku+1 = 8$ rows and $n = 9$ columns as follows:

*	*	*	*	*	+	+	+	+
*	*	*	*	+	+	+	+	+
*	*	*	14	25	36	47	58	69
*	*	13	24	35	46	57	68	79
*	12	23	34	45	56	67	78	89
11	22	33	44	55	66	77	88	99
21	32	43	54	65	76	87	98	*
31	42	53	64	75	86	97	*	*

The asterisks in the $(kl+ku)$-by-$(kl+ku)$ triangle at the upper left corner and in the kl-by-kl triangle at the lower right corner represent elements of **ab** that are not referenced, and the plus signs in the first kl rows indicate elements that may be filled in during the factorization. Thus, if a_{ij} is an element within the band of A, then it is stored in **ab**$(kl+ku+1+i-j,j)$.

Therefore, the columns of A are stored in the columns of **ab**, and the diagonals of A are stored in the rows of **ab**, such that the principal diagonal is stored in row $kl+ku+1$ of **ab**.

Usage

LAPACK:

```
INTEGER*4          info, kl, ku, ldab, m, n
INTEGER*4          ipiv(min(m,n))
REAL*4             ab(ldab, n)
CALL SGBTRF(m, n, kl, ku, ab, ldab, ipiv, info)

INTEGER*4          info, kl, ku, ldab, m, n
INTEGER*4          ipiv(min(m,n))
REAL*8             ab(ldab, n)
CALL DGBTRF(m, n, kl, ku, ab, ldab, ipiv, info)

INTEGER*4          info, kl, ku, ldab, m, n
INTEGER*4          ipiv(min(m,n))
COMPLEX*8          ab(ldab, n)
CALL CGBTRF(m, n, kl, ku, ab, ldab, ipiv, info)

INTEGER*4          info, kl, ku, ldab, m, n
INTEGER*4          ipiv(min(m,n))
COMPLEX*16         ab(ldab, n)
```

```
CALL ZGBTRF(m, n, kl, ku, ab, ldab, ipiv, info)
```

LAPACK8:

```
INTEGER*8          info, kl, ku, ldab, m, n
INTEGER*8          ipiv(min(m,n))
REAL*8             ab(ldab, n)
CALL SGBTRF(m, n, kl, ku, ab, ldab, ipiv, info)

INTEGER*8          info, kl, ku, ldab, m, n
INTEGER*8          ipiv(min(m,n))
COMPLEX*16         ab(ldab, n)
CALL CGBTRF(m, n, kl, ku, ab, ldab, ipiv, info)
```

Input

m The number of rows of the matrix A. $\mathbf{m} \geq 0$.

n The number of columns of the matrix A. $\mathbf{n} \geq 0$.

kl The number of subdiagonals within the band of A. $\mathbf{kl} \geq 0$.

ku The number of superdiagonals within the band of A. $\mathbf{ku} \geq 0$.

ab The matrix A in band storage, in rows **kl**+1 to 2**kl**+**ku**+1; rows 1 to **kl** of array **ab** need not be set. The j-th column of A is stored in the j-th column of array **ab** as follows: $\mathbf{ab}(\mathbf{kl}+\mathbf{ku}+1+i-j,j) = A(i,j)$ for $\max(1,j-\mathbf{ku}) \leq i \leq \min(\mathbf{m},j+\mathbf{kl})$

ldab The leading dimension of array **ab** in the calling program unit. $\mathbf{ldab} \geq 2\mathbf{kl}+\mathbf{ku}+1$.

Output

ab On successful exit, details of the factorization. U is an upper triangular band matrix with **kl**+**ku** superdiagonals, stored in rows 1 to **kl**+**ku**+1. The multipliers, L, used during the factorization, are stored in rows **kl**+**ku**+2 to 2**kl**+**ku**+1.

ipiv On successful exit, the pivot indices; for $1 \leq i \leq \min(\mathbf{m},\mathbf{n})$, row i of the matrix was interchanged with row **ipiv**(i).

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, $U(k,k)$ is zero. The factorization has been completed, but the factor U is singular, and division by zero will occur if it is used to solve a system of equations.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11) may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
kl < 0,
ku < 0, and
ldab < **2kl+ku+1**.

NAME

SGBTRS/DGBTRS/CGBTRS/ZGBTRS – Solve General Band System

Purpose

These subprograms solve a system of linear equations $AX = B$, $A^TX = B$, or $A^*X = B$ with a general band matrix A using the LU factorization computed by _GBTRF, where A^T is the transpose of A, and A^* is the conjugate transpose.

Usage

LAPACK:

```
CHARACTER*1     trans
INTEGER*4       info, kl, ku, ldab, ldb, n, nrhs
INTEGER*4       ipiv(n)
REAL*4          ab(ldab, n), b(ldb, nrhs)
CALL SGBTRS(trans, n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*4       info, kl, ku, ldab, ldb, n, nrhs
INTEGER*4       ipiv(n)
REAL*8          ab(ldab, n), b(ldb, nrhs)
CALL DGBTRS(trans, n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*4       info, kl, ku, ldab, ldb, n, nrhs
INTEGER*4       ipiv(n)
COMPLEX*8       ab(ldab, n), b(ldb, nrhs)
CALL CGBTRS(trans, n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*4       info, kl, ku, ldab, ldb, n, nrhs
INTEGER*4       ipiv(n)
COMPLEX*16      ab(ldab, n), b(ldb, nrhs)
CALL ZGBTRS(trans, n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1     trans
INTEGER*8       info, kl, ku, ldab, ldb, n, nrhs
INTEGER*8       ipiv(n)
REAL*8          ab(ldab, n), b(ldb, nrhs)
CALL SGBTRS(trans, n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*8       info, kl, ku, ldab, ldb, n, nrhs
INTEGER*8       ipiv(n)
COMPLEX*16      ab(ldab, n), b(ldb, nrhs)
CALL CGBTRS(trans, n, kl, ku, nrhs, ab, ldab, ipiv, b, ldb, info)
```

Input

trans Specifies the form of the system of equations, as follows:

trans = 'N' or 'n': Solve $AX = B$.

trans = 'T' or 't': Solve $A^TX = B$.

trans = 'C' or 'c': Solve $A^*X = B$.

n The order of the matrix A. **n** ≥ 0.

kl The number of subdiagonals within the band of A. **kl** ≥ 0.

ku The number of superdiagonals within the band of A. **ku** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ab Details of the LU factorization of the band matrix A, as computed by _GBTRF. U is an upper triangular band matrix with **kl+ku** superdiagonals, stored in the first **kl+ku**+1 rows. The multipliers, L, used during the factorization, are stored in rows **kl+ku**+2 to 2**kl+ku**+1.

ldab The leading dimension of array **ab** in the calling program unit. **ldab** ≥ 2**kl+ku**+1.

ipiv The pivot indices; for $1 \le i \le$ **n**, row i of the matrix was interchanged with row **ipiv**(i).

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

Output

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info Status response:

info = 0: Successful exit.

info < 0: If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

trans ≠ 'N' or 'n' or 'T' or 't' or 'C' or 'c',
n < 0,
kl < 0,
ku < 0,
nrhs < 0,
ldab < 2**kl**+**ku**+1, and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **trans** argument as 'NotTransposed' for 'N', 'Transposed' for 'T', or 'ConjugateTransposed' for 'C'.

NAME

SGECON/.../ZGECON – Condition Number of General Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a general matrix A, in either the 1-norm or the ∞-norm, using the LU factorization computed by _GETRF.

An estimate is obtained for $||A^{-1}||$ and the reciprocal of the condition number is computed as **rcond** = $(||A||\ ||A^{-1}||)^{-1}$.

Usage

LAPACK:

```
CHARACTER*1        norm
INTEGER*4          info, lda, n
REAL*4             anorm, rcond
INTEGER*4          iwork(n)
REAL*4             a(lda, n), work(4*n)
CALL SGECON(norm, n, a, lda, anorm, rcond, work, iwork, info)

CHARACTER*1        norm
INTEGER*4          info, lda, n
REAL*8             anorm, rcond
INTEGER*4          iwork(n)
REAL*8             a(lda, n), work(4*n)
CALL DGECON(norm, n, a, lda, anorm, rcond, work, iwork, info)

CHARACTER*1        norm
INTEGER*4          info, lda, n
REAL*4             anorm, rcond, rwork(2*n)
COMPLEX*8          a(lda, n), work(2*n)
CALL CGECON(norm, n, a, lda, anorm, rcond, work, rwork, info)

CHARACTER*1        norm
INTEGER*4          info, lda, n
REAL*8             anorm, rcond, rwork(2*n)
COMPLEX*16         a(lda, n), work(2*n)
CALL ZGECON(norm, n, a, lda, anorm, rcond, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1        norm
INTEGER*8          info, lda, n
REAL*8             anorm, rcond
INTEGER*8          iwork(n)
REAL*8             a(lda, n), work(4*n)
CALL SGECON(norm, n, a, lda, anorm, rcond, work, iwork, info)
```

```
CHARACTER*1     norm
INTEGER*8       info, lda, n
REAL*8          anorm, rcond, rwork(2*n)
COMPLEX*16      a(lda, n), work(2*n)
CALL CGECON(norm, n, a, lda, anorm, rcond, work, rwork, info)
```

Input

norm — Specifies whether to use the 1-norm or the ∞-norm to estimate the condition number, as follows:

norm = '1', 'O', or 'o':	Use $\|\|\ \|\|_1$.
norm = 'I' or 'i':	Use $\|\|\ \|\|_\infty$.

n — The order of the matrix A. **n** ≥ 0.

a — The factors L and U from the factorization $A = PLU$ as computed by _GETRF.

lda — The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

anorm — If **norm** = '1' or 'O' or 'o', $\|A\|_1$ of the original matrix A.

If **norm** = 'I' or 'i', $\|A\|_\infty$ of the original matrix A.

Working Storage

work, iwork, rwork — Arrays used for work space.

Output

rcond — On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as

rcond = $(\|A\|\ \|A^{-1}\|)^{-1}$, using the norm specified by **norm**. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info — Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

norm ≠ '1' or 'O' or 'o' or 'I' or 'i',
n < 0,
lda < max(1,**n**), and
anorm < 0.0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **norm** argument as 'Infinity-Norm' for 'I' or '1-norm' for '1'.

NAME

SGETRF/DGETRF/CGETRF/ZGETRF – Factor General Matrix

Purpose

These subprograms compute 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 $m < n$).

Usage

LAPACK:

```
INTEGER*4          info, lda, m, n
INTEGER*4          ipiv(min(m,n))
REAL*4             a(lda, n)
CALL SGETRF(m, n, a, lda, ipiv, info)

INTEGER*4          info, lda, m, n
INTEGER*4          ipiv(min(m,n))
REAL*8             a(lda, n)
CALL DGETRF(m, n, a, lda, ipiv, info)

INTEGER*4          info, lda, m, n
INTEGER*4          ipiv(min(m,n))
COMPLEX*8          a(lda, n)
CALL CGETRF(m, n, a, lda, ipiv, info)

INTEGER*4          info, lda, m, n
INTEGER*4          ipiv(min(m,n))
COMPLEX*16         a(lda, n)
CALL ZGETRF(m, n, a, lda, ipiv, info)
```

LAPACK8:

```
INTEGER*8          info, lda, m, n
INTEGER*8          ipiv(min(m,n))
REAL*8             a(lda, n)
CALL SGETRF(m, n, a, lda, ipiv, info)

INTEGER*8          info, lda, m, n
INTEGER*8          ipiv(min(m,n))
COMPLEX*16         a(lda, n)
CALL CGETRF(m, n, a, lda, ipiv, info)
```

Input

m	The number of rows of the matrix A. $\mathbf{m} \geq 0$.
n	The number of columns of the matrix A. $\mathbf{n} \geq 0$.
a	The **m**-by-**n** matrix A to be factored.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**m**).

Output

a On successful exit, the factors L and U from the factorization $A = PLU$; the unit diagonal elements of L are not stored.

ipiv On successful exit, the pivot indices; for $1 \le i \le \min(\mathbf{m},\mathbf{n})$, row i of the matrix was interchanged with row **ipiv**(i).

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, $U(k,k)$ is zero. The factorization has been completed, but the factor U is singular, and division by zero will occur if it is used to solve a system of equations.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0, and
lda < max(1,**m**).

NAME

SGETRI/DGETRI/CGETRI/ZGETRI – Invert General Matrix

Purpose

These subprograms compute the inverse of a general matrix using the *LU* factorization computed by _GETRF.

Usage

LAPACK:

```
INTEGER*4. info, lda, lwork, n
INTEGER*4. ipiv(n)
REAL*4 . a(lda, n), work(lwork)
CALL SGETRI. (n, a, lda, ipiv, work, lwork, info)

INTEGER*4. info, lda, lwork, n
INTEGER*4. ipiv(n)
REAL*8 . a(lda, n), work(lwork)
CALL DGETRI. (n, a, lda, ipiv, work, lwork, info)

INTEGER*4. info, lda, lwork, n
INTEGER*4. ipiv(n)
COMPLEX*8. a(lda, n), work(lwork)
CALL CGETRI. (n, a, lda, ipiv, work, lwork, info)

INTEGER*4. info, lda, lwork, n
INTEGER*4. ipiv(n)
COMPLEX*16. a(lda, n), work(lwork)
CALL ZGETRI. (n, a, lda, ipiv, work, lwork, info)
```

LAPACK8:

```
INTEGER*8. info, lda, lwork, n
INTEGER*8. ipiv(n)
REAL*8 . a(lda, n), work(lwork)
CALL SGETRI. (n, a, lda, ipiv, work, lwork, info)

INTEGER*8. info, lda, lwork, n
INTEGER*8. ipiv(n)
COMPLEX*16. a(lda, n), work(lwork)
CALL CGETRI. (n, a, lda, ipiv, work, lwork, info)
```

Input

n The order of the matrix A. $\mathbf{n} \geq 0$.

a The factors L and U from the factorization $A = PLU$ as computed by _GETRF.

lda The leading dimension of array **a** in the calling program unit. $\mathbf{lda} \geq \max(1,\mathbf{n})$.

ipiv The pivot indices from _GETRF; for $1 \leq i \leq \mathbf{n}$, row i of the matrix was interchanged with row **ipiv**(i).

lwork The length of array **work**. $\mathbf{lwork} \geq \max(1,\mathbf{n})$. For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the inverse of the original matrix A overwrites the input.

info Status response:

info = 0: .	Successful exit.
info < 0: .	If **info** = $-k$, the k-th argument had an invalid value.
info > 0: .	If **info** = k, $U(k,k)$ is zero; the matrix is singular and its inverse could not be computed.

Notes

It is almost never necessary to compute the inverse of a matrix. While papers and reference books extensively use the notation "$A^{-1}b$" to mean "the solution x of the system of linear equations $Ax = b$," it is almost always more efficient and more accurate to compute the solution directly than to invert the coefficient matrix and multiply the inverse times the right hand side vector. This is true even if there are many systems of equations, all using the same coefficient matrix; the matrix may be factored once and the systems may be solved from the factors usually just as efficiently—and more accurately—than by matrix multiplication by the inverse.

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

n < 0,
lda < max(1,**n**), and
lwork < max(1,**n**).

NAME

SGETRS/DGETRS/CGETRS/ZGETRS – Solve General Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, $A^TX = B$, or $A^*X = B$ with a general matrix A using the LU factorization computed by _GETRF, where A^T is the transpose of A, and A^* is the conjugate transpose.

Usage

LAPACK:

```
CHARACTER*1     trans
INTEGER*4       info, lda, ldb, n, nrhs
INTEGER*4       ipiv(n)
REAL*4          a(lda, n), b(ldb, nrhs)
CALL SGETRS(trans, n, nrhs, a, lda, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*4       info, lda, ldb, n, nrhs
INTEGER*4       ipiv(n)
REAL*8          a(lda, n), b(ldb, nrhs)
CALL DGETRS(trans, n, nrhs, a, lda, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*4       info, lda, ldb, n, nrhs
INTEGER*4       ipiv(n)
COMPLEX*8       a(lda, n), b(ldb, nrhs)
CALL CGETRS(trans, n, nrhs, a, lda, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*4       info, lda, ldb, n, nrhs
INTEGER*4       ipiv(n)
COMPLEX*16      a(lda, n), b(ldb, nrhs)
CALL ZGETRS(trans, n, nrhs, a, lda, ipiv, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1     trans
INTEGER*8       info, lda, ldb, n, nrhs
INTEGER*8       ipiv(n)
REAL*8          a(lda, n), b(ldb, nrhs)
CALL SGETRS(trans, n, nrhs, a, lda, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*8       info, lda, ldb, n, nrhs
INTEGER*8       ipiv(n)
COMPLEX*16      a(lda, n), b(ldb, nrhs)
CALL CGETRS(trans, n, nrhs, a, lda, ipiv, b, ldb, info)
```

Input

trans Specifies the form of the system of equations, as follows:

trans = 'N' or 'n':	Solve $AX = B$.
trans = 'T' or 't':	Solve $A^TX = B$.
trans = 'C' or 'c':	Solve $A^*X = B$.

n The order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

a The factors L and U from the factorization $A = PLU$ as computed by _GETRF.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

ipiv The pivot indices from _GETRF; for $1 \le i \le$ **n**, row i of the matrix was interchanged with row **ipiv**(i).

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(**1**,**n**).

Output

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

trans ≠ 'N' or 'n' or 'T' or 't' or 'C' or 'c',
n < 0,
nrhs < 0,
lda < max(1,**n**), and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **trans** argument as 'NotTransposed' for 'N', 'Transposed' for 'T', or 'ConjugateTransposed' for 'C'.

NAME

SGTCON/.../ZGTCON – Condition Number of General Tridiagonal Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a general tridiagonal matrix A, in either the 1-norm or the ∞-norm, using the LU factorization computed by _GTTRF.

An estimate is obtained for $||A^{-1}||$, and the reciprocal of the condition number is computed as **rcond** = $(||A||\ ||A^{-1}||)^{-1}$.

Usage

LAPACK:

```
CHARACTER*1     norm
INTEGER*4       info, n
REAL*4          anorm, rcond
INTEGER*4       ipiv(n), iwork(n)
REAL*4          d(n), dl(n–1), du(n–1), du2(n–2), work(n)
CALL SGTCON(norm, n, dl, d, du, du2, ipiv, anorm, rcond, work, iwork,
   info)

CHARACTER*1     norm
INTEGER*4       info, n
REAL*8          anorm, rcond
INTEGER*4       ipiv(n), iwork(n)
REAL*8          d(n), dl(n–1), du(n–1), du2(n–2), work(n)
CALL DGTCON(norm, n, dl, d, du, du2, ipiv, anorm, rcond, work, iwork,
   info)

CHARACTER*1     norm
INTEGER*4       info, n
REAL*4          anorm, rcond
INTEGER*4       ipiv(n)
COMPLEX*8       d(n), dl(n–1), du(n–1), du2(n–2), work(n)
CALL CGTCON(norm, n, dl, d, du, du2, ipiv, anorm, rcond, work, info)

CHARACTER*1     norm
INTEGER*4       info, n
REAL*8          anorm, rcond
INTEGER*4       ipiv(n)
COMPLEX*16      d(n), dl(n–1), du(n–1), du2(n–2), work(n)
CALL ZGTCON(norm, n, dl, d, du, du2, ipiv, anorm, rcond, work, info)
```

LAPACK8:

```
CHARACTER*1     norm
INTEGER*8       info, n
REAL*8          anorm, rcond
INTEGER*8       ipiv(n), iwork(n)
```

```
REAL*8          d(n), dl(n–1), du(n–1), du2(n–2), work(n)
CALL SGTCON(norm, n, dl, d, du, du2, ipiv, anorm, rcond, work, iwork,
  info)
CHARACTER*1     norm
INTEGER*8       info, n
REAL*8          anorm, rcond
INTEGER*8       ipiv(n)
COMPLEX*16      d(n), dl(n–1), du(n–1), du2(n–2), work(n)
CALL CGTCON(norm, n, dl, d, du, du2, ipiv, anorm, rcond, work, info)
```

Input

norm Specifies whether to use the 1-norm or the ∞-norm to estimate the condition number, as follows:

norm = '1', 'O', or 'o':	Use $\|\ \|_1$.
norm = 'I' or 'i':	Use $\|\ \|_\infty$.

n The order of the matrix A. $\mathbf{n} \geq 0$.

dl The **n**–1 multipliers that define the matrix L from the LU factorization of A.

d The **n** diagonal elements of the upper triangular matrix U from the LU factorization of A.

du The **n**–1 elements of the first superdiagonal of U.

du2 The **n**–2 elements of the second superdiagonal of U.

ipiv The pivot indices; for $1 \leq i \leq \mathbf{n}$, row i of the matrix was interchanged with row **ipiv**(i).

anorm If **norm** = '1' or 'O' or 'o', $\|A\|_1$ of the original matrix A.

If **norm** = 'I' or 'i', $\|A\|_\infty$ of the original matrix A.

Working Storage

work, iwork Arrays used for work space.

Output

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as

rcond = $(\|A\| \, \|A^{-1}\|)^{-1}$, using the norm specified by **norm**. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11) may be replaced with a user-supplied version to change the error procedure. Error conditions are

norm ≠ '1' or 'O' or 'o' or 'I' or 'i',
n < 0, and
anorm < 0.0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **norm** argument as 'One-norm' for 'O' or 'Infinity-norm' for 'I'.

NAME

SGTTRF/DGTTRF/.../ZGTTRF – Factor General Tridiagonal Matrix

Purpose

These subprograms compute an LU factorization of a general tridiagonal matrix A using partial pivoting with row interchanges. A matrix $A = (a_{ij})$ is tridiagonal if its nonzero elements lie only on the principal diagonal ($i = j$), the subdiagonal ($i = j+1$), and the superdiagonal ($i = j-1$) of the matrix.

Given such a matrix A, these subprograms compute the factorization of the form $A = LU$ where L is a product of permutation and unit lower bidiagonal matrices and U is upper triangular with nonzeros on only the principal diagonal and first two superdiagonals.

Matrix Storage

The following example illustrates the storage of general tridiagonal matrices. Consider the following tridiagonal matrix of order $n = 7$:

11	12	0	0	0	0	0
21	22	23	0	0	0	0
0	32	33	34	0	0	0
0	0	43	44	45	0	0
0	0	0	54	55	56	0
0	0	0	0	65	66	67
0	0	0	0	0	76	77

The subdiagonal is stored in array **dl**, the principal diagonal is stored in array **d**, and the superdiagonal is stored in array **du**, as follows:

i	**dl**(i)	**d**(i)	**du**(i)
1	21	11	12
2	32	22	23
3	43	33	34
4	54	44	45
5	65	55	56
6	76	66	67
7		77	

Usage

LAPACK:

```
INTEGER*4          info, n
INTEGER*4          ipiv(n)
REAL*4             d(n), dl(n–1), du(n–1), du2(n–2)
CALL SGTTRF(n, dl, d, du, du2, ipiv, info)

INTEGER*4          info, n
INTEGER*4          ipiv(n)
REAL*8             d(n), dl(n–1), du(n–1), du2(n–2)
CALL DGTTRF(n, dl, d, du, du2, ipiv, info)

INTEGER*4          info, n
INTEGER*4          ipiv(n)
COMPLEX*8          d(n), dl(n–1), du(n–1), du2(n–2)
CALL CGTTRF(n, dl, d, du, du2, ipiv, info)

INTEGER*4          info, n
INTEGER*4          ipiv(n)
COMPLEX*16         d(n), dl(n–1), du(n–1), du2(n–2)
CALL ZGTTRF(n, dl, d, du, du2, ipiv, info)
```

LAPACK8:

```
INTEGER*8          info, n
INTEGER*8          ipiv(n)
REAL*8             d(n), dl(n–1), du(n–1), du2(n–2)
CALL SGTTRF(n, dl, d, du, du2, ipiv, info)

INTEGER*8          info, n
INTEGER*8          ipiv(n)
COMPLEX*16         d(n), dl(n–1), du(n–1), du2(n–2)
CALL CGTTRF(n, dl, d, du, du2, ipiv, info)
```

Input

n	The order of the matrix A. **n** ≥ 0.
dl	The **n**–1 subdiagonal elements of A.
d	The diagonal elements of A.
du	The **n**–1 superdiagonal elements of A.

Output

dl	On successful exit, the **n**–1 multipliers that define the matrix L from the LU factorization of A.
d	On successful exit, the **n** diagonal elements of the upper triangular matrix U from the LU factorization of A.
du	On successful exit, the **n**–1 elements of the first superdiagonal of U.

du2 On successful exit, the **n**–2 elements of the second superdiagonal of U.

ipiv On successful exit, the pivot indices from the LU factorization of A; row i of the matrix was interchanged with row **ipiv**(i). **ipiv**(i) will always be either i or i+1; **ipiv**(i) = i indicates a row interchange was not required.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = –k, the k-th argument had an invalid value.
info > 0:	If **info** = k, $U(k,k)$ is zero. The factorization has been completed, but the factor U is singular, and division by zero will occur if it is used to solve a system of equations.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11) may be replaced with a user-supplied version to change the error procedure. Error conditions are

n < 0.

NAME

SGTTRS/DGTTRS/.../ZGTTRS – Solve General Tridiagonal System

Purpose

These subprograms solve a system of linear equations $AX = B, A^TX = B$, or $A^*X = B$ with a general tridiagonal matrix A using the LU factorization computed by _GTTRF, where A^T is the transpose of A, and A^* is the conjugate transpose.

Usage

LAPACK:

```
CHARACTER*1     trans
INTEGER*4       info, ldb, n, nrhs
INTEGER*4       ipiv(n)
REAL*4          b(ldb, nrhs), d(n), dl(n-1), du(n-1), du2(n-2)
CALL SGTTRS(trans, n, nrhs, dl, d, du, du2, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*4       info, ldb, n, nrhs
INTEGER*4       ipiv(n)
REAL*8          b(ldb, nrhs), d(n), dl(n-1), du(n-1), du2(n-2)
CALL DGTTRS(trans, n, nrhs, dl, d, du, du2, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*4       info, ldb, n, nrhs
INTEGER*4       ipiv(n)
COMPLEX*8       b(ldb, nrhs), d(n), dl(n-1), du(n-1), du2(n-2)
CALL CGTTRS(trans, n, nrhs, dl, d, du, du2, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*4       info, ldb, n, nrhs
INTEGER*4       ipiv(n)
COMPLEX*16      b(ldb, nrhs), d(n), dl(n-1), du(n-1), du2(n-2)
CALL ZGTTRS(trans, n, nrhs, dl, d, du, du2, ipiv, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1     trans
INTEGER*8       info, ldb, n, nrhs
INTEGER*8       ipiv(n)
REAL*8          b(ldb, nrhs), d(n), dl(n-1), du(n-1), du2(n-2)
CALL SGTTRS(trans, n, nrhs, dl, d, du, du2, ipiv, b, ldb, info)

CHARACTER*1     trans
INTEGER*8       info, ldb, n, nrhs
INTEGER*8       ipiv(n)
COMPLEX*16      b(ldb, nrhs), d(n), dl(n-1), du(n-1), du2(n-2)
CALL CGTTRS(trans, n, nrhs, dl, d, du, du2, ipiv, b, ldb, info)
```

Input

trans Specifies the form of the system of equations, as follows:

trans = 'N' or 'n': Solve $AX = B$.

trans = 'T' or 't': Solve $A^TX = B$.

trans = 'C' or 'c': Solve $A^*X = B$.

n The order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

dl The **n**–1 multipliers that define the matrix L from the LU factorization of A.

d The **n** diagonal elements of the upper triangular matrix U from the LU factorization of A.

du The **n**–1 elements of the first superdiagonal of U.

du2 The **n**–2 elements of the second superdiagonal of U.

ipiv The pivot indices; for $1 \leq i \leq$ **n**, row i of the matrix was interchanged with row **ipiv**(i).

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** $\geq$ max(1,**n**).

Output

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info Status response:

info = 0: Successful exit.

info < 0: If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

trans ≠ 'N' or 'n' or 'T' or 't' or 'C' or 'c',
n < 0,
nrhs < 0, and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **trans** argument as 'NotTransposed' for 'N', 'Transposed' for 'T', or 'ConjugateTransposed' for 'C'.

NAME

SPBCON/.../ZPBCON – Condition Number of Positive Definite Band Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a real symmetric or complex Hermitian positive definite band matrix A using the Cholesky factorization computed by _PBTRF.

An estimate is obtained for $||A^{-1}||$, and the reciprocal of the condition number is computed as **rcond** = $(||A||_1 \, ||A^{-1}||_1)^{-1}$.

Usage

LAPACK:

```
CHARACTER*1     uplo
INTEGER*4       info, kd, ldab, n
REAL*4          anorm, rcond
INTEGER*4       iwork(n)
REAL*4          ab(ldab, n), work(3*n)
CALL SPBCON(uplo, n, kd, ab, ldab, anorm, rcond, work, iwork, info)

CHARACTER*1     uplo
INTEGER*4       info, kd, ldab, n
REAL*8          anorm, rcond
INTEGER*4       iwork(n)
REAL*8          ab(ldab, n), work(3*n)
CALL DPBCON(uplo, n, kd, ab, ldab, anorm, rcond, work, iwork, info)

CHARACTER*1     uplo
INTEGER*4       info, kd, ldab, n
REAL*4          anorm, rcond
REAL*4          rwork(n)
COMPLEX*8       ab(ldab, n), work(2*n)
CALL CPBCON(uplo, n, kd, ab, ldab, anorm, rcond, work, rwork, info)

CHARACTER*1     uplo
INTEGER*4       info, kd, ldab, n
REAL*8          anorm, rcond
REAL*8          rwork(n)
COMPLEX*16      ab(ldab, n), work(2*n)
CALL ZPBCON(uplo, n, kd, ab, ldab, anorm, rcond, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1     uplo
INTEGER*8       info, kd, ldab, n
REAL*8          anorm, rcond
INTEGER*8       iwork(n)
REAL*8          ab(ldab, n), work(3*n)
```

```
CALL SPBCON(uplo, n, kd, ab, ldab, anorm, rcond, work, iwork, info)
CHARACTER*1     uplo
INTEGER*8       info, kd, ldab, n
REAL*8          anorm, rcond
REAL*8          rwork(n)
COMPLEX*16      ab(ldab, n), work(2*n)
CALL CPBCON(uplo, n, kd, ab, ldab, anorm, rcond, work, rwork, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': U, the upper triangular factor of A is stored.
- **uplo** = 'L' or '1': L, the lower triangular factor of A is stored.

n The order of the matrix A. **n** ≥ 0.

kd The number of super-diagonals of the matrix A if **uplo** = 'U' or 'u', or the number of sub-diagonals if **uplo** = 'L' or '1'. **kd** ≥ 0.

ab The triangular factor U or L from the Cholesky factorization $A = U^*U$ or $A = LL^*$ of the band matrix A, stored in the first **kd**+1 rows of the array. The j-th column of U or L is stored in the array **ab** as follows:

If **uplo** = 'U' or 'u', **ab**(**kd**+1+i–j,j) = $U(i,j)$ for max(1,j–**kd**) ≤ i ≤ j;

If **uplo** = 'L' or '1', **ab**(1+i–j,j) = $L(i,j)$ for j ≤ i ≤ min(**n**,j+**kd**).

ldab The leading dimension of array **ab** in the calling program unit. **ldab** ≥ **kd**+1.

anorm $\|A\|_1$ (= $\|A\|_\infty$) of the original symmetric or Hermitian band matrix A. **anorm** ≥ 0.

Working Storage

work, iwork, rwork Arrays used for work space.

Output

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as **rcond** = $(\|A\|_1 \|A^{-1}\|_1)^{-1}$. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
kd < 0,
ldab < **kd**+1, and
anorm < 0.0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPBTRF/DPBTRF/.../ZPBTRF – Factor Positive Definite Band Matrix

Purpose

These subprograms compute the Cholesky factorization of a real symmetric or complex Hermitian positive definite band matrix A. A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x; a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

A positive definite band matrix is a positive definite matrix whose nonzero elements all lie fairly near the principal diagonal. Specifically, $a_{ij} = 0$ if $|i-j| > kd$ for some integer kd. The smallest such kd for a given matrix is called the half bandwidth, and $2kd+1$ is called the total bandwidth.

Tridiagonal matrices are the special case $kd = 1$. They can be handled more efficiently by the LAPACK subprograms SPTTRF, DPTTRF, CPTTRF, and ZPTTRF.

Given such a matrix A, these subprograms compute the Cholesky factorization of the form $A = U^*U$ or $A = LL^*$ where U is an upper triangular matrix and L is a lower triangular matrix.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, and since either triangle of A may be obtained from the other, you need only provide the band within one triangle of A. Compared to storing the entire matrix, this can save memory in two ways: only the elements within the band are stored, and of them, only the upper or the lower triangle.

The following examples illustrate the storage of positive definite band matrices. Consider the following matrix A of order $n = 7$ and half bandwidth $kd = 2$:

11	12	13	0	0	0	0
12	22	23	24	0	0	0
13	23	33	34	35	0	0
0	24	34	44	45	46	0
0	0	35	45	55	56	57
0	0	0	46	56	66	67
0	0	0	0	57	67	77

Upper triangular storage. The upper triangle of A is stored in an array **ab** with at least $kd+1 = 3$ rows and 7 columns as follows:

*	*	13	24	35	46	57
*	12	23	34	45	56	67
11	22	33	44	55	66	77

The asterisks represent elements in the kd-by-kd triangle at the upper left corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the upper triangle of A, it is stored in **ab**($kd+1+i-j,j$). Therefore, the columns of the upper triangle of A are stored in the columns of **ab**, and the diagonals of the upper triangle of A are stored in the rows of **ab**.

Lower triangular storage. The lower triangle of A is stored in the array **ab** as follows:

11	22	33	44	55	66	77
12	23	34	45	56	67	*
13	24	35	46	57	*	*

The asterisks represent elements in the kd-by-kd triangle at the lower right corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the lower triangle of A, it is stored in **ab**($1+i-j,j$). Therefore, the columns of the lower triangle of A are stored in the columns of **ab**, and the diagonals of the lower triangle of A are stored in the rows of **ab**.

Usage

LAPACK:

```
CHARACTER*1        uplo
INTEGER*4          info, kd, ldab, n
REAL*4             ab(ldab, n)
CALL SPBTRF(uplo, n, kd, ab, ldab, info)

CHARACTER*1        uplo
INTEGER*4          info, kd, ldab, n
REAL*8             ab(ldab, n)
CALL DPBTRF(uplo, n, kd, ab, ldab, info)

CHARACTER*1        uplo
INTEGER*4          info, kd, ldab, n
COMPLEX*8          ab(ldab, n)
CALL CPBTRF(uplo, n, kd, ab, ldab, info)

CHARACTER*1        uplo
INTEGER*4          info, kd, ldab, n
COMPLEX*16         ab(ldab, n)
CALL ZPBTRF(uplo, n, kd, ab, ldab, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, kd, ldab, n
REAL*8             ab(ldab, n)
CALL SPBTRF(uplo, n, kd, ab, ldab, info)

CHARACTER*1        uplo
INTEGER*8          info, kd, ldab, n
COMPLEX*16         ab(ldab, n)
CALL CPBTRF(uplo, n, kd, ab, ldab, info)
```

Input

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or 'l': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

kd The number of super-diagonals of the matrix A if **uplo** = 'U' or 'u', or the number of sub-diagonals if **uplo** = 'L' or 'l'. $\mathbf{kd} \geq 0$.

ab The upper or lower triangle of the symmetric or Hermitian band matrix A, stored in the first **kd**+1 rows of the array. The j-th column of A is stored in the j-th column of array **ab** as follows:

If **uplo** = 'U' or 'u', $\mathbf{ab}(\mathbf{kd}+1+i-j,j) = A(i,j)$ for $\max(1,j-\mathbf{kd}) \leq i \leq j$;

If **uplo** = 'L' or 'l', $\mathbf{ab}(1+i-j,j) = A(i,j)$ for $j \leq i \leq \min(\mathbf{n},j+\mathbf{kd})$.

ldab The leading dimension of array **ab** in the calling program unit. $\mathbf{ldab} \geq \mathbf{kd}+1$.

Output

ab On successful exit, the triangular factor U or L from the Cholesky factorization of A in the same storage format as A overwrites the input.

info Status response:

- **info** = 0: Successful exit.
- **info** < 0: If **info** = $-k$, the k-th argument had an invalid value.

info > 0:	If **info** = k, the leading minor of order k is not positive definite, and the factorization could not be completed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
kd < 0, and
ldab < **kd**+1.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPBTRS/.../ZPBTRS – Solve Positive Definite Band System

Purpose

These subprograms solve a system of linear equations $AX = B$ with a real symmetric or complex Hermitian positive definite band matrix A using the Cholesky factorization computed by _PBTRF.

Usage

LAPACK:

```
CHARACTER*1     uplo
INTEGER*4       info, kd, ldab, ldb, n, nrhs
REAL*4          ab(ldab, n), b(ldb, nrhs)
CALL SPBTRS(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)

CHARACTER*1     uplo
INTEGER*4       info, kd, ldab, ldb, n, nrhs
REAL*8          ab(ldab, n), b(ldb, nrhs)
CALL DPBTRS(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)

CHARACTER*1     uplo
INTEGER*4       info, kd, ldab, ldb, n, nrhs
COMPLEX*8       ab(ldab, n), b(ldb, nrhs)
CALL CPBTRS(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)

CHARACTER*1     uplo
INTEGER*4       info, kd, ldab, ldb, n, nrhs
COMPLEX*16      ab(ldab, n), b(ldb, nrhs)
CALL ZPBTRS(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1     uplo
INTEGER*8       info, kd, ldab, ldb, n, nrhs
REAL*8          ab(ldab, n), b(ldb, nrhs)
CALL SPBTRS(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)

CHARACTER*1     uplo
INTEGER*8       info, kd, ldab, ldb, n, nrhs
COMPLEX*16      ab(ldab, n), b(ldb, nrhs)
CALL CPBTRS(uplo, n, kd, nrhs, ab, ldab, b, ldb, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

uplo = 'U' or 'u': U, the upper triangular factor of A is stored.

uplo = 'L' or '1': L, the lower triangular factor of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

kd The number of super-diagonals of the matrix A if **uplo** = 'U' or 'u', or the number of sub-diagonals if **uplo** = 'L' or '1'. $\mathbf{kd} \geq 0$.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. $\mathbf{nrhs} \geq 0$.

ab The triangular factor U or L from the Cholesky factorization of the band matrix A, stored in the first **kd**+1 rows of the array. The j-th column of U or L is stored in the array **ab** as follows:

If **uplo** = 'U' or 'u', $\mathbf{ab}(\mathbf{kd}+1+i-j,j) = U(i,j)$ for $\max(1,j-\mathbf{kd}) \leq i \leq j$;

If **uplo** = 'L' or '1', $\mathbf{ab}(1+i-j,j) = L(i,j)$ for $j \leq i \leq \min(\mathbf{n},j+\mathbf{kd})$.

ldab The leading dimension of array **ab** in the calling program unit. $\mathbf{ldab} \geq \mathbf{kd}+1$.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. $\mathbf{ldb} \geq \max(1,\mathbf{n})$.

Output

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info Status response:

info = 0: Successful exit.

info < 0: If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
kd < 0,
nrhs < 0,
ldab < **kd**+1, and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPOCON/.../ZPOCON – Condition Number of Positive Definite Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a real symmetric or complex Hermitian positive definite matrix A using the Cholesky factorization computed by _POTRF.

An estimate is obtained for $\|A^{-1}\|_1$, and the reciprocal of the condition number is computed as **rcond** = $(\|A\|_1 \|A^{-1}\|_1)^{-1}$.

Usage

LAPACK:

```
CHARACTER*1        uplo
INTEGER*4          info, lda, n
REAL*4             anorm, rcond
INTEGER*4          iwork(n)
REAL*4             a(lda, n), work(3*n)
CALL SPOCON(uplo, n, a, lda, anorm, rcond, work, iwork, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, n
REAL*8             anorm, rcond
INTEGER*4          iwork(n)
REAL*8             a(lda, n), work(3*n)
CALL DPOCON(uplo, n, a, lda, anorm, rcond, work, iwork, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, n
REAL*4             anorm, rcond, rwork(n)
COMPLEX*8          a(lda, n), work(2*n)
CALL CPOCON(uplo, n, a, lda, anorm, rcond, work, rwork, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, n
REAL*8             anorm, rcond, rwork(n)
COMPLEX*16         a(lda, n), work(2*n)
CALL ZPOCON(uplo, n, a, lda, anorm, rcond, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, lda, n
REAL*8             anorm, rcond
INTEGER*8          iwork(n)
REAL*8             a(lda, n), work(3*n)
CALL SPOCON(uplo, n, a, lda, anorm, rcond, work, iwork, info)
```

```
CHARACTER*1     uplo
INTEGER*8       info, lda, n
REAL*8          anorm, rcond, rwork(n)
COMPLEX*16      a(lda, n), work(2*n)
CALL CPOCON(uplo, n, a, lda, anorm, rcond, work, rwork, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': U, the upper triangular factor of A is stored.
- **uplo** = 'L' or 'l': L, the lower triangular factor of A is stored.

n The order of the matrix A. **n** ≥ 0.

a The triangular factor U or L from the Cholesky factorization as computed by _POTRF.

lda The leading dimension of array **a** in the calling program unit. **lda** $\geq \max(1,$**n**$)$.

anorm $\|A\|_1$ $(= \|A\|_\infty)$ of the original symmetric or Hermitian matrix A. **anorm** ≥ 0.

Working Storage

work, iwork, rwork Arrays used for work space

Output

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as

rcond $= (\|A\|_1 \|A^{-1}\|_1)^{-1}$. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info Status response:

- **info** = 0: Successful exit.
- **info** < 0: If **info** $= -k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
lda < max(1,**n**), and
anorm < 0.0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPOTRF/DPOTRF/CPOTRF/ZPOTRF – Factor Positive Definite Matrix

Purpose

These subprograms compute the Cholesky factorization of a real symmetric or complex Hermitian positive definite matrix A. A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x; a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

Given such a matrix A, these subprograms compute the Cholesky factorization of the form $A = U^*U$ or $A = LL^*$ where U is an upper triangular matrix, L is a lower triangular matrix.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A. You may supply either the upper or the lower triangle of A, in a two-dimensional array large enough to hold the entire matrix. The other triangle of the array is not referenced.

Usage

LAPACK:

```
CHARACTER*1          uplo
INTEGER*4            info, lda, n
REAL*4               a(lda, n)
CALL SPOTRF(uplo, n, a, lda, info)

CHARACTER*1          uplo
INTEGER*4            info, lda, n
REAL*8               a(lda, n)
CALL DPOTRF(uplo, n, a, lda, info)

CHARACTER*1          uplo
INTEGER*4            info, lda, n
COMPLEX*8            a(lda, n)
CALL CPOTRF(uplo, n, a, lda, info)

CHARACTER*1          uplo
INTEGER*4            info, lda, n
COMPLEX*16           a(lda, n)
CALL ZPOTRF(uplo, n, a, lda, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, lda, n
REAL*8             a(lda, n)
CALL SPOTRF(uplo, n, a, lda, info)

CHARACTER*1        uplo
INTEGER*8          info, lda, n
COMPLEX*16         a(lda, n)
CALL CPOTRF(uplo, n, a, lda, info)
```

Input

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or 'l': The lower triangular part of A is stored.

n The order of the matrix A. **n** ≥ 0.

a The symmetric or Hermitian matrix A.

If **uplo** = 'U' or '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' or '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 The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

Output

a On successful exit, the Cholesky factor U or L overwrites the input.

info Status response:

- **info** = 0: Successful exit.
- **info** < 0: If **info** = $-k$, the k-th argument had an invalid value.
- **info** > 0: If **info** = k, the leading minor of order k is not positive definite, and the factorization could not be completed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0, and
lda < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPOTRI/DPOTRI/CPOTRI/ZPOTRI – Invert Positive Definite Matrix

Purpose

These subprograms compute the inverse of a real symmetric or complex Hermitian positive definite matrix *A* using the Cholesky factorization computed by _POTRF.

Usage

LAPACK:

```
CHARACTER*1        uplo
INTEGER*4          info, lda, n
REAL*4             a(lda, n)
CALL SPOTRI(uplo, n, a, lda, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, n
REAL*8             a(lda, n)
CALL DPOTRI(uplo, n, a, lda, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, n
COMPLEX*8          a(lda, n)
CALL CPOTRI(uplo, n, a, lda, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, n
COMPLEX*16         a(lda, n)
CALL ZPOTRI(uplo, n, a, lda, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, lda, n
REAL*8             a(lda, n)
CALL SPOTRI(uplo, n, a, lda, info)

CHARACTER*1        uplo
INTEGER*8          info, lda, n
COMPLEX*16         a(lda, n)
CALL CPOTRI(uplo, n, a, lda, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': U, the upper triangular factor of A is stored.
- **uplo** = 'L' or 'l': L, the lower triangular factor of A is stored.

n The order of the matrix A. **n** ≥ 0.

a The triangular factor U or L from the Cholesky factorization as computed by _POTRF.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

Output

a On successful exit, the upper or lower triangle of the symmetric or Hermitian inverse of A, overwriting the input factor U or L.

info Status response:

- **info** = 0: Successful exit.
- **info** < 0: If **info** = $-k$, the k-th argument had an invalid value.
- **info** > 0: If **info** = k, the (k,k) element of the factor U or L is zero; the matrix is singular and its inverse could not be computed.

Notes

It is almost never necessary to compute the inverse of a matrix. While papers and reference books extensively use the notation "$A^{-1}b$" to mean "the solution x of the system of linear equations $Ax = b$," it is almost always more efficient and more accurate to compute the solution directly than to invert the coefficient matrix and multiply the inverse times the right hand side vector. This is true even if there are many systems of equations, all using the same coefficient matrix; the matrix may be factored once and the systems may be solved from the factors usually just as efficiently—and more accurately—than by matrix multiplication by the inverse.

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0, and
lda < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPOTRS/DPOTRS/.../ZPOTRS – Solve Positive Definite Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$ with a real symmetric or complex Hermitian positive definite matrix A using the Cholesky factorization computed by _POTRF.

Usage

LAPACK:

```
CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
REAL*4             a(lda, n), b(ldb, nrhs)
CALL SPOTRS(uplo, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
REAL*8             a(lda, n), b(ldb, nrhs)
CALL DPOTRS(uplo, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
COMPLEX*8          a(lda, n), b(ldb, nrhs)
CALL CPOTRS(uplo, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
COMPLEX*16         a(lda, n), b(ldb, nrhs)
CALL ZPOTRS(uplo, n, nrhs, a, lda, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, lda, ldb, n, nrhs
REAL*8             a(lda, n), b(ldb, nrhs)
CALL SPOTRS(uplo, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1        uplo
INTEGER*8          info, lda, ldb, n, nrhs
COMPLEX*16         a(lda, n), b(ldb, nrhs)
CALL CPOTRS(uplo, n, nrhs, a, lda, b, ldb, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': U, the upper triangular factor of A is stored.
- **uplo** = 'L' or 'l': L, the lower triangular factor of A is stored.

n The order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

a The triangular factor U or L from the Cholesky factorization as computed by _POTRF.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

Output

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info Status response:

- **info** = 0: Successful exit.
- **info** < 0: If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
nrhs < 0,
lda < max(1,**n**), and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPPCON/... – Condition Number of Positive Definite Packed Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a real symmetric or complex Hermitian positive definite matrix A that is stored in an array in packed form, using the Cholesky factorization computed by _PPTRF.

An estimate is obtained for $\|A^{-1}\|_1$, and the reciprocal of the condition number is computed as **rcond** = $(\|A\|_1 \|A^{-1}\|_1)^{-1}$.

Usage

LAPACK:

```
CHARACTER*1        uplo
INTEGER*4          info, n
REAL*4             anorm, rcond
INTEGER*4          iwork(n)
REAL*4             ap((n*(n+1))/2), work(3*n)
CALL SPPCON(uplo, n, ap, anorm, rcond, work, iwork, info)

CHARACTER*1        uplo
INTEGER*4          info, n
REAL*8             anorm, rcond
INTEGER*4          iwork(n)
REAL*8             ap((n*(n+1))/2), work(3*n)
CALL DPPCON(uplo, n, ap, anorm, rcond, work, iwork, info)

CHARACTER*1        uplo
INTEGER*4          info, n
REAL*4             anorm, rcond
REAL*4             rwork(n)
COMPLEX*8          ap((n*(n+1))/2), work(2*n)
CALL CPPCON(uplo, n, ap, anorm, rcond, work, rwork, info)

CHARACTER*1        uplo
INTEGER*4          info, n
REAL*8             anorm, rcond
REAL*8             rwork(n)
COMPLEX*16         ap((n*(n+1))/2), work(2*n)
CALL ZPPCON(uplo, n, ap, anorm, rcond, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, n
REAL*8             anorm, rcond
INTEGER*8          iwork(n)
REAL*8             ap((n*(n+1))/2), work(3*n)
CALL SPPCON(uplo, n, ap, anorm, rcond, work, iwork, info)
CHARACTER*1        uplo
INTEGER*8          info, n
REAL*8             anorm, rcond
REAL*8             rwork(n)
COMPLEX*16         ap((n*(n+1))/2), work(2*n)
CALL CPPCON(uplo, n, ap, anorm, rcond, work, rwork, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': U, the upper triangular factor of A is stored.
- **uplo** = 'L' or '1': L, the lower triangular factor of A is stored.

n The order of the matrix A. **n** ≥ 0.

ap The triangular factor U or L from the Cholesky factorization as computed by _PPTRF.

anorm $||A||_1$ (= $||A||_\infty$) of the original symmetric or Hermitian matrix A. **anorm** ≥ 0.

Working Storage

work, iwork, rwork Arrays used for work space

Output

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as

rcond = $(||A||_1 \, ||A^{-1}||_1)^{-1}$. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0, and
anorm < 0.0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPPTRF/DPPTRF/.../ZPPTRF – Factor Positive Definite Packed Matrix

Purpose

These subprograms compute the Cholesky factorization of a real symmetric or complex Hermitian positive definite matrix A that is stored in an array in packed form. A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x; a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

Given such a matrix A, these subprograms compute the Cholesky factorization of the form $A = U^*U$ or $A = LL^*$ where U is an upper triangular matrix, L is a lower triangular matrix.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A, either the upper or the lower triangle. Compared to storing the entire matrix, you save memory by supplying that triangle stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**($i+j\times(j-1)/2$).

Lower triangular storage. If the lower triangle of A is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**(i+(j–1)×(2n–j)/2).

Usage

LAPACK:

```
CHARACTER*1          uplo
INTEGER*4            info, n
REAL*4               ap((n*(n+1))/2)
CALL SPPTRF(uplo, n, ap, info)

CHARACTER*1          uplo
INTEGER*4            info, n
REAL*8               ap((n*(n+1))/2)
CALL DPPTRF(uplo, n, ap, info)

CHARACTER*1          uplo
INTEGER*4            info, n
COMPLEX*8            ap((n*(n+1))/2)
CALL CPPTRF(uplo, n, ap, info)

CHARACTER*1          uplo
INTEGER*4            info, n
COMPLEX*16           ap((n*(n+1))/2)
CALL ZPPTRF(uplo, n, ap, info)
```

LAPACK8:

```
CHARACTER*1          uplo
INTEGER*8            info, n
REAL*8               ap((n*(n+1))/2)
CALL SPPTRF(uplo, n, ap, info)

CHARACTER*1          uplo
INTEGER*8            info, n
COMPLEX*16           ap((n*(n+1))/2)
CALL CPPTRF(uplo, n, ap, info)
```

Input

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or 'l': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

ap The upper or lower triangular part of the symmetric or Hermitian matrix A, packed columnwise in a linear array as follows:

If **uplo** = 'U' or 'u', $\mathbf{ap}(i + (j-1) \times j/2) = A(i,j)$ for $1 \leq i \leq j$;

If **uplo** = 'L' or 'l', $\mathbf{ap}(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \leq i \leq \mathbf{n}$.

Output

ap On successful exit, the Cholesky factor U or L overwrites the input.

info Status response:

- **info** = 0: Successful exit.
- **info** < 0: If **info** = $-k$, the k-th argument had an invalid value.
- **info** > 0: If **info** = k, the leading minor of order k is not positive definite, and the factorization could not be completed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u', and
n < 0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPPTRI/DPPTRI/.../ZPPTRI – Invert Positive Definite Packed Matrix

Purpose

These subprograms compute the inverse of a real symmetric or complex Hermitian positive definite matrix A that is stored in an array in packed form, using the Cholesky factorization computed by _PPTRF.

Matrix Storage

Because either triangle of A^{-1} may be obtained from that triangle of the Cholesky factorization of A or from the other triangle of A^{-1}, you need only provide one triangle of the factorization, and only the corresponding triangle of A^{-1} is computed. Compared to storing the entire matrix, you save memory by supplying only either the upper or the lower triangle of the factorization of A, stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A^{-1} is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then $(\alpha_{ij}) = A^{-1}$ is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element α_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular storage. If the lower triangle of A^{-1} is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then $(\alpha_{ij}) = A^{-1}$ is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element α_{ij} is stored in array element **ap**(i+(j–1)×(2n–j)/2).

Usage

LAPACK:

```
CHARACTER*1        uplo
INTEGER*4          info, n
REAL*4             ap((n*(n+1))/2)
CALL SPPTRI(uplo, n, ap, info)

CHARACTER*1        uplo
INTEGER*4          info, n
REAL*8             ap((n*(n+1))/2)
CALL DPPTRI(uplo, n, ap, info)

CHARACTER*1        uplo
INTEGER*4          info, n
COMPLEX*8          ap((n*(n+1))/2)
CALL CPPTRI(uplo, n, ap, info)

CHARACTER*1        uplo
INTEGER*4          info, n
COMPLEX*16         ap((n*(n+1))/2)
CALL ZPPTRI(uplo, n, ap, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, n
REAL*8             ap((n*(n+1))/2)
CALL SPPTRI(uplo, n, ap, info)

CHARACTER*1        uplo
INTEGER*8          info, n
COMPLEX*16         ap((n*(n+1))/2)
CALL CPPTRI(uplo, n, ap, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': U, the upper triangular factor of A is stored.
- **uplo** = 'L' or 'l': L, the lower triangular factor of A is stored.

n The order of the matrix A. **n** ≥ 0.

ap The triangular factor U or L from the Cholesky factorization as computed by _PPTRF.

Output

ap On successful exit, the upper or lower triangle of the symmetric or Hermitian inverse of A overwrites the input, as follows:

If **uplo** = 'U' or 'u', $\mathbf{ap}(i + (j-1) \times j/2) = A^{-1}(i,j)$ for $1 \le i \le j$;

If **uplo** = 'L' or '1', $\mathbf{ap}(i + (j-1) \times (2\mathbf{n}-j)/2) = A^{-1}(i,j)$ for $j \le i \le \mathbf{n}$.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, the (k,k) element of the factor U or L is zero; the matrix is singular and its inverse could not be computed.

Notes

It is almost never necessary to compute the inverse of a matrix. While papers and reference books extensively use the notation "$A^{-1}b$" to mean "the solution x of the system of linear equations $Ax = b$," it is almost always more efficient and more accurate to compute the solution directly than to invert the coefficient matrix and multiply the inverse times the right hand side vector. This is true even if there are many systems of equations, all using the same coefficient matrix; the matrix may be factored once and the systems may be solved from the factors usually just as efficiently—and more accurately—than by matrix multiplication by the inverse.

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or '1' or 'U' or 'u',
n < 0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPPTRS/.../ZPPTRS – Solve Positive Definite Packed Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$ with a real symmetric or complex Hermitian positive definite matrix A that is stored in an array in packed form, using the Cholesky factorization computed by _PPTRF.

Usage

LAPACK:

```
CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
REAL*4               ap((n*(n+1))/2), b(ldb, nrhs)
CALL SPPTRS(uplo, n, nrhs, ap, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
REAL*8               ap((n*(n+1))/2), b(ldb, nrhs)
CALL DPPTRS(uplo, n, nrhs, ap, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
COMPLEX*8            ap((n*(n+1))/2), b(ldb, nrhs)
CALL CPPTRS(uplo, n, nrhs, ap, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
COMPLEX*16           ap((n*(n+1))/2), b(ldb, nrhs)
CALL ZPPTRS(uplo, n, nrhs, ap, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1          uplo
INTEGER*8            info, ldb, n, nrhs
REAL*8               ap((n*(n+1))/2), b(ldb, nrhs)
CALL SPPTRS(uplo, n, nrhs, ap, b, ldb, info)

CHARACTER*1          uplo
INTEGER*8            info, ldb, n, nrhs
COMPLEX*16           ap((n*(n+1))/2), b(ldb, nrhs)
CALL CPPTRS(uplo, n, nrhs, ap, b, ldb, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

uplo = 'U' or 'u':	U, the upper triangular factor of A is stored.
uplo = 'L' or 'l':	L, the lower triangular factor of A is stored.

n The order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ap The triangular factor U or L from the Cholesky factorization as computed by _PPTRF.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

Output

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
nrhs < 0, and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SPTCON/... – Condition Number of Positive Definite Tridiagonal Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a real symmetric or complex Hermitian positive definite tridiagonal matrix A using the Cholesky factorization computed by _PTTRF.

An estimate is obtained for $||A^{-1}||$, and the reciprocal of the condition number is computed as **rcond** = $(||A||_1 \, ||A^{-1}||_1)^{-1}$.

Usage

LAPACK:

```
INTEGER*4          info, n
REAL*4             anorm, rcond
REAL*4             d(n), e(n–1), work(n)
CALL SPTCON(n, d, e, anorm, rcond, work, info)

INTEGER*4          info, n
REAL*8             anorm, rcond
REAL*8             d(n), e(n–1), work(n)
CALL DPTCON(n, d, e, anorm, rcond, work, info)

INTEGER*4          info, n
REAL*4             anorm, rcond
REAL*4             d(n), rwork(n)
COMPLEX*8          e(n–1)
CALL CPTCON(n, d, e, anorm, rcond, rwork, info)

INTEGER*4          info, n
REAL*8             anorm, rcond
REAL*8             d(n), rwork(n)
COMPLEX*16         e(n–1)
CALL ZPTCON(n, d, e, anorm, rcond, rwork, info)
```

LAPACK8:

```
INTEGER*8          info, n
REAL*8             anorm, rcond
REAL*8             d(n), e(n–1), work(n)
CALL SPTCON(n, d, e, anorm, rcond, work, info)

INTEGER*8          info, n
REAL*8             anorm, rcond
REAL*8             d(n), rwork(n)
COMPLEX*16         e(n–1)
CALL CPTCON(n, d, e, anorm, rcond, rwork, info)
```

Input

n The order of the matrix A. $\mathbf{n} \geq 0$.

d The **n** diagonal elements of the diagonal matrix D from the LDL^* factorization of A.

e The **n**–1 subdiagonal elements of the unit bidiagonal factor L from the LDL^* factorization of A. **e** can also be regarded as the superdiagonal of the unit bidiagonal factor U from the U^*DU factorization of A.

anorm $\|A\|_1$ (= $\|A\|_\infty$) of the original symmetric or Hermitian tridiagonal matrix A. **anorm** ≥ 0.

Working Storage

work, rwork Arrays used for work space.

Output

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as

rcond = $(\|A\|_1 \|A^{-1}\|_1)^{-1}$. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

n < 0, and
anorm < 0.0.

NAME

SPTTRF/.../ZPTTRF – Factor Positive Definite Tridiagonal Matrix

Purpose

These subprograms compute the Cholesky factorization of a real symmetric or complex Hermitian positive definite tridiagonal matrix A. A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A real symmetric matrix A is positive definite if the quadratic form x^TAx is positive for all nonzero real vectors x; a complex Hermitian matrix A is positive definite if the quadratic form x^*Ax is positive for all nonzero complex vectors x.

A matrix $A = (a_{ij})$ is tridiagonal if its nonzero elements lie only on the principal diagonal ($i = j$), the subdiagonal ($i = j+1$), and the superdiagonal ($i = j-1$) of the matrix.

Given such a matrix A, these subprograms compute the Cholesky factorization of the form $A = LDL^*$ where L is a unit lower bidiagonal matrix and D is a diagonal matrix. Alternatively, the factorization can be viewed as $A = U^*DU$.

Matrix Storage

The following example illustrates the storage of symmetric or Hermitian tridiagonal matrices. Consider the following symmetric tridiagonal matrix of order $n = 7$:

11	21	0	0	0	0	0
21	22	32	0	0	0	0
0	32	33	43	0	0	0
0	0	43	44	54	0	0
0	0	0	54	55	65	0
0	0	0	0	65	66	76
0	0	0	0	0	76	77

The subdiagonal is stored in array **e** and the principal diagonal is stored in array **d**, as follows:

i	**e**(i)	**d**(i)
1	21	11
2	32	22
3	43	33
4	54	44
5	65	55
6	76	66
7		77

Usage

LAPACK:

```
INTEGER*4          info, n
REAL*4             d(n), e(n–1)
CALL SPTTRF(n, d, e, info)

INTEGER*4          info, n
REAL*8             d(n), e(n–1)
CALL DPTTRF(n, d, e, info)

INTEGER*4          info, n
REAL*4             d(n)
COMPLEX*8          e(n–1)
CALL CPTTRF(n, d, e, info)

INTEGER*4          info, n
REAL*8             d(n)
COMPLEX*16         e(n–1)
CALL ZPTTRF(n, d, e, info)
```

LAPACK8:

```
INTEGER*8          info, n
REAL*8             d(n), e(n–1)
CALL SPTTRF(n, d, e, info)

INTEGER*8          info, n
REAL*8             d(n)
COMPLEX*16         e(n–1)
CALL CPTTRF(n, d, e, info)
```

Input

n	The order of the matrix A. **n** ≥ 0.
d	The **n** diagonal elements of the tridiagonal matrix A.
e	The **n**–1 subdiagonal elements of the tridiagonal matrix A.

Output

d On successful exit, the **n** diagonal elements of the diagonal matrix D from the LDL^* factorization of A.

e On successful exit, the **n**–1 subdiagonal elements of the unit lower bidiagonal factor L from the LDL^* factorization of A. **e** can also be regarded as the superdiagonal of the unit upper bidiagonal factor U from the U^*DU factorization of A.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, the leading minor of order k is not positive definite; if k < **n**, the factorization could not be completed, while if k = **n**, the factorization was completed but $D(n) = 0$.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

n < 0.

NAME

SPTTRS/.../ZPTTRS – Solve Positive Definite Tridiagonal System

Purpose

These subprograms solve a system of linear equations $AX = B$ with a real symmetric or complex Hermitian positive definite tridiagonal matrix A using the Cholesky factorization computed by _PTTRF.

Usage

LAPACK:

```
INTEGER*4          info, ldb, n, nrhs
REAL*4             b(ldb, nrhs), d(n), e(n–1)
CALL SPTTRS(n, nrhs, d, e, b, ldb, info)

INTEGER*4          info, ldb, n, nrhs
REAL*8             b(ldb, nrhs), d(n), e(n–1)
CALL DPTTRS(n, nrhs, d, e, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, ldb, n, nrhs
REAL*4             d(n)
COMPLEX*8          b(ldb, nrhs), e(n–1)
CALL CPTTRS(uplo, n, nrhs, d, e, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, ldb, n, nrhs
REAL*8             d(n)
COMPLEX*16         b(ldb, nrhs), e(n–1)
CALL ZPTTRS(uplo, n, nrhs, d, e, b, ldb, info)
```

LAPACK8:

```
INTEGER*8          info, ldb, n, nrhs
REAL*8             b(ldb, nrhs), d(n), e(n–1)
CALL SPTTRS(n, nrhs, d, e, b, ldb, info)

CHARACTER*1        uplo
INTEGER*8          info, ldb, n, nrhs
REAL*8             d(n)
COMPLEX*16         b(ldb, nrhs), e(n–1)
CALL CPTTRS(uplo, n, nrhs, d, e, b, ldb, info)
```

Input

uplo Specifies the form of the factorization and whether the array **e** contains the superdiagonal of the upper bidiagonal factor U or the subdiagonal of the lower bidiagonal factor L, as follows:

uplo = 'U' or 'u': $A = U^T DU$ and **e** is the superdiagonal of U.

uplo = 'L' or 'l': $A = LDL^T$ and **e** is the superdiagonal of L.

n The order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

d The **n** diagonal elements of the diagonal matrix D from the LDL^* factorization of A.

e The **n**–1 subdiagonal elements of the unit bidiagonal factor L from the LDL^* factorization of A. **e** can also be regarded as the superdiagonal of the unit bidiagonal factor U from the U^*DU factorization of A.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

Output

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info Status response:

info = 0: Successful exit.

info < 0: If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
nrhs < 0, and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SSPCON/... – Condition Number of Symmetric or Hermitian Packed Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a real or complex symmetric or complex Hermitian matrix A that is stored in an array in packed form, using the Bunch-Kaufman factorization computed by _SPTRF or _HPTRF.

The structure of A is indicated by the name of the subprogram used:

SSPCON	or	DSPCON	A is a real symmetric packed matrix.
CSPCON	or	ZSPCON	A is a complex symmetric packed matrix.
CHPCON	or	ZHPCON	A is a complex Hermitian packed matrix.

An estimate is obtained for $||A^{-1}||$, and the reciprocal of the condition number is computed as **rcond** = $(||A||\ ||A^{-1}||)^{-1}$.

Usage

LAPACK:

```
CHARACTER*1          uplo
INTEGER*4            info, n
REAL*4               anorm, rcond
INTEGER*4            ipiv(n), iwork(n)
REAL*4               ap((n*(n+1))/2), work(2*n)
CALL SSPCON(uplo, n, ap, ipiv, anorm, rcond, work, iwork, info)

CHARACTER*1          uplo
INTEGER*4            info, n
REAL*8               anorm, rcond
INTEGER*4            ipiv(n), iwork(n)
REAL*8               ap((n*(n+1))/2), work(2*n)
CALL DSPCON(uplo, n, ap, ipiv, anorm, rcond, work, iwork, info)

CHARACTER*1          uplo
INTEGER*4            info, n
REAL*4               anorm, rcond
INTEGER*4            ipiv(n)
COMPLEX*8            ap((n*(n+1))/2), work(2*n)
CALL CHPCON(uplo, n, ap, ipiv, anorm, rcond, work, info)

CHARACTER*1          uplo
INTEGER*4            info, n
REAL*4               anorm, rcond
INTEGER*4            ipiv(n)
COMPLEX*8            ap((n*(n+1))/2), work(2*n)
CALL CSPCON(uplo, n, ap, ipiv, anorm, rcond, work, info)
```

```
CHARACTER*1     uplo
INTEGER*4       info, n
REAL*8          anorm, rcond
INTEGER*4       ipiv(n)
COMPLEX*16      ap((n*(n+1))/2), work(2*n)
CALL ZHPCON(uplo, n, ap, ipiv, anorm, rcond, work, info)
```

```
CHARACTER*1     uplo
INTEGER*4       info, n
REAL*8          anorm, rcond
INTEGER*4       ipiv(n)
COMPLEX*16      ap((n*(n+1))/2), work(2*n)
CALL ZSPCON(uplo, n, ap, ipiv, anorm, rcond, work, info)
```

LAPACK8:

```
CHARACTER*1     uplo
INTEGER*8       info, n
REAL*8          anorm, rcond
INTEGER*8       ipiv(n), iwork(n)
REAL*8          ap((n*(n+1))/2), work(2*n)
CALL SSPCON(uplo, n, ap, ipiv, anorm, rcond, work, iwork, info)
```

```
CHARACTER*1     uplo
INTEGER*8       info, n
REAL*8          anorm, rcond
INTEGER*8       ipiv(n)
COMPLEX*16      ap((n*(n+1))/2), work(2*n)
CALL CHPCON(uplo, n, ap, ipiv, anorm, rcond, work, info)
```

```
CHARACTER*1     uplo
INTEGER*8       info, n
REAL*8          anorm, rcond
INTEGER*8       ipiv(n)
COMPLEX*16      ap((n*(n+1))/2), work(2*n)
CALL CSPCON(uplo, n, ap, ipiv, anorm, rcond, work, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular factor of A is stored.
- **uplo** = 'L' or 'l': The lower triangular factor of A is stored.

n The order of the matrix A. $n \geq 0$.

ap The block diagonal matrix D and the multipliers used to obtain the factor U or L as computed by _SPTRF or _HPTRF.

ipiv Details of the interchanges and the block structure of D as determined by _SPTRF or _HPTRF.

anorm $\|A\|_1$ (= $\|A\|_\infty$) of the original symmetric or Hermitian matrix A. **anorm** ≥ 0.

Working Storage

work, iwork Arrays used for work space.

Output

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as

rcond = $(\|A\|_1 \|A^{-1}\|_1)^{-1}$. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',

n < 0, and

anorm < 0.0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SSPTRF/.../ZSPTRF – Factor Symmetric or Hermitian Packed Matrix

Purpose

These subprograms compute the factorization of a real or complex symmetric or complex Hermitian matrix A that is stored in an array in packed form, using the Bunch-Kaufman diagonal pivoting method. If A is known to be positive definite, other subprograms in this chapter, specifically designed for positive definite matrices, are more efficient than these subprograms.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

The structure of A is indicated by the name of the subprogram used:

SSPTRF	or	DSPTRF	A is a real symmetric packed matrix.
CSPTRF	or	ZSPTRF	A is a complex symmetric packed matrix.
CHPTRF	or	ZHPTRF	A is a complex Hermitian packed matrix.

If A is real or complex symmetric, the factorization has the form $A = UDU^T$ or $A = LDL^T$ where U is a product of permutation and unit upper triangular matrices, L is a product of permutation and unit lower triangular matrices, and D is symmetric and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

If A is complex Hermitian, the factorization has the form $A = UDU^*$ or $A = LDL^*$ where U and L are as above, and D is Hermitian and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A, either the upper or the lower triangle. Compared to storing the entire matrix, you save memory by supplying that triangle stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**($i+j\times(j-1)/2$).

Lower triangular storage. If the lower triangle of A is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**($i+(j-1)\times(2n-j)/2$).

Usage

LAPACK:

```
CHARACTER*1        uplo
INTEGER*4          info, n
INTEGER*4          ipiv(n)
REAL*4             ap((n*(n+1))/2)
CALL SSPTRF(uplo, n, ap, ipiv, info)

CHARACTER*1        uplo
INTEGER*4          info, n
INTEGER*4          ipiv(n)
REAL*8             ap((n*(n+1))/2)
CALL DSPTRF(uplo, n, ap, ipiv, info)

CHARACTER*1        uplo
```

```
INTEGER*4          info, n
INTEGER*4          ipiv(n)
COMPLEX*8          ap((n*(n+1))/2)
CALL CHPTRF(uplo, n, ap, ipiv, info)

CHARACTER*1        uplo
INTEGER*4          info, n
INTEGER*4          ipiv(n)
COMPLEX*8          ap((n*(n+1))/2)
CALL CSPTRF(uplo, n, ap, ipiv, info)

CHARACTER*1        uplo
INTEGER*4          info, n
INTEGER*4          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2)
CALL ZHPTRF(uplo, n, ap, ipiv, info)

CHARACTER*1        uplo
INTEGER*4          info, n
INTEGER*4          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2)
CALL ZSPTRF(uplo, n, ap, ipiv, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, n
INTEGER*8          ipiv(n)
REAL*8             ap((n*(n+1))/2)
CALL SSPTRF(uplo, n, ap, ipiv, info)

CHARACTER*1        uplo
INTEGER*8          info, n
INTEGER*8          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2)
CALL CHPTRF(uplo, n, ap, ipiv, info)

CHARACTER*1        uplo
INTEGER*8          info, n
INTEGER*8          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2)
CALL CSPTRF(uplo, n, ap, ipiv, info)
```

Input

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

uplo = 'U' or 'u':	The upper triangular part of A is stored.
uplo = 'L' or 'l':	The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

ap The upper or lower triangular part of the symmetric or Hermitian matrix A, packed columnwise in a linear array as follows:

If **uplo** = 'U' or 'u', $\mathbf{ap}(i + (j-1) \times j/2) = A(i,j)$ for $1 \leq i \leq j$;

If **uplo** = 'L' or 'l', $\mathbf{ap}(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \leq i \leq \mathbf{n}$.

Output

ap On successful exit, the block diagonal matrix D and the multipliers used to obtain the factor U or L overwrites the input.

ipiv On successful exit, details of the interchanges and the block structure of D:

If $\mathbf{ipiv}(k) > 0$, then rows and columns k and $\mathbf{ipiv}(k)$ were interchanged and $D(k,k)$ is a 1-by-1 diagonal block.

If **uplo** = 'U' or 'u' and $\mathbf{ipiv}(k) = \mathbf{ipiv}(k-1) < 0$, then rows and columns $k-1$ and $-\mathbf{ipiv}(k)$ were interchanged and $D(k-1:k,k-1:k)$ is a 2-by-2 diagonal block.

If **uplo** = 'L' or 'l' and $\mathbf{ipiv}(k) = \mathbf{ipiv}(k+1) < 0$, then rows and columns $k+1$ and $-\mathbf{ipiv}(k)$ were interchanged and $D(k:k+1,k:k+1)$ is a 2-by-2 diagonal block.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, $D(k,k)$ is zero. The factorization has been completed, but the block diagonal matrix D is singular, and division by zero will occur if it is used to solve a system of equations.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u', and
n < 0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SSPTRI/.../ZSPTRI – Invert Symmetric or Hermitian Packed Matrix

Purpose

These subprograms compute the inverse of a real or complex symmetric or complex Hermitian matrix A that is stored in an array in packed form, using the Bunch-Kaufman factorization computed by _SPTRF or _HPTRF.

The structure of A is indicated by the name of the subprogram used:

SSPTRI	or DSPTRI	A is a real symmetric matrix.
CSPTRI	or ZSPTRI	A is a complex symmetric matrix.
CHPTRI	or ZHPTRI	A is a complex Hermitian matrix.

Matrix Storage

Because either triangle of A^{-1} may be obtained from that triangle of the Bunch-Kaufman factorization of A or from the other triangle of A^{-1}, you need only provide one triangle of the factorization, and only the corresponding triangle of A^{-1} is computed. Compared to storing the entire matrix, you save memory by supplying only either the upper or the lower triangle of the factorization of A, stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A^{-1} is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then $(\alpha_{ij}) = A^{-1}$ is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element α_{ij} is stored in array element **ap**($i+j\times(j-1)/2$).

Lower triangular storage. If the lower triangle of A^{-1} is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then $(\alpha_{ij}) = A^{-1}$ is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element α_{ij} is stored in array element **ap**$(i+(j-1)\times(2n-j)/2)$.

Usage

LAPACK:

```
CHARACTER*1          uplo
INTEGER*4            info, n
INTEGER*4            ipiv(n)
REAL*4               ap((n*(n+1))/2), work(n)
CALL SSPTRI(uplo, n, ap, ipiv, work, info)

CHARACTER*1          uplo
INTEGER*4            info, n
INTEGER*4            ipiv(n)
REAL*8               ap((n*(n+1))/2), work(n)
CALL DSPTRI(uplo, n, ap, ipiv, work, info)

CHARACTER*1          uplo
INTEGER*4            info, n
INTEGER*4            ipiv(n)
COMPLEX*8            ap((n*(n+1))/2), work(n)
CALL CHPTRI(uplo, n, ap, ipiv, work, info)

CHARACTER*1          uplo
INTEGER*4            info, n
INTEGER*4            ipiv(n)
COMPLEX*8            ap((n*(n+1))/2), work(n)
CALL CSPTRI(uplo, n, ap, ipiv, work, info)

CHARACTER*1          uplo
INTEGER*4            info, n
INTEGER*4            ipiv(n)
COMPLEX*16           ap((n*(n+1))/2), work(n)
CALL ZHPTRI(uplo, n, ap, ipiv, work, info)
```

```
CHARACTER*1        uplo
INTEGER*4          info, n
INTEGER*4          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2), work(n)
CALL ZSPTRI(uplo, n, ap, ipiv, work, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, n
INTEGER*8          ipiv(n)
REAL*8             ap((n*(n+1))/2), work(n)
CALL SSPTRI(uplo, n, ap, ipiv, work, info)
```

```
CHARACTER*1        uplo
INTEGER*8          info, n
INTEGER*8          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2), work(n)
CALL CHPTRI(uplo, n, ap, ipiv, work, info)
```

```
CHARACTER*1        uplo
INTEGER*8          info, n
INTEGER*8          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2), work(n)
CALL CSPTRI(uplo, n, ap, ipiv, work, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular factor of A is stored.
- **uplo** = 'L' or 'l': The lower triangular factor of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

ap The block diagonal matrix D and the multipliers used to obtain the factor U or L as computed by _SPTRF or _HPTRF.

ipiv Details of the interchanges and the block structure of D as determined by _SPTRF or _HPTRF.

Working Storage

work An array used for work space.

Output

ap On successful exit, the upper or lower triangle of the symmetric or Hermitian inverse of A overwrites the input, as follows:

If **uplo** = 'U' or 'u', $\mathbf{ap}(i + (j-1) \times j/2) = A^{-1}(i,j)$ for $1 \le i \le j$;

If **uplo** = 'L' or '1', $\mathbf{ap}(i + (j-1) \times (2\mathbf{n}-j)/2) = A^{-1}(i,j)$ for $j \le i \le \mathbf{n}$.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, $D(k,k)$ is zero; the matrix is singular and its inverse could not be computed.

Notes

It is almost never necessary to compute the inverse of a matrix. While papers and reference books extensively use the notation "$A^{-1}b$" to mean "the solution x of the system of linear equations $Ax = b$," it is almost always more efficient and more accurate to compute the solution directly than to invert the coefficient matrix and multiply the inverse times the right hand side vector. This is true even if there are many systems of equations, all using the same coefficient matrix; the matrix may be factored once and the systems may be solved from the factors usually just as efficiently—and more accurately—than by matrix multiplication by the inverse.

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or '1' or 'U' or 'u',
n < 0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SSPTRS/.../ZSPTRS – Solve Symmetric or Hermitian Packed System

Purpose

These subprograms solve a system of linear equations $AX = B$ with a real or complex symmetric or complex Hermitian matrix A that is stored in an array in packed form, using the Bunch-Kaufman factorization computed by _SPTRF or _HPTRF.

The structure of A is indicated by the name of the subprogram used:

SSPTRS	or	DSPTRS	A is a real symmetric packed matrix.
CSPTRS	or	ZSPTRS	A is a complex symmetric packed matrix.
CHETRS	or	ZHETRS	A is a complex Hermitian matrix.

Usage

LAPACK:

```
CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
INTEGER*4            ipiv(n)
REAL*4               ap((n*(n+1))/2), b(ldb, nrhs)
CALL SSPTRS(uplo, n, nrhs, ap, ipiv, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
INTEGER*4            ipiv(n)
REAL*8               ap((n*(n+1))/2), b(ldb, nrhs)
CALL DSPTRS(uplo, n, nrhs, ap, ipiv, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
INTEGER*4            ipiv(n)
COMPLEX*8            ap((n*(n+1))/2), b(ldb, nrhs)
CALL CHPTRS(uplo, n, nrhs, ap, ipiv, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
INTEGER*4            ipiv(n)
COMPLEX*8            ap((n*(n+1))/2), b(ldb, nrhs)
CALL CSPTRS(uplo, n, nrhs, ap, ipiv, b, ldb, info)

CHARACTER*1          uplo
INTEGER*4            info, ldb, n, nrhs
INTEGER*4            ipiv(n)
COMPLEX*16           ap((n*(n+1))/2), b(ldb, nrhs)
CALL ZHPTRS(uplo, n, nrhs, ap, ipiv, b, ldb, info)
```

```
CHARACTER*1        uplo
INTEGER*4          info, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2), b(ldb, nrhs)
CALL ZSPTRS(uplo, n, nrhs, ap, ipiv, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, ldb, n, nrhs
INTEGER*8          ipiv(n)
REAL*8             ap((n*(n+1))/2), b(ldb, nrhs)
CALL SSPTRS(uplo, n, nrhs, ap, ipiv, b, ldb, info)
```

```
CHARACTER*1        uplo
INTEGER*8          info, ldb, n, nrhs
INTEGER*8          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2), b(ldb, nrhs)
CALL CHPTRS(uplo, n, nrhs, ap, ipiv, b, ldb, info)
```

```
CHARACTER*1        uplo
INTEGER*8          info, ldb, n, nrhs
INTEGER*8          ipiv(n)
COMPLEX*16         ap((n*(n+1))/2), b(ldb, nrhs)
CALL CSPTRS(uplo, n, nrhs, ap, ipiv, b, ldb, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular factor of A is stored.
- **uplo** = 'L' or 'l': The lower triangular factor of A is stored.

n The order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ap The block diagonal matrix D and the multipliers used to obtain the factor U or L as computed by _SPTRF or _HPTRF.

ipiv Details of the interchanges and the block structure of D as determined by _SPTRF or _HPTRF.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

Output

b	On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
nrhs < 0, and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SSYCON/... – Condition Number of Symmetric or Hermitian Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a real or complex symmetric or complex Hermitian matrix A using the Bunch-Kaufman factorization computed by _SYTRF or _HETRF.

The structure of A is indicated by the name of the subprogram used:

SSYCON	or DSYCON	A is a real symmetric matrix.
CSYCON	or ZSYCON	A is a complex symmetric matrix.
CHECON	or ZHECON	A is a complex Hermitian matrix.

An estimate is obtained for $||A^{-1}||$, and the reciprocal of the condition number is computed as **rcond** = $(||A||\ ||A^{-1}||)^{-1}$.

Usage

LAPACK:

```
CHARACTER*1     uplo
INTEGER*4       info, lda, n
REAL*4          anorm, rcond
INTEGER*4       ipiv(n), iwork(n)
REAL*4          a(lda, n), work(2*n)
CALL SSYCON(uplo, n, a, lda, ipiv, anorm, rcond, work, iwork, info)
```

```
CHARACTER*1     uplo
INTEGER*4       info, lda, n
REAL*8          anorm, rcond
INTEGER*4       ipiv(n), iwork(n)
REAL*8          a(lda, n), work(2*n)
CALL DSYCON(uplo, n, a, lda, ipiv, anorm, rcond, work, iwork, info)
```

```
CHARACTER*1     uplo
INTEGER*4       info, lda, n
REAL*4          anorm, rcond
INTEGER*4       ipiv(n)
COMPLEX*8       a(lda, n), work(2*n)
CALL CHECON(uplo, n, a, lda, ipiv, anorm, rcond, work, info)
```

```
CHARACTER*1     uplo
INTEGER*4       info, lda, n
REAL*4          anorm, rcond
INTEGER*4       ipiv(n)
COMPLEX*8       a(lda, n), work(2*n)
CALL CSYCON(uplo, n, a, lda, ipiv, anorm, rcond, work, info)
```

```
CHARACTER*1     uplo
INTEGER*4       info, lda, n
REAL*8          anorm, rcond
INTEGER*4       ipiv(n)
COMPLEX*16      a(lda, n), work(2*n)
CALL ZHECON(uplo, n, a, lda, ipiv, anorm, rcond, work, info)

CHARACTER*1     uplo
INTEGER*4       info, lda, n
REAL*8          anorm, rcond
INTEGER*4       ipiv(n)
COMPLEX*16      a(lda, n), work(2*n)
CALL ZSYCON(uplo, n, a, lda, ipiv, anorm, rcond, work, info)
```

LAPACK8:

```
CHARACTER*1     uplo
INTEGER*8       info, lda, n
REAL*8          anorm, rcond
INTEGER*8       ipiv(n), iwork(n)
REAL*8          a(lda, n), work(2*n)
CALL SSYCON(uplo, n, a, lda, ipiv, anorm, rcond, work, iwork, info)

CHARACTER*1     uplo
INTEGER*8       info, lda, n
REAL*8          anorm, rcond
INTEGER*8       ipiv(n)
COMPLEX*16      a(lda, n), work(2*n)
CALL CHECON(uplo, n, a, lda, ipiv, anorm, rcond, work, info)

CHARACTER*1     uplo
INTEGER*8       info, lda, n
REAL*8          anorm, rcond
INTEGER*8       ipiv(n)
COMPLEX*16      a(lda, n), work(2*n)
CALL CSYCON(uplo, n, a, lda, ipiv, anorm, rcond, work, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular factor of A is stored.
- **uplo** = 'L' or '1': The lower triangular factor of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

a The block diagonal matrix D and the multipliers used to obtain the factor U or L as computed by _SYTRF or _HETRF.

lda — The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

ipiv — Details of the interchanges and the block structure of D as determined by _SYTRF or _HETRF.

anorm — $\|A\|_1$ (= $\|A\|_1$) of the original symmetric or Hermitian matrix A. **anorm** ≥ 0.

Working Storage

work, iwork — Arrays used for work space.

Output

rcond — On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as

rcond = $(\|A\|_1 \|A^{-1}\|_1)^{-1}$. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info — Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
lda < max(1,**n**), and
anorm < 0.0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SSYTRF/.../ZHETRF/ZSYTRF – Factor Symmetric or Hermitian Matrix

Purpose

These subprograms compute the factorization of a real or complex symmetric or complex Hermitian matrix A using the Bunch-Kaufman diagonal pivoting method. If A is known to be positive definite, other subprograms in this chapter, specifically designed for positive definite matrices, are more efficient than these subprograms.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

The structure of A is indicated by the name of the subprogram used:

SSYTRF	or	DSYTRF	A is a real symmetric matrix.
CSYTRF	or	ZSYTRF	A is a complex symmetric matrix.
CHETRF	or	ZHETRF	A is a complex Hermitian matrix.

If A is real or complex symmetric, the factorization has the form $A = UDU^T$ or $A = LDL^T$ where U is a product of permutation and unit upper triangular matrices, L is a product of permutation and unit lower triangular matrices, and D is symmetric and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

If A is complex Hermitian, the factorization has the form $A = UDU^*$ or $A = LDL^*$ where U and L are as above, and D is Hermitian and block diagonal with 1-by-1 and 2-by-2 diagonal blocks.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A. You may supply either the upper or the lower triangle of A, in a two-dimensional array large enough to hold the entire matrix. The other triangle of the array is not referenced.

Usage

LAPACK:

```
CHARACTER*1     uplo
INTEGER*4       info, lda, lwork, n
INTEGER*4       ipiv(n)
REAL*4          a(lda, n), work(lwork)
CALL SSYTRF(uplo, n, a, lda, ipiv, work, lwork, info)
```

```
CHARACTER*1          uplo
INTEGER*4            info, lda, lwork, n
INTEGER*4            ipiv(n)
REAL*8               a(lda, n), work(lwork)
CALL DSYTRF(uplo, n, a, lda, ipiv, work, lwork, info)

CHARACTER*1          uplo
INTEGER*4            info, lda, lwork, n
INTEGER*4            ipiv(n)
COMPLEX*8            a(lda, n), work(lwork)
CALL CHETRF(uplo, n, a, lda, ipiv, work, lwork, info)

CHARACTER*1          uplo
INTEGER*4            info, lda, lwork, n
INTEGER*4            ipiv(n)
COMPLEX*8            a(lda, n), work(lwork)
CALL CSYTRF(uplo, n, a, lda, ipiv, work, lwork, info)

CHARACTER*1          uplo
INTEGER*4            info, lda, lwork, n
INTEGER*4            ipiv(n)
COMPLEX*16           a(lda, n), work(lwork)
CALL ZHETRF(uplo, n, a, lda, ipiv, work, lwork, info)

CHARACTER*1          uplo
INTEGER*4            info, lda, lwork, n
INTEGER*4            ipiv(n)
COMPLEX*16           a(lda, n), work(lwork)
CALL ZSYTRF(uplo, n, a, lda, ipiv, work, lwork, info)
```

LAPACK8:

```
CHARACTER*1          uplo
INTEGER*8            info, lda, lwork, n
INTEGER*8            ipiv(n)
REAL*8               a(lda, n), work(lwork)
CALL SSYTRF(uplo, n, a, lda, ipiv, work, lwork, info)

CHARACTER*1          uplo
INTEGER*8            info, lda, lwork, n
INTEGER*8            ipiv(n)
COMPLEX*16           a(lda, n), work(lwork)
CALL CHETRF(uplo, n, a, lda, ipiv, work, lwork, info)

CHARACTER*1          uplo
INTEGER*8            info, lda, lwork, n
INTEGER*8            ipiv(n)
COMPLEX*16           a(lda, n), work(lwork)
CALL CSYTRF(uplo, n, a, lda, ipiv, work, lwork, info)
```

Input

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or 'l': The lower triangular part of A is stored.

n The order of the matrix A. **n** ≥ 0.

a The symmetric or Hermitian matrix A, as follows:

If **uplo** = 'U' or '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' or '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 The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

lwork The length of array **work**. **lwork** ≥ max(1,**n**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the block diagonal matrix D and the multipliers used to obtain the factor U or L overwrites the input.

ipiv On successful exit, details of the interchanges and the block structure of D:

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' or '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' or '1' 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 Status response:

info = 0:	Successful exit.
info < 0:	If **info** = –k, the k-th argument had an invalid value.
info > 0:	If **info** = k, $D(k,k)$ is zero. The factorization has been completed, but the block diagonal matrix D is singular, and division by zero will occur if it is used to solve a system of equations.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or '1' or 'U' or 'u',
n < 0,
lda < max(1,**n**), and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SSYTRI/.../ZHETRI/ZSYTRI – Invert Symmetric or Hermitian Matrix

Purpose

These subprograms compute the inverse of a real or complex symmetric or complex Hermitian matrix A using the Bunch-Kaufman factorization computed by _SYTRF or _HETRF.

The structure of A is indicated by the name of the subprogram used:

SSYTRI	or	DSYTRI	A is a real symmetric matrix.
CSYTRI	or	ZSYTRI	A is a complex symmetric matrix.
CHETRI	or	ZHETRI	A is a complex Hermitian matrix.

Matrix Storage

Because either triangle of A^{-1} may be obtained from that triangle of the Bunch-Kaufman factorization of A or from the other triangle of A^{-1}, you need only provide one triangle of the factorization, and only the corresponding triangle of A^{-1} is computed. You may supply either the upper or the lower triangle of the factorization of A, in a two-dimensional array large enough to hold the entire matrix. The other triangle of the array is not referenced.

Usage

LAPACK:

```
CHARACTER*1          uplo
INTEGER*4            info, lda, n
INTEGER*4            ipiv(n)
REAL*4               a(lda, n), work(n)
CALL SSYTRI(uplo, n, a, lda, ipiv, work, info)

CHARACTER*1          uplo
INTEGER*4            info, lda, n
INTEGER*4            ipiv(n)
REAL*8               a(lda, n), work(n)
CALL DSYTRI(uplo, n, a, lda, ipiv, work, info)

CHARACTER*1          uplo
INTEGER*4            info, lda, n
INTEGER*4            ipiv(n)
COMPLEX*8            a(lda, n), work(n)
CALL CHETRI(uplo, n, a, lda, ipiv, work, info)
```

```
CHARACTER*1        uplo
INTEGER*4          info, lda, n
INTEGER*4          ipiv(n)
COMPLEX*8          a(lda, n), work(n)
CALL CSYTRI(uplo, n, a, lda, ipiv, work, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, n
INTEGER*4          ipiv(n)
COMPLEX*16         a(lda, n), work(n)
CALL ZHETRI(uplo, n, a, lda, ipiv, work, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, n
INTEGER*4          ipiv(n)
COMPLEX*16         a(lda, n), work(n)
CALL ZSYTRI(uplo, n, a, lda, ipiv, work, info)
```

LAPACK8:

```
CHARACTER*1        uplo
INTEGER*8          info, lda, n
INTEGER*8          ipiv(n)
REAL*8             a(lda, n), work(n)
CALL SSYTRI(uplo, n, a, lda, ipiv, work, info)

CHARACTER*1        uplo
INTEGER*8          info, lda, n
INTEGER*8          ipiv(n)
COMPLEX*16         a(lda, n), work(n)
CALL CHETRI(uplo, n, a, lda, ipiv, work, info)

CHARACTER*1        uplo
INTEGER*8          info, lda, n
INTEGER*8          ipiv(n)
COMPLEX*16         a(lda, n), work(n)
CALL CSYTRI(uplo, n, a, lda, ipiv, work, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular factor of A is stored.
- **uplo** = 'L' or 'l': The lower triangular factor of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

a The block diagonal matrix D and the multipliers used to obtain the factor U or L as computed by _SYTRF or _HETRF.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

ipiv Details of the interchanges and the block structure of D as determined by _SYTRF or _HETRF.

Working Storage

work An array used for work space.

Output

a On successful exit, the upper or lower triangle of the symmetric or Hermitian inverse of A overwrites the input, as follows:

If **uplo** = 'U' or 'u', the upper triangular part of A^{-1}overwrites the leading **n**-by-**n** upper triangular part of **a**, and the strictly lower triangular part of **a** is not referenced.

If **uplo** = 'L' or 'u', the lower triangular part of A^{-1}overwrites the leading **n**-by-**n** lower triangular part of **a**, and the strictly upper triangular part of **a** is not referenced.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, $D(k,k)$ is zero; the matrix is singular and its inverse could not be computed.

Notes

It is almost never necessary to compute the inverse of a matrix. While papers and reference books extensively use the notation "$A^{-1}b$" to mean "the solution x of the system of linear equations $Ax = b$," it is almost always more efficient and more accurate to compute the solution directly than to invert the coefficient matrix and multiply the inverse times the right hand side vector. This is true even if there are many systems of equations, all using the same coefficient matrix; the matrix may be factored once and the systems may be solved from the factors usually just as efficiently—and more accurately—than by matrix multiplication by the inverse.

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0, and
lda < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

SSYTRS/.../ZHETRS/ZSYTRS – Solve Symmetric or Hermitian System

Purpose

These subprograms solve a system of linear equations $AX = B$ with a real or complex symmetric or complex Hermitian matrix A using the Bunch-Kaufman factorization computed by _SYTRF or _HETRF.

The structure of A is indicated by the name of the subprogram used:

SSYTRS	or	DSYTRS	A is a real symmetric matrix.
CSYTRS	or	ZSYTRS	A is a complex Hermitian matrix.
CHETRS	or	ZHETRS	A is a complex Hermitian matrix.

Usage

LAPACK:

```
CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
INTEGER*4          ipiv(n)
REAL*4             a(lda, n), b(ldb, nrhs)
CALL SSYTRS(uplo, n, nrhs, a, lda, ipiv, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
INTEGER*4          ipiv(n)
REAL*8             a(lda, n), b(ldb, nrhs)
CALL DSYTRS(uplo, n, nrhs, a, lda, ipiv, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*8          a(lda, n), b(ldb, nrhs)
CALL CHETRS(uplo, n, nrhs, a, lda, ipiv, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*8          a(lda, n), b(ldb, nrhs)
CALL CSYTRS(uplo, n, nrhs, a, lda, ipiv, b, ldb, info)

CHARACTER*1        uplo
INTEGER*4          info, lda, ldb, n, nrhs
INTEGER*4          ipiv(n)
COMPLEX*16         a(lda, n), b(ldb, nrhs)
CALL ZHETRS(uplo, n, nrhs, a, lda, ipiv, b, ldb, info)
```

```
CHARACTER*1     uplo
INTEGER*4       info, lda, ldb, n, nrhs
INTEGER*4       ipiv(n)
COMPLEX*16      a(lda, n), b(ldb, nrhs)
CALL ZSYTRS(uplo, n, nrhs, a, lda, ipiv, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1     uplo
INTEGER*8       info, lda, ldb, n, nrhs
INTEGER*8       ipiv(n)
REAL*8          a(lda, n), b(ldb, nrhs)
CALL SSYTRS(uplo, n, nrhs, a, lda, ipiv, b, ldb, info)
```

```
CHARACTER*1     uplo
INTEGER*8       info, lda, ldb, n, nrhs
INTEGER*8       ipiv(n)
COMPLEX*16      a(lda, n), b(ldb, nrhs)
CALL CHETRS(uplo, n, nrhs, a, lda, ipiv, b, ldb, info)
```

```
CHARACTER*1     uplo
INTEGER*8       info, lda, ldb, n, nrhs
INTEGER*8       ipiv(n)
COMPLEX*16      a(lda, n), b(ldb, nrhs)
CALL CSYTRS(uplo, n, nrhs, a, lda, ipiv, b, ldb, info)
```

Input

uplo Specifies whether the upper or lower triangular factor of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular factor of A is stored.
- **uplo** = 'L' or 'l': The lower triangular factor of A is stored.

n The order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

a The block diagonal matrix D and the multipliers used to obtain the factor U or L as computed by _SYTRF or _HETRF.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

ipiv Details of the interchanges and the block structure of D as determined by _SYTRF or _HETRF.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb — The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

Output

b — On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info — Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
nrhs < 0,
lda < max(1,**n**), and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

STBCON/.../ZTBCON – Condition Number of Triangular Band Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a triangular band matrix A, in either the 1-norm or the ∞-norm.

$||A||$ is computed, an estimate is obtained for $||A^{-1}||$, and the reciprocal of the condition number is computed as **rcond** = $(||A||\ ||A^{-1}||)^{-1}$.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, and since A is triangular, you need only provide the band within the triangle of A. Compared to storing the entire matrix, this can save memory in two ways: only the elements within the band are stored, and of them, only the relevant triangle.

Upper triangular matrix. Consider the following upper triangular matrix A of order n = 7and bandwidth kd = 2:

11	12	13	0	0	0	0
0	22	23	24	0	0	0
0	0	33	34	35	0	0
0	0	0	44	45	46	0
0	0	0	0	55	56	57
0	0	0	0	0	66	67
0	0	0	0	0	0	77

A is stored in an array **ab** with at least kd+1 = 3 rows and 7 columns as follows:

*	*	13	24	35	46	57
*	12	23	34	45	56	67
11	22	33	44	55	66	77

The asterisks represent elements in the kd-by-kd triangle at the upper left corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the upper triangle of A, it is stored in **ab**(kd+1+i–j,j). Therefore, the columns of the upper triangle of A are stored in the columns of **ab**, and the diagonals of the upper triangle of A are stored in the rows of **ab**.

Lower triangular matrix. Consider the following lower triangular matrix A of order n = 7and bandwidth kd = 2:

11	0	0	0	0	0	0
21	22	0	0	0	0	0
31	32	33	0	0	0	0
0	42	43	44	0	0	0
0	0	53	54	55	0	0
0	0	0	64	65	66	0
0	0	0	0	75	76	77

The lower triangle of A is stored in the array **ab** as follows:

11	22	33	44	55	66	77
21	32	43	54	65	76	*
31	42	53	64	75	*	*

The asterisks represent elements in the kd-by-kd triangle at the lower right corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the lower triangle of A, it is stored in **ab**$(1+i-j,j)$. Therefore, the columns of the lower triangle of A are stored in the columns of **ab**, and the diagonals of the lower triangle of A are stored in the rows of **ab**.

Usage

LAPACK:

```
CHARACTER*1          diag, norm, uplo
INTEGER*4            info, kd, ldab, n
REAL*4               rcond
INTEGER*4            iwork(n)
REAL*4               ab(ldab, n), work(3*n)
CALL STBCON(norm, uplo, diag, n, kd, ab, ldab, rcond, work, iwork, info)

CHARACTER*1          diag, norm, uplo
INTEGER*4            info, kd, ldab, n
REAL*8               rcond
INTEGER*4            iwork(n)
REAL*8               ab(ldab, n), work(3*n)
CALL DTBCON(norm, uplo, diag, n, kd, ab, ldab, rcond, work, iwork,
  info)

CHARACTER*1          diag, norm, uplo
INTEGER*4            info, kd, ldab, n
REAL*4               rcond, rwork(n)
COMPLEX*8            ab(ldab, n), work(2*n)
CALL CTBCON(norm, uplo, diag, n, kd, ab, ldab, rcond, work, rwork,
  info)
```

```
CHARACTER*1     diag, norm, uplo
INTEGER*4       info, kd, ldab, n
REAL*8          rcond, rwork(n)
COMPLEX*16      ab(ldab, n), work(2*n)
CALL ZTBCON(norm, uplo, diag, n, kd, ab, ldab, rcond, work, rwork,
   info)
```

LAPACK8:

```
CHARACTER*1     diag, norm, uplo
INTEGER*8       info, kd, ldab, n
REAL*8          rcond
INTEGER*8       iwork(n)
REAL*8          ab(ldab, n), work(3*n)
CALL STBCON(norm, uplo, diag, n, kd, ab, ldab, rcond, work, iwork, info)

CHARACTER*1     diag, norm, uplo
INTEGER*8       info, kd, ldab, n
REAL*8          rcond, rwork(n)
COMPLEX*16      ab(ldab, n), work(2*n)
CALL CTBCON(norm, uplo, diag, n, kd, ab, ldab, rcond, work, rwork,
   info)
```

Input

norm Specifies whether to use the 1-norm or the ∞-norm to estimate the condition number, as follows:

norm = '1', 'O', or 'o':	Use $\|\|\ \|\|_1$.
norm = 'I' or 'i':	Use $\|\|\ \|\|_\infty$.

uplo Specifies whether the matrix A is an upper or lower triangular band matrix, as follows:

uplo = 'U' or 'u':	A is an upper triangular band matrix.
uplo = 'L' or 'l':	A is a lower triangular band matrix.

diag Specifies whether the matrix A is unit triangular, that is, $a_{ii} = 1$, or not, as follows:

diag = 'N' or 'n':	The diagonal of A is stored in the array.
diag = 'U' or 'u':	The diagonal of A consists of unstored ones.

n The order of the matrix A. **n** ≥ 0.

kd The number of super-diagonals of the matrix A if **uplo** = 'U' or 'u', or the number of sub-diagonals if **uplo** = 'L' or 'l'. **kd** ≥ 0.

ab — The upper or lower triangular band matrix A, stored in the first **kd**+1 rows of the array. The j-th column of A is stored in the j-th column of array **ab** as follows:

If **uplo** = 'U' or 'u', **ab**(**kd**+1+i–j,j) = $A(i,j)$ for max(1,j–**kd**) ≤ i ≤ j;

If **uplo** = 'L' or 'l', **ab**(1+i–j,j) = $A(i,j)$ for j ≤ i ≤ min(**n**,j+**kd**).

If **diag** = 'U' or 'u', the diagonal elements of A are not referenced and are assumed to be 1.

ldab — The leading dimension of array **ab** in the calling program unit. **ldab** ≥ **kd**+1.

Working Storage

work, iwork, rwork — Arrays used for work space.

Output

rcond — On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as

rcond = $(\|A\| \|A^{-1}\|)^{-1}$, using the norm specified by **norm**. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info — Status response:

info = 0:	Successful exit.
info < 0:	If **info** = –k, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

norm ≠ '1' or 'O' or 'o' or 'I' or 'i',
uplo ≠ 'L' or 'l' or 'U' or 'u',
diag ≠ 'N' or 'n' or 'U' or 'u',
n < 0,
kd < 0, and
ldab < **kd**+1.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **norm** argument as 'Infinity-Norm' for 'I' or '1-norm' for '1'.

NAME

STBTRS/DTBTRS/.../ZTBTRS – Solve Triangular Band Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, $A^TX = B$, or $A^*X = B$ with an upper or lower triangular band matrix A, where A^T is the transpose of A, and A^* is the conjugate transpose.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, and since A is triangular, you need only provide the band within the triangle of A. Compared to storing the entire matrix, this can save memory in two ways: only the elements within the band are stored, and of them, only the relevant triangle.

Upper triangular matrix. Consider the following upper triangular matrix A of order $n = 7$and bandwidth $kd = 2$:

11	12	13	0	0	0	0
0	22	23	24	0	0	0
0	0	33	34	35	0	0
0	0	0	44	45	46	0
0	0	0	0	55	56	57
0	0	0	0	0	66	67
0	0	0	0	0	0	77

A is stored in an array **ab** with at least $kd+1 = 3$ rows and 7 columns as follows:

*	*	13	24	35	46	57
*	12	23	34	45	56	67
11	22	33	44	55	66	77

The asterisks represent elements in the kd-by-kd triangle at the upper left corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the upper triangle of A, it is stored in **ab**($kd+1+i-j,j$). Therefore, the columns of the upper triangle of A are stored in the columns of **ab**, and the diagonals of the upper triangle of A are stored in the rows of **ab**.

Lower triangular matrix. Consider the following lower triangular matrix A of order $n = 7$and bandwidth $kd = 2$:

11	0	0	0	0	0	0
21	22	0	0	0	0	0
31	32	33	0	0	0	0
0	42	43	44	0	0	0
0	0	53	54	55	0	0
0	0	0	64	65	66	0
0	0	0	0	75	76	77

The lower triangle of A is stored in the array **ab** as follows:

11	22	33	44	55	66	77
21	32	43	54	65	76	*
31	42	53	64	75	*	*

The asterisks represent elements in the *kd*-by-*kd* triangle at the lower right corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the lower triangle of A, it is stored in **ab**$(1+i-j,j)$. Therefore, the columns of the lower triangle of A are stored in the columns of **ab**, and the diagonals of the lower triangle of A are stored in the rows of **ab**.

Usage

LAPACK:

```
CHARACTER*1        diag, trans, uplo
INTEGER*4          info, kd, ldab, ldb, n, nrhs
REAL*4             ab(ldab, n), b(ldb, nrhs)
CALL STBTRS(uplo, trans, diag, n, kd, nrhs, ab, ldab, b, ldb, info)

CHARACTER*1        diag, trans, uplo
INTEGER*4          info, kd, ldab, ldb, n, nrhs
REAL*8             ab(ldab, n), b(ldb, nrhs)
CALL DTBTRS(uplo, trans, diag, n, kd, nrhs, ab, ldab, b, ldb, info)

CHARACTER*1        diag, trans, uplo
INTEGER*4          info, kd, ldab, ldb, n, nrhs
COMPLEX*8          ab(ldab, n), b(ldb, nrhs)
CALL CTBTRS(uplo, trans, diag, n, kd, nrhs, ab, ldab, b, ldb, info)

CHARACTER*1        diag, trans, uplo
INTEGER*4          info, kd, ldab, ldb, n, nrhs
COMPLEX*16         ab(ldab, n), b(ldb, nrhs)
CALL ZTBTRS(uplo, trans, diag, n, kd, nrhs, ab, ldab, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1        diag, trans, uplo
INTEGER*8          info, kd, ldab, ldb, n, nrhs
REAL*8             ab(ldab, n), b(ldb, nrhs)
CALL STBTRS(uplo, trans, diag, n, kd, nrhs, ab, ldab, b, ldb, info)

CHARACTER*1        diag, trans, uplo
INTEGER*8          info, kd, ldab, ldb, n, nrhs
COMPLEX*16         ab(ldab, n), b(ldb, nrhs)
CALL CTBTRS(uplo, trans, diag, n, kd, nrhs, ab, ldab, b, ldb, info)
```

Input

uplo Specifies whether the matrix A is an upper or lower triangular band matrix, as follows:

- **uplo** = 'U' or 'u': A is an upper triangular band matrix.
- **uplo** = 'L' or '1': A is a lower triangular band matrix.

trans Specifies the form of the system of equations, as follows:

- **trans** = 'N' or 'n': Solve $AX = B$.
- **trans** = 'T' or 't': Solve $A^TX = B$.
- **trans** = 'C' or 'c': Solve $A^*X = B$.

diag Specifies whether the matrix A is unit triangular, that is, $a_{ii} = 1$, or not, as follows:

- **diag** = 'N' or 'n': The diagonal of A is stored in the array.
- **diag** = 'U' or 'u': The diagonal of A consists of unstored ones.

n The order of the matrix A. **n** ≥ 0.

kd The number of super-diagonals of the matrix A if **uplo** = 'U' or 'u', or the number of sub-diagonals if **uplo** = 'L' or '1'. **kd** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ab The upper or lower triangular band matrix A, stored in the first **kd**+1 rows of the array. The j-th column of A is stored in the j-th column of array **ab** as follows:

If **uplo** = 'U' or 'u', **ab**(**kd**+1+i–j,j) = $A(i,j)$ for max(1,j–**kd**) $\leq i \leq j$;

If **uplo** = 'L' or '1', **ab**(1+i–j,j) = $A(i,j)$ for $j \leq i \leq$ min(**n**,j+**kd**).

If **diag** = 'U' or 'u', the diagonal elements of A are not referenced and are assumed to be 1.

ldab — The leading dimension of array **ab** in the calling program unit. **ldab** ≥ **kd**+1.

b — The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb — The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

Output

b — On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info — Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, $A(k,k)$ is zero; the matrix is singular and the solution could not be computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
trans ≠ 'N' or 'n' or 'T' or 't' or 'C' or 'c',
diag ≠ 'N' or 'n' or 'U' or 'u',
n < 0,
kd < 0,
nrhs < 0,
ldab < **kd**+1,
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME STPCON/... – Condition Number of Triangular Packed Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a triangular matrix A that is stored in an array in packed form. The condition number can be estimated in either the 1-norm or the ∞-norm.

$||A||$ is computed, an estimate is obtained for $||A^{-1}||$, and the reciprocal of the condition number is computed as **rcond** = $(||A||\ ||A^{-1}||)^{-1}$.

Matrix Storage

You supply the upper or lower triangle of A, stored column-by-column in packed form in a 1-dimensional array. This saves memory compared to storing the entire matrix.

The following examples illustrate the storage of triangular packed matrices.

Upper triangular matrix. If A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ 0 & 22 & 23 & 24 \\ 0 & 0 & 33 & 34 \\ 0 & 0 & 0 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular matrix. If A is

$$\begin{matrix} 11 & 0 & 0 & 0 \\ 21 & 22 & 0 & 0 \\ 31 & 32 & 33 & 0 \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**(i+(j–1)×(2n–j)/2).

Usage

LAPACK:

```
CHARACTER*1     diag, norm, uplo
INTEGER*4       info, n
REAL*4          rcond
INTEGER*4       iwork(n)
REAL*4          ap((n*(n+1))/2), work(3*n)
CALL STPCON(norm, uplo, diag, n, ap, rcond, work, iwork, info)

CHARACTER*1     diag, norm, uplo
INTEGER*4       info, n
REAL*8          rcond
INTEGER*4       iwork(n)
REAL*8          ap((n*(n+1))/2), work(3*n)
CALL DTPCON(norm, uplo, diag, n, ap, rcond, work, iwork, info)

CHARACTER*1     diag, norm, uplo
INTEGER*4       info, n
REAL*4          rcond, rwork(n)
COMPLEX*8       ap((n*(n+1))/2), work(2*n)
CALL CTPCON(norm, uplo, diag, n, ap, rcond, work, rwork, info)

CHARACTER*1     diag, norm, uplo
INTEGER*4       info, n
REAL*8          rcond, rwork(n)
COMPLEX*16      ap((n*(n+1))/2), work(2*n)
CALL ZTPCON(norm, uplo, diag, n, ap, rcond, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1     diag, norm, uplo
INTEGER*8       info, n
REAL*8          rcond
INTEGER*8       iwork(n)
REAL*8          ap((n*(n+1))/2), work(3*n)
CALL STPCON(norm, uplo, diag, n, ap, rcond, work, iwork, info)

CHARACTER*1     diag, norm, uplo
INTEGER*8       info, n
REAL*8          rcond, rwork(n)
COMPLEX*16      ap((n*(n+1))/2), work(2*n)
CALL CTPCON(norm, uplo, diag, n, ap, rcond, work, rwork, info)
```

Input

norm Specifies whether to use the 1-norm or the ∞-norm to estimate the condition number, as follows:

norm = '1', 'O', or 'o': Use $\| \ \|_1$.

norm = 'I' or 'i': Use $\| \ \|_\infty$.

uplo Specifies whether the matrix A is an upper or lower triangular matrix, as follows:

uplo = 'U' or 'u': A is an upper triangular matrix.

uplo = 'L' or 'l': A is a lower triangular matrix.

diag Specifies whether the matrix A is unit triangular, that is, $a_{ii} = 1$, or not, as follows:

diag = 'N' or 'n': The diagonal of A is stored in the array.

diag = 'U' or 'u': The diagonal of A consists of unstored ones.

n The order of the matrix A. $\mathbf{n} \geq 0$.

ap The **n**-by-**n** 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' or 'u', $\mathbf{ap}(i + (j-1) \times j/2) = A(i,j)$ for $1 \leq i \leq j$;

If **uplo** = 'L' or 'l', $\mathbf{ap}(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \leq i \leq \mathbf{n}$.

If **diag** = 'U' or 'u', the diagonal elements of A are not referenced and are assumed to be 1.

Working Storage

work, iwork, rwork Arrays used for work space.

Output

rcond On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as

rcond = $(\|A\| \, \|A^{-1}\|)^{-1}$, using the norm specified by **norm**. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

norm ≠ '1' or 'O' or 'o' or 'I' or 'i',
uplo ≠ 'L' or 'l' or 'U' or 'u',
diag ≠ 'N' or 'n' or 'U' or 'u', and
n < 0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **norm** argument as 'Infinity-Norm' for 'I' or '1-norm' for '1'.

NAME

STPTRI/DTPTRI/CTPTRI/ZTPTRI – Invert Triangular Packed Matrix

Purpose

These subprograms compute the inverse of an upper or lower triangular matrix A that is stored in an array in packed form.

Matrix Storage

You supply the upper or lower triangle of A, stored column-by-column in packed form in a 1-dimensional array. This saves memory compared to storing the entire matrix.

The following examples illustrate the storage of triangular packed matrices.

Upper triangular matrix. If A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ 0 & 22 & 23 & 24 \\ 0 & 0 & 33 & 34 \\ 0 & 0 & 0 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular matrix. If A is

$$\begin{matrix} 11 & 0 & 0 & 0 \\ 21 & 22 & 0 & 0 \\ 31 & 32 & 33 & 0 \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**(i+(j–1)×(2n–j)/2).

Usage

LAPACK:

```
CHARACTER*1        diag, uplo
INTEGER*4          info, n
REAL*4             ap((n*(n+1))/2)
CALL STPTRI(uplo, diag, n, ap, info)

CHARACTER*1        diag, uplo
INTEGER*4          info, n
REAL*8             ap((n*(n+1))/2)
CALL DTPTRI(uplo, diag, n, ap, info)

CHARACTER*1        diag, uplo
INTEGER*4          info, n
COMPLEX*8          ap((n*(n+1))/2)
CALL CTPTRI(uplo, diag, n, ap, info)

CHARACTER*1        diag, uplo
INTEGER*4          info, n
COMPLEX*16         ap((n*(n+1))/2)
CALL ZTPTRI(uplo, diag, n, ap, info)
```

LAPACK8:

```
CHARACTER*1        diag, uplo
INTEGER*8          info, n
REAL*8             ap((n*(n+1))/2)
CALL STPTRI(uplo, diag, n, ap, info)

CHARACTER*1        diag, uplo
INTEGER*8          info, n
COMPLEX*16         ap((n*(n+1))/2)
CALL CTPTRI(uplo, diag, n, ap, info)
```

Input

uplo Specifies whether the matrix A is an upper or lower triangular matrix, as follows:

- **uplo** = 'U' or 'u': A is an upper triangular matrix.
- **uplo** = 'L' or 'l': A is a lower triangular matrix.

diag Specifies whether the matrix A is unit triangular, that is, $a_{ii} = 1$, or not, as follows:

- **diag** = 'N' or 'n': The diagonal of A is stored in the array.
- **diag** = 'U' or 'u': The diagonal of A consists of unstored ones.

n The order of the matrix A. **n** ≥ 0.

ap The **n**-by-**n** 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' or 'u', **ap**$(i + (j-1) \times j/2) = A(i,j)$ for $1 \le i \le j$;

If **uplo** = 'L' or 'l', **ap**$(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \le i \le \mathbf{n}$.

If **diag** = 'U' or 'u', the diagonal elements of A are not referenced and are assumed to be 1.

Output

ap On successful exit, A^{-1} overwrites the input.

If **diag** = 'U' or 'u', then A^{-1} also will have an unstored unit diagonal.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, $A(k,k)$ is zero; the matrix is singular and its inverse could not be computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
diag ≠ 'N' or 'n' or 'U' or 'u', and
n < 0.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

STPTRS/DTPTRS/.../ZTPTRS – Solve Triangular Packed Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, $A^TX = B$, or $A^*X = B$ with an upper or lower triangular matrix A that is stored in an array in packed form, where A^T is the transpose of A, and A^* is the conjugate transpose.

Matrix Storage

You supply the upper or lower triangle of A, stored column-by-column in packed form in a 1-dimensional array. This saves memory compared to storing the entire matrix.

The following examples illustrate the storage of triangular packed matrices.

Upper triangular matrix. If A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ 0 & 22 & 23 & 24 \\ 0 & 0 & 33 & 34 \\ 0 & 0 & 0 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular matrix. If A is

$$\begin{matrix} 11 & 0 & 0 & 0 \\ 21 & 22 & 0 & 0 \\ 31 & 32 & 33 & 0 \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**(i+(j–1)×(2n–j)/2).

Usage

LAPACK:

```
CHARACTER*1        diag, trans, uplo
INTEGER*4          info, ldb, n, nrhs
REAL*4             ap((n*(n+1))/2), b(ldb, nrhs)
CALL STPTRS(uplo, trans, diag, n, nrhs, ap, b, ldb, info)

CHARACTER*1        diag, trans, uplo
INTEGER*4          info, ldb, n, nrhs
REAL*8             ap((n*(n+1))/2), b(ldb, nrhs)
CALL DTPTRS(uplo, trans, diag, n, nrhs, ap, b, ldb, info)

CHARACTER*1        diag, trans, uplo
INTEGER*4          info, ldb, n, nrhs
COMPLEX*8          ap((n*(n+1))/2), b(ldb, nrhs)
CALL CTPTRS(uplo, trans, diag, n, nrhs, ap, b, ldb, info)

CHARACTER*1        diag, trans, uplo
INTEGER*4          info, ldb, n, nrhs
COMPLEX*16         ap((n*(n+1))/2), b(ldb, nrhs)
CALL ZTPTRS(uplo, trans, diag, n, nrhs, ap, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1        diag, trans, uplo
INTEGER*8          info, ldb, n, nrhs
REAL*8             ap((n*(n+1))/2), b(ldb, nrhs)
CALL STPTRS(uplo, trans, diag, n, nrhs, ap, b, ldb, info)

CHARACTER*1        diag, trans, uplo
INTEGER*8          info, ldb, n, nrhs
COMPLEX*16         ap((n*(n+1))/2), b(ldb, nrhs)
CALL CTPTRS(uplo, trans, diag, n, nrhs, ap, b, ldb, info)
```

Input

uplo Specifies whether the matrix A is an upper or lower triangular matrix, as follows:

- **uplo** = 'U' or 'u': A is an upper triangular matrix.
- **uplo** = 'L' or 'l': A is a lower triangular matrix.

trans Specifies the form of the system of equations, as follows:

- **trans** = 'N' or 'n': Solve $AX = B$.
- **trans** = 'T' or 't': Solve $A^TX = B$.
- **trans** = 'C' or 'c': Solve $A^*X = B$.

diag Specifies whether the matrix A is unit triangular, that is, $a_{ii} = 1$, or not, as follows:

diag = 'N' or 'n': The diagonal of A is stored in the array.

diag = 'U' or 'u': The diagonal of A consists of unstored ones.

n The order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

ap The **n**-by-**n** 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' or 'u', **ap**$(i + (j-1) \times j/2) = A(i,j)$ for $1 \leq i \leq j$;

If **uplo** = 'L' or 'l', **ap**$(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \leq i \leq \mathbf{n}$.

If **diag** = 'U' or 'u', the diagonal elements of A are not referenced and are assumed to be 1.

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** $\geq \max(1,\mathbf{n})$.

Output

b On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.

info Status response:

info = 0: Successful exit.

info < 0: If **info** = $-k$, the k-th argument had an invalid value.

info > 0: If **info** = k, $A(k,k)$ is zero; the matrix is singular and the solution could not be computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
trans ≠ 'N' or 'n' or 'T' or 't' or 'C' or 'c',
diag ≠ 'N' or 'n' or 'U' or 'u',
n < 0,
nrhs < 0, and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

STRCON/.../ZTRCON – Condition Number of Triangular Matrix

Purpose

These subprograms estimate the reciprocal of the condition number of a triangular matrix A, in either the 1-norm or the ∞-norm.

$||A||$ is computed, an estimate is obtained for $||A^{-1}||$, and the reciprocal of the condition number is computed as **rcond** = $(||A||\ ||A^{-1}||)^{-1}$.

Matrix Storage

For these subprograms, you supply A in a two-dimensional array large enough to hold a square matrix. The other triangle of the array is not referenced. If A has an unstored unit diagonal (see input argument **diag**), then the diagonal elements of the array also will not be referenced.

Usage

LAPACK:

```
CHARACTER*1        diag, norm, uplo
INTEGER*4          info, lda, n
REAL*4             rcond
INTEGER*4          iwork(n)
REAL*4             a(lda, n), work(3*n)
CALL STRCON(norm, uplo, diag, n, a, lda, rcond, work, iwork, info)

CHARACTER*1        diag, norm, uplo
INTEGER*4          info, lda, n
REAL*8             rcond
INTEGER*4          iwork(n)
REAL*8             a(lda, n), work(3*n)
CALL DTRCON(norm, uplo, diag, n, a, lda, rcond, work, iwork, info)

CHARACTER*1        diag, norm, uplo
INTEGER*4          info, lda, n
REAL*4             rcond, rwork(n)
COMPLEX*8          a(lda, n), work(2*n)
CALL CTRCON(norm, uplo, diag, n, a, lda, rcond, work, rwork, info)

CHARACTER*1        diag, norm, uplo
INTEGER*4          info, lda, n
REAL*8             rcond, rwork(n)
COMPLEX*16         a(lda, n), work(2*n)
CALL ZTRCON(norm, uplo, diag, n, a, lda, rcond, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1     diag, norm, uplo
INTEGER*8       info, lda, n
REAL*8          rcond
INTEGER*8       iwork(n)
REAL*8          a(lda, n), work(3*n)
CALL STRCON(norm, uplo, diag, n, a, lda, rcond, work, iwork, info)

CHARACTER*1     diag, norm, uplo
INTEGER*8       info, lda, n
REAL*8          rcond, rwork(n)
COMPLEX*16      a(lda, n), work(2*n)
CALL CTRCON(norm, uplo, diag, n, a, lda, rcond, work, rwork, info)
```

Input

norm Specifies whether to use the 1-norm or the ∞-norm to estimate the condition number, as follows:

norm = 'I', 'O', or 'o': Use $\| \ \|_1$.

norm = 'I' or 'i': Use $\| \ \|_\infty$.

uplo Specifies whether the matrix A is an upper or lower triangular matrix, as follows:

uplo = 'U' or 'u': A is an upper triangular matrix.

uplo = 'L' or 'l': A is a lower triangular matrix.

diag Specifies whether the matrix A is unit triangular, that is, $a_{ii} = 1$, or not, as follows:

diag = 'N' or 'n': The diagonal of A is stored in the array.

diag = 'U' or 'u': The diagonal of A consists of unstored ones.

n The order of the matrix A. **n** ≥ 0.

a The **n**-by-**n** triangular matrix A.

If **uplo** = 'U' or 'u', the leading **n**-by-**n** upper triangular part of **a** contains the upper triangular matrix A, and the strictly lower triangular part of **a** is not referenced.

If **uplo** = 'L' or 'l', the leading **n**-by-**n** lower triangular part of **a** contains the lower triangular matrix A, and the strictly upper triangular part of **a** is not referenced.

If **diag** = 'U' or 'u', the diagonal elements of A are not referenced and are assumed to be 1.

lda — The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

Working Storage

work, iwork, rwork — Arrays used for work space.

Output

rcond — On successful exit, the estimate of the reciprocal condition number of the matrix A, computed as

rcond = $(\|A\| \, \|A^{-1}\|)^{-1}$, using the norm specified by **norm**. If **rcond** is small enough so that the logical expression

1.0 + **rcond** .EQ. 1.0

is true, then A can be regarded as singular to working precision. If **rcond** is zero, then the companion subprograms for solving and computing the inverse may divide by zero.

info — Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

norm ≠ 'I' or 'O' or 'o' or '1' or 'i',
uplo ≠ 'L' or 'l' or 'U' or 'u',
diag ≠ 'N' or 'n' or 'U' or 'u',
n < 0, and
lda < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **norm** argument as 'Infinity-Norm' for 'I' or '1-norm' for '1'.

NAME

STRTRI/DTRTRI/CTRTRI/ZTRTRI – Invert Triangular Matrix

Purpose

These subprograms compute the inverse of an upper or lower triangular matrix A.

Matrix Storage

For these subprograms, you supply A in a two-dimensional array large enough to hold a square matrix. The other triangle of the array is not referenced. If A has an unstored unit diagonal (see input argument **diag**), then A^{-1} also will have an unstored unit diagonal and the diagonal elements of the array also will not be referenced.

Usage

LAPACK:

```
CHARACTER*1        diag, uplo
INTEGER*4          info, lda, n
REAL*4             a(lda, n)
CALL STRTRI(uplo, diag, n, a, lda, info)

CHARACTER*1        diag, uplo
INTEGER*4          info, lda, n
REAL*8             a(lda, n)
CALL DTRTRI(uplo, diag, n, a, lda, info)

CHARACTER*1        diag, uplo
INTEGER*4          info, lda, n
COMPLEX*8          a(lda, n)
CALL CTRTRI(uplo, diag, n, a, lda, info)

CHARACTER*1        diag, uplo
INTEGER*4          info, lda, n
COMPLEX*16         a(lda, n)
CALL ZTRTRI(uplo, diag, n, a, lda, info)
```

LAPACK8:

```
CHARACTER*1        diag, uplo
INTEGER*8          info, lda, n
REAL*8             a(lda, n)
CALL STRTRI(uplo, diag, n, a, lda, info)

CHARACTER*1        diag, uplo
INTEGER*8          info, lda, n
COMPLEX*16         a(lda, n)
CALL CTRTRI(uplo, diag, n, a, lda, info)
```

Input

uplo Specifies whether the matrix A is an upper or lower triangular matrix, as follows:

- **uplo** = 'U' or 'u': A is an upper triangular matrix.
- **uplo** = 'L' or 'l': A is a lower triangular matrix.

diag Specifies whether the matrix A is unit triangular, that is, $a_{ii} = 1$, or not, as follows:

- **diag** = 'N' or 'n': The diagonal of A is stored in the array.
- **diag** = 'U' or 'u': The diagonal of A consists of unstored ones.

n The order of the matrix A. **n** ≥ 0.

a The **n**-by-**n** triangular matrix A.

If **uplo** = 'U' or 'u', the leading **n**-by-**n** upper triangular part of **a** contains the upper triangular matrix A, and the strictly lower triangular part of **a** is not referenced.

If **uplo** = 'L' or 'l', the leading **n**-by-**n** lower triangular part of **a** contains the lower triangular matrix A, and the strictly upper triangular part of **a** is not referenced.

If **diag** = 'U' or 'u', the diagonal elements of A are not referenced and are assumed to be 1.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

Output

a On successful exit, A^{-1} overwrites the triangle of **a** that contained the input matrix. The other triangle of **a** is not referenced.

If **diag** = 'U' or 'u', then A^{-1} also will have an unstored unit diagonal and the diagonal elements of the array also will not be referenced.

info Status response:

- **info** = 0: Successful exit.
- **info** < 0: If **info** = $-k$, the k-th argument had an invalid value.

info > 0:	If **info** = k, $A(k,k)$ is zero; the matrix is singular and its inverse could not be computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
diag ≠ 'N' or 'n' or 'U' or 'u',
n < 0, and
lda < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME

STRTRS/DTRTRS/.../ZTRTRS – Solve Triangular Linear System

Purpose

These subprograms solve a system of linear equations $AX = B$, $A^TX = B$, or $A^*X = B$ with an upper or lower triangular matrix A, where A^T is the transpose of A, and A^* is the conjugate transpose.

Matrix Storage

For these subprograms, you supply A in a two-dimensional array large enough to hold a square matrix. The other triangle of the array is not referenced. If A has an unstored unit diagonal (see input argument **diag**), then the diagonal elements of the array also will not be referenced.

Usage

LAPACK:

```
CHARACTER*1      diag, trans, uplo
INTEGER*4        info, lda, ldb, n, nrhs
REAL*4           a(lda, n), b(ldb, nrhs)
CALL STRTRS(uplo, trans, diag, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1      diag, trans, uplo
INTEGER*4        info, lda, ldb, n, nrhs
REAL*8           a(lda, n), b(ldb, nrhs)
CALL DTRTRS(uplo, trans, diag, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1      diag, trans, uplo
INTEGER*4        info, lda, ldb, n, nrhs
COMPLEX*8        a(lda, n), b(ldb, nrhs)
CALL CTRTRS(uplo, trans, diag, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1      diag, trans, uplo
INTEGER*4        info, lda, ldb, n, nrhs
COMPLEX*16       a(lda, n), b(ldb, nrhs)
CALL ZTRTRS(uplo, trans, diag, n, nrhs, a, lda, b, ldb, info)
```

LAPACK8:

```
CHARACTER*1      diag, trans, uplo
INTEGER*8        info, lda, ldb, n, nrhs
REAL*8           a(lda, n), b(ldb, nrhs)
CALL STRTRS(uplo, trans, diag, n, nrhs, a, lda, b, ldb, info)

CHARACTER*1      diag, trans, uplo
INTEGER*8        info, lda, ldb, n, nrhs
COMPLEX*16       a(lda, n), b(ldb, nrhs)
CALL CTRTRS(uplo, trans, diag, n, nrhs, a, lda, b, ldb, info)
```

Input

uplo Specifies whether the matrix A is an upper or lower triangular matrix, as follows:

uplo = 'U' or 'u': A is an upper triangular matrix.

uplo = 'L' or 'l': A is a lower triangular matrix.

trans Specifies the form of the system of equations, as follows:

trans = 'N' or 'n': Solve $AX = B$.

trans = 'T' or 't': Solve $A^TX = B$.

trans = 'C' or 'c': Solve $A^*X = B$.

diag Specifies whether the matrix A is unit triangular, that is, $a_{ii} = 1$, or not, as follows:

diag = 'N' or 'n': The diagonal of A is stored in the array.

diag = 'U' or 'u': The diagonal of A consists of unstored ones.

n The order of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides, that is, the number of columns of the matrix B. **nrhs** ≥ 0.

a The **n**-by-**n** triangular matrix A.

If **uplo** = 'U' or 'u', the leading **n**-by-**n** upper triangular part of **a** contains the upper triangular matrix A, and the strictly lower triangular part of **a** is not referenced.

If **uplo** = 'L' or 'l', the leading **n**-by-**n** lower triangular part of **a** contains the lower triangular matrix A, and the strictly upper triangular part of **a** is not referenced.

If **diag** = 'U' or 'u', the diagonal elements of A are not referenced and are assumed to be 1.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

b The **n**-by-**nrhs** matrix of right hand side vectors for the system of linear equations $AX = B$.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

Output

b	On successful exit, the **n**-by-**nrhs** matrix of solution vectors X overwrites the input.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k, $A(k,k)$ is zero; the matrix is singular and the solution could not be computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

uplo ≠ 'L' or 'l' or 'U' or 'u',
trans ≠ 'N' or 'n' or 'T' or 't' or 'C' or 'c',
diag ≠ 'N' or 'n' or 'U' or 'u',
n < 0,
nrhs < 0,
lda < max(1,**n**), and
ldb < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **uplo** argument as 'Lower' for 'L' or 'Upper' for 'U'.

NAME Subprograms not in this Guide –

Although LAPACK includes all computational subprograms for linear equations, as defined in Table 1-5, the following subprograms are not documented in the *HP MLIB LAPACK User's Guide*. Refer to (Anderson *et al.*) for documentation for these subprograms.

Subprograms not in this Guide

Name	Function
SGBEQU	Equilibrate a General Band Matrix
DGBEQU	Equilibrate a General Band Matrix
CGBEQU	Equilibrate a General Band Matrix
ZGBEQU	Equilibrate a General Band Matrix
SGBRFS	Iteratively Refine the Solution of a General Band Linear System
DGBRFS	Iteratively Refine the Solution of a General Band Linear System
CGBRFS	Iteratively Refine the Solution of a General Band Linear System
ZGBRFS	Iteratively Refine the Solution of a General Band Linear System
SGEEQU	Equilibrate a General Full Matrix
DGEEQU	Equilibrate a General Full Matrix
CGEEQU	Equilibrate a General Full Matrix
ZGEEQU	Equilibrate a General Full Matrix
SGERFS	Iteratively Refine the Solution of a General Full Linear System
DGERFS	Iteratively Refine the Solution of a General Full Linear System
CGERFS	Iteratively Refine the Solution of a General Full Linear System
ZGERFS	Iteratively Refine the Solution of a General Full Linear System
SGTRFS	Iteratively Refine the Solution of a General Tridiagonal Linear System
DGTRFS	Iteratively Refine the Solution of a General Tridiagonal Linear System
CGTRFS	Iteratively Refine the Solution of a General Tridiagonal Linear System
ZGTRFS	Iteratively Refine the Solution of a General Tridiagonal Linear System
CHERFS	Iteratively Refine the Solution of a Hermitian Indefinite Linear System
ZHERFS	Iteratively Refine the Solution of a Hermitian Indefinite Linear System
CHPRFS	Iteratively Refine the Solution of a Hermitian Indefinite Packed Linear System
ZHPRFS	Iteratively Refine the Solution of a Hermitian Indefinite Packed Linear System
SPBEQU	Equilibrate a Positive Definite Band Matrix
DPBEQU	Equilibrate a Positive Definite Band Matrix
CPBEQU	Equilibrate a Positive Definite Band Matrix

Name	Function
ZPBEQU	Equilibrate a Positive Definite Band Matrix
SPBRFS	Iteratively Refine the Solution of a Positive Definite Band Linear System
DPBRFS	Iteratively Refine the Solution of a Positive Definite Band Linear System
CPBRFS	Iteratively Refine the Solution of a Positive Definite Band Linear System
ZPBRFS	Iteratively Refine the Solution of a Positive Definite Band Linear System
SPOEQU	Equilibrate a Positive Definite Full Matrix
DPOEQU	Equilibrate a Positive Definite Full Matrix
CPOEQU	Equilibrate a Positive Definite Full Matrix
ZPOEQU	Equilibrate a Positive Definite Full Matrix
SPORFS	Iteratively Refine the Solution of a Positive Definite Full Linear System
DPORFS	Iteratively Refine the Solution of a Positive Definite Full Linear System
CPORFS	Iteratively Refine the Solution of a Positive Definite Full Linear System
ZPORFS	Iteratively Refine the Solution of a Positive Definite Full Linear System
SPPEQU	Equilibrate a Positive Definite Packed Matrix
DPPEQU	Equilibrate a Positive Definite Packed Matrix
CPPEQU	Equilibrate a Positive Definite Packed Matrix
ZPPEQU	Equilibrate a Positive Definite Packed Matrix
SPPRFS	Iteratively Refine the Solution of a Positive Definite Packed Linear System
DPPRFS	Iteratively Refine the Solution of a Positive Definite Packed Linear System
CPPRFS	Iteratively Refine the Solution of a Positive Definite Packed Linear System
ZPPRFS	Iteratively Refine the Solution of a Positive Definite Packed Linear System
SPTRFS	Iteratively Refine the Solution of a Positive Definite Tridiagonal Linear System
DPTRFS	Iteratively Refine the Solution of a Positive Definite Tridiagonal Linear System
CPTRFS	Iteratively Refine the Solution of a Positive Definite Tridiagonal Linear System
ZPTRFS	Iteratively Refine the Solution of a Positive Definite Tridiagonal Linear System
SSPRFS	Iteratively Refine the Solution of a Symmetric Indefinite Packed Linear System

Name	Function
DSPRFS	Iteratively Refine the Solution of a Symmetric Indefinite Packed Linear System
CSPRFS	Iteratively Refine the Solution of a Symmetric Packed Linear System
ZSPRFS	Iteratively Refine the Solution of a Symmetric Packed Linear System
SSYRFS	Iteratively Refine the Solution of a Symmetric Indefinite Linear System
DSYRFS	Iteratively Refine the Solution of a Symmetric Indefinite Linear System
CSYRFS	Iteratively Refine the Solution of a Symmetric Linear System
ZSYRFS	Iteratively Refine the Solution of a Symmetric Linear System
STBRFS	Iteratively Refine the Solution of a Triangular Band Linear System
DTBRFS	Iteratively Refine the Solution of a Triangular Band Linear System
CTBRFS	Iteratively Refine the Solution of a Triangular Band Linear System
ZTBRFS	Iteratively Refine the Solution of a Triangular Band Linear System
STPRFS	Iteratively Refine the Solution of a Triangular Packed Linear System
DTPRFS	Iteratively Refine the Solution of a Triangular Packed Linear System
CTPRFS	Iteratively Refine the Solution of a Triangular Packed Linear System
ZTPRFS	Iteratively Refine the Solution of a Triangular Packed Linear System
STRRFS	Iteratively Refine the Solution of a Triangular Linear System
DTRRFS	Iteratively Refine the Solution of a Triangular Linear System
CTRRFS	Iteratively Refine the Solution of a Triangular Linear System
ZTRRFS	Iteratively Refine the Solution of a Triangular Linear System

Subprograms not in this Guide –

5 Drivers for Linear Least Squares Problems

Overview

This chapter explains how to use LAPACK drivers to solve linear least squares problems for under- and over-determined systems of linear equations. The operations covered are:

- Solve least squares problems using the *QR* factorization
- Solve least squares problems using the singular value decomposition
- Solve least squares problems using the complete orthogonal factorization
- Solve generalized linear regression model (GLM) problems
- Solve general least squares problems with linear equality constraints

The following documents provide supplemental material for this chapter:

- Golub, G.H. and C.F. Van Loan. *Matrix Computations*, 2nd Edition. Baltimore, MD: The Johns Hopkins University Press. 1989.
- Lawson, C.L. and R.J. Hanson. *Solving Least Squares Problems*. Englewood Cliffs, NJ: Prentice-Hall, Inc. 1974.

Chapter Objectives

After reading this chapter you will

- Know about the various types of least squares problems
- Understand the weaknesses of the normal equations solution method
- Know how to use the described subprograms

What You Need to Know to Use These Subprograms

The Linear Least Squares Problem

If A is a given m-by-n matrix and b is a given m-dimensional vector, the problem of finding an n-dimensional vector x satisfying $Ax = b$ is said to be *overdetermined* if $m > n$, that is, if there are more equations than unknowns.

Usually an overdetermined system has no exact solution, so it is common to try to find an approximate solution that minimizes $\|Ax - b\|$ for some suitable norm.If you choose the Euclidean norm, the minimization problem itself is linear and the problem is called *the least squares problem* (because the solution has the least sum of squares of the residual vector $r = Ax - b$). If A has full column rank, that is, if the columns of A are linearly independent, then the least squares solution is unique.

On the other hand, if $m < n$ then the system $Ax = b$ is said to be *underdetermined.*

If the problem is underdetermined or if A does not have full column rank, then there are an infinite number of solutions to the least squares problem, for if x minimizes $\|Ax - b\|^2$ and y is in the null space of A, then $x+y$ is also a minimizer. As the set of all minimizers is convex, there exists a unique minimizer with minimum Euclidean norm, called the *minimum-norm solution.*

The LAPACK drivers described in this chapter provide several options for handling over- or underdetermined linear least squares problems.

The Method of Normal Equations

Probably due to its simple exposition, the relative ease of solving small problems by hand, and the low sophistication of software required to implement it on a computer, the method of normal equations is widely used for solving linear least squares problems $Ax \approx b$ when the matrix A is of size m-by-n with $m > n$ and A has full column rank. Solving the normal equations is theoretically important and is effective in certain cases, but it is not implemented in any of the subprograms described in this chapter.

The method of normal equations reduces the problem of minimizing $\|Ax - b\|_2$ to the seemingly simpler problem of solving $A^TAx = A^Tb$. The matrix A^TA is of size only n-by-n, which is attractive if $m >> n$. If A has full column rank, then A^TA, if computed exactly, is positive definite, so the normal equations can be solved by Cholesky factorization.

The following points are gleaned from (Golub and Van Loan), where the condition number, $\kappa_2(A)$, is the ratio of largest and smallest singular values of A, and $\rho = min||Ax - b||_2$.

- The sensitivity of the least squares solution to changes in A and b is roughly proportional to the quantity $\kappa_2(A) + \rho\kappa_2(A)^2$.
- The method of normal equations produces a computed solution that has a relative error given approximately by $\varepsilon\kappa_2(A)^2$.
- The orthogonal factorization methods in LAPACK produce a solution that has a relative error given approximately by $\varepsilon(\kappa_2(A) + \rho\kappa_2(A)^2)$.

Thus, if ρ is small and $\kappa_2(A)$ is large, the method of normal equations usually gives a least squares solution that is less accurate than given by the subprograms described in this chapter. In addition, when applied to ill-conditioned problems, the LAPACK subprograms usually will not break down as easily as the normal equations.

In the full-rank case (rank(A) = $min(m,n)$), the orthogonal factorization method of _GELS is often appropriate. But in the rank deficient case (rank(A) < $min(m,n)$), a different method should be used, either the SVD of _GELSS or the complete orthogonal factorization of _GELSX.

NAME

SGELS/DGELS/CGELS/ZGELS – Using Orthogonal Factorization

Purpose

These subprograms solve square or over- and under-determined linear systems involving the m-by-n matrix A and the right hand side B using orthogonal factorization of A. A must have full rank, that is, rank(A) = $min(m,n)$.

There are several cases, depending on the values of m and n and a transposition option:

1. $m \geq n$, **trans** = 'N' or 'n': Solve the least squares problem of finding X to minimize the Euclidean norm of each column of $AX–B$, where A is an m-by-n matrix, B is an m-by-$nrhs$ matrix, and X is an n-by-$nrhs$ matrix. After computing the QR factorization

$$A = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} R \\ 0 \end{bmatrix}$$

where Q_1 is m-by-n, Q_2 is m-by-$(m–n)$, R is n-by-n, and 0 is an $(m–n)$-by-n matrix of zeros, the least squares solution is $X = R^{-1}Q_1{}^*B$.

2. $m \geq n$, **trans** = 'T' or 't' or 'C' or 'c': Solve the underdetermined system $A^TX = B$ or $A^*X = B$, where A^T is the transpose of the real matrix A and A^* is the conjugate transpose of the complex matrix A. After computing the QR factorization

$$A = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} R \\ 0 \end{bmatrix}$$

where Q_1 is m-by-n, Q_2 is m-by-$(m–n)$, R is n-by-n, and 0 is an $(m–n)$-by-n matrix of zeros, the minimum-norm solution is $X = Q_1R^{-*}B$, where R^{-*} is the inverse of the conjugate transpose of R.

3. $m < n$, **trans** = 'N' or 'n': Solve the underdetermined system $AX = B$. After computing the LQ factorization

$$A = \begin{bmatrix} L & 0 \end{bmatrix} \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$$

where L is m-by-m, 0 is an m-by-$(n-m)$ matrix of zeros, Q_1 is m-by-n, and Q_2 is $(n-m)$-by-n, the minimum-norm solution is $X = Q_1{}^*L^{-1}B$.

4. $m < n$, **trans** = 'T' or 't' or 'C' or 'c': Solve the least squares problem of finding X to minimize the Euclidean norm of each column of A^TX-B or A^*X-B, where A is an m-by-n matrix, A^T is the transpose of the real matrix A, A^* is the conjugate transpose of the complex matrix A, B is an m-by-*nrhs* matrix, and X is an n-by-*nrhs* matrix. After computing the LQ factorization

$$A = \begin{bmatrix} L & 0 \end{bmatrix} \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$$

where L is m-by-m, 0 is an m-by-$(n-m)$ matrix of zeros, Q_1 is m-by-n, and Q_2 is $(n-m)$-by-n, the least squares solution is $X = L^{-*}Q_1B$, where L^{-*} is the inverse of the conjugate transpose of L.

Usage

LAPACK:

```
CHARACTER*1      trans
INTEGER*4        info, lda, ldb, lwork, m, n, nrhs
REAL*4           a(lda, n), b(ldb, nrhs), work(lwork)
CALL SGELS(trans, m, n, nrhs, a, lda, b, ldb, work, lwork, info)
CHARACTER*1      trans
INTEGER*4        info, lda, ldb, lwork, m, n, nrhs
REAL*8           a(lda, n), b(ldb, nrhs), work(lwork)
CALL DGELS(trans, m, n, nrhs, a, lda, b, ldb, work, lwork, info)
CHARACTER*1      trans
INTEGER*4        info, lda, ldb, lwork, m, n, nrhs
COMPLEX*8        a(lda, n), b(ldb, nrhs), work(lwork)
CALL CGELS(trans, m, n, nrhs, a, lda, b, ldb, work, lwork, info)
CHARACTER*1      trans
INTEGER*4        info, lda, ldb, lwork, m, n, nrhs
COMPLEX*16       a(lda, n), b(ldb, nrhs), work(lwork)
CALL ZGELS(trans, m, n, nrhs, a, lda, b, ldb, work, lwork, info)
```

LAPACK8:

```
CHARACTER*1        trans
INTEGER*8          info, lda, ldb, lwork, m, n, nrhs
REAL*8             a(lda, n), b(ldb, nrhs), work(lwork)
CALL SGELS(trans, m, n, nrhs, a, lda, b, ldb, work, lwork, info)
CHARACTER*1        trans
INTEGER*8          info, lda, ldb, lwork, m, n, nrhs
COMPLEX*16         a(lda, n), b(ldb, nrhs), work(lwork)
CALL CGELS(trans, m, n, nrhs, a, lda, b, ldb, work, lwork, info)
```

Input

trans Transposition option for the matrix A:

trans = 'N' or 'n': Solve $AX = B$.

trans = 'T' or 't': Solve $A^TX = B$.

trans = 'C' or 'c': Solve $A^*X = B$.

trans = 'T' or 't' is valid only in subprograms SGELS and DGELS, and **trans** = 'C' or 'c' is valid only in subprograms CGELS and ZGELS.

m The number of rows of the matrix A. **m** ≥ 0.

n The number of columns of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides; that is, the number of columns of the matrix B. **nrhs** ≥0.

a The **m**-by-**n** matrix A.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**m**).

b If **trans** = 'N' or 'n', the **m**-by-**nrhs** right hand side matrix B.

If **trans** = 'T' or 't' or 'C' or 'c', the **n**-by-**nrhs** right hand side matrix B.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**m**,**n**).

lwork The length of array **work**. **lwork** ≥ max(1,min(**m**,**n**) + max(**m**,**n**,**nrhs**)). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a If **m** ≥ **n**, **a** has been overwritten by the QR factorization of A.

If **m** < **n**, **a** has been overwritten by the LQ factorization of A.

b On successful exit, if **m** ≥ **n** and **trans** = 'N' or '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.

On successful exit, if **m** ≥ **n** and **trans** = 'T' or 't', the **m**-by-**nrhs** minimum-norm solution.

On successful exit, if **m** < **n** and **trans** = 'N' or 'n', the **n**-by-**nrhs** minimum-norm solution.

On successful exit, if **m** < **n** and **trans** = 'T' or 't', 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.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

trans ≠ 'N' or 'n' or 'T' or 't' or 'C' or 'c',
m < 0,
n < 0,
nrhs < 0,
lda < max(1,**m**),
ldb too small, and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **trans** argument as 'NotTransposed' for 'N', 'Transposed' for 'T', or 'ConjugateTransposed' for 'C'.

NAME

SGELSS/DGELSS/CGELSS/ZGELSS – Using Singular Value Decomposition

Purpose

These subprograms use 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 an m-by-n matrix, B is an m-by-$nrhs$ matrix, and X is an n-by-$nrhs$ matrix. If $m \geq n$, the problem is overdetermined and the least squares solution is computed. If $m < n$, the problem is underdetermined; in this case a minimum-norm solution is returned.

The singular values of A that are smaller than a specified tolerance times the largest singular value are treated as zero in solving the least squares problem; in this case a minimum-norm solution is returned.

Usage

LAPACK:

```
INTEGER*4          info, lda, ldb, lwork, m, n, nrhs, rank
REAL*4             rcond
REAL*4             a(lda, n), b(ldb, nrhs), s(min(m,n)), work(lwork)
CALL SGELSS(m, n, nrhs, a, lda, b, ldb, s, rcond, rank, work, lwork, info)
INTEGER*4          info, lda, ldb, lwork, m, n, nrhs, rank
REAL*8             rcond
REAL*8             a(lda, n), b(ldb, nrhs), s(min(m,n)), work(lwork)
CALL DGELSS(m, n, nrhs, a, lda, b, ldb, s, rcond, rank, work, lwork, info)
INTEGER*4          info, lda, ldb, lwork, m, n, nrhs, rank
REAL*4             rcond
REAL*4             rwork(max(1,5*min(m,n)–1)), s(min(m,n))
COMPLEX*8          a(lda, n), b(ldb, nrhs), work(lwork)
CALL CGELSS(m, n, nrhs, a, lda, b, ldb, s, rcond, rank, work, lwork,
                   rwork, info)
INTEGER*4          info, lda, ldb, lwork, m, n, nrhs, rank
REAL*8             rcond
REAL*8             rwork(max(1,5*min(m,n)–1)), s(min(m,n))
COMPLEX*16         a(lda, n), b(ldb, nrhs), work(lwork)
CALL ZGELSS(m, n, nrhs, a, lda, b, ldb, s, rcond, rank, work, lwork,
                   rwork, info)
```

LAPACK8:

```
INTEGER*8          info, lda, ldb, lwork, m, n, nrhs, rank
REAL*8             rcond
REAL*8             a(lda, n), b(ldb, nrhs), s(min(m,n)), work(lwork)
CALL SGELSS(m, n, nrhs, a, lda, b, ldb, s, rcond, rank, work, lwork, info)
```

```
INTEGER*8          info, lda, ldb, lwork, m, n, nrhs, rank
REAL*8             rcond
REAL*8             rwork(max(1,5*min(m,n)-1)), s(min(m,n))
COMPLEX*16         a(lda, n), b(ldb, nrhs), work(lwork)
CALL CGELSS(m, n, nrhs, a, lda, b, ldb, s, rcond, rank, work, lwork,
                   rwork, info)
```

Input

m The number of rows of the matrix A. **m** ≥ 0.

n The number of columns of the matrix A. **n** ≥ 0.

nrhs The number of right hand sides; that is, the number of columns of the matrix B. **nrhs** ≥0.

a The matrix A specifying the least squares problem.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**m**).

b The **m**-by-**nrhs** matrix of right hand side vectors for the least squares problem.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**m**,**n**).

rcond A tolerance: the singular values of A that are less than or equal to **rcond** times the largest singular value are treated as zero in solving the least squares problem. If **rcond** is negative, the machine precision is used instead. For example, if $Sx = b$ were the least squares problem, where S is a diagonal matrix of singular values and x and b are vectors, the i-th component of the solution would be

$$x_i = \begin{cases} b_i/s_{ii} & \text{if } s_{ii} > \textbf{rcond} \times \max_j(s_{jj}) \\ 0 & \text{if } s_{ii} \le \textbf{rcond} \times \max_j(s_{jj}) \end{cases}$$

lwork The length of array **work**.

For SGELSS and DGELSS, **lwork** ≥ max(1,3min(**m**,**n**) + max(2min(**m**,**n**), **m**,**n**,**nrhs**)).

For CGELSS and ZGELSS, **lwork** ≥ max(1,2min(**m**,**n**) + max(**m**,**n**, **nrhs**)).

For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work, rwork Arrays used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the input has been overwritten with the right singular vectors of A.

b On successful exit, the solution X in rows 1 through **n**.

s On successful exit, the singular values of A, sorted into decreasing order.

rank On successful exit, the number of singular values of A that are greater than **rcond** times the largest singular value.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, the algorithm terminated with k unconverged elements of an intermediate bidiagonal matrix.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
nrhs < 0,
lda < max(1,**m**),
ldb < max(1,**m**,**n**), and
lwork too small.

NAME

SGELSX/DGELSX/.../ZGELSX – Using Complete Orthogonal Factorization

Purpose

Solve the least squares problem of finding X to minimize the Euclidean norm of each column of $AX–B$, where A is an m-by-n matrix, B is an m-by-$nrhs$ matrix, and X is an n-by-$nrhs$ matrix using a complete orthogonal factorization. The subprograms compute the QR factorization of A with column pivoting

$$AP = Q \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix}$$

where P is a permutation matrix designed to make R_{11} the largest leading square submatrix whose condition number is less than 1/**rcond**. Then, treating R_{22} as negligible, R_{12} is annihilated by orthogonal or unitary transformations from the right, giving

$$AP = Q \begin{bmatrix} T_{11} & 0 \\ 0 & 0 \end{bmatrix} Y$$

from which the minimum-norm solution is

$$X = PY* \begin{bmatrix} T_{11}^{-1} Q_1 * B \\ 0 \end{bmatrix}$$

where Q_1 is the submatrix of Q having the same number of columns as T_{11}.

Usage

LAPACK:

```
INTEGER*4       info, lda, ldb, m, n, nrhs, rank
REAL*4          rcond
INTEGER*4       jpvt(n)
REAL*4          a(lda, n), b(ldb, nrhs), work(lwork)
CALL SGELSX(m, n, nrhs, a, lda, b, ldb, jpvt, rcond, rank, work, info)
INTEGER*4       info, lda, ldb, m, n, nrhs, rank
REAL*8          rcond
INTEGER*4       jpvt(n)
REAL*8          a(lda, n), b(ldb, nrhs), work(lwork)
CALL DGELSX(m, n, nrhs, a, lda, b, ldb, jpvt, rcond, rank, work, info)
```

```
INTEGER*4          info, lda, ldb, m, n, nrhs, rank
REAL*4             rcond
INTEGER*4          jpvt(n)
REAL*4             rwork(2*n)
COMPLEX*8          a(lda, n), b(ldb, nrhs), work(lwork)
CALL CGELSX(m, n, nrhs, a, lda, b, ldb, jpvt, rcond, rank, work, rwork,
                   info)
INTEGER*4          info, lda, ldb, m, n, nrhs, rank
REAL*8             rcond
INTEGER*4          jpvt(n)
REAL*8             rwork(2*n)
COMPLEX*16         a(lda, n), b(ldb, nrhs), work(lwork)
CALL ZGELSX(m, n, nrhs, a, lda, b, ldb, jpvt, rcond, rank, work, rwork,
                   info)
```

LAPACK8:

```
INTEGER*8          info, lda, ldb, m, n, nrhs, rank
REAL*8             rcond
INTEGER*8          jpvt(n)
REAL*8             a(lda, n), b(ldb, nrhs), work(lwork)
CALL SGELSX(m, n, nrhs, a, lda, b, ldb, jpvt, rcond, rank, work, info)
INTEGER*8          info, lda, ldb, m, n, nrhs, rank
REAL*8             rcond
INTEGER*8          jpvt(n)
REAL*8             rwork(2*n)
COMPLEX*16         a(lda, n), b(ldb, nrhs), work(lwork)
CALL CGELSX(m, n, nrhs, a, lda, b, ldb, jpvt, rcond, rank, work, rwork,
                   info)
```

Input

m	The number of rows of the matrix A. **m** ≥ 0.
n	The number of columns of the matrix A. **n** ≥ 0.
nrhs	The number of right hand sides; that is, the number of columns of the matrix B. **nrhs** ≥ 0.
a	The **m**-by-**n** matrix A.
lda	The leading dimension of array **a** in the calling program unit. **lda** $\geq \max(1,\mathbf{m})$.
b	The **m**-by-**nrhs** matrix of right hand side vectors for the least squares problem.
ldb	The leading dimension of array **b** in the calling program unit. **ldb** $\geq \max(1,\mathbf{m},\mathbf{n})$.
jpvt	If **jpvt**(j) $\neq 0$, column j is permuted to the front of AP; otherwise, column j is a free column.

rcond A tolerance: the goal of the complete orthogonal factorization is to identify a well-conditioned triangular matrix whose condition number is less than 1/**rcond**.

Working Storage

work An array of length **lwork** = max(min(**m**,**n**)+3**n**, 2min(**m**,**n**)+**nrhs**), used for work space.

rwork An array used for work space.

Output

a On successful exit, the input has been overwritten by the complete orthogonal factorization of A.

b On successful exit, the first **n** rows of **b** contain the minimum-norm solution.

jpvt On successful exit, if **jpvt**(j) = k, then the j-th column of AP was the k-th column of A.

rank On successful exit, the size of the largest leading triangular matrix in the QR factorization (with pivoting) of A, whose condition number is less than 1/**rcond**.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
nrhs < 0,
lda < max(1,**m**), and
ldb < max(1,**m**,**n**).

NAME

SGGGLM/DGGGLM/CGGGLM/ZGGGLM – Generalized Linear Regression

Purpose

These subprograms solve a generalized linear regression model (GLM) problem:

$$\min_{x,y} ||y||_2 \qquad \text{subject to} \qquad d = Ax + By$$

using a generalized QR factorization of matrices A and B, where A is an n-by-m matrix, B is an n-by-p matrix, and $||\ \ ||_2$ denotes the Euclidean vector norm.

These subprograms require that $m \le n \le m+p$, and

$$\text{rank}(A) = m \qquad \text{and} \qquad \text{rank}([A \quad B]) = n.$$

Under these conditions, the constraint equation is always consistent and there is a unique solution x and a minimal 2-norm solution y.

In particular, if matrix B is square and nonsingular, then the GLM problem is equivalent to the following weighted linear least squares problem

$$\min_x ||B^{-1}(b-Ax)||_2.$$

Usage

LAPACK:

```
INTEGER*4          info, lda, ldb, lwork, m, n, p
REAL*4             a(lda, m), b(ldb, p), d(n), work(lwork), x(m), y(p)
CALL SGGGLM(n, m, p, a, lda, b, ldb, d, x, y, work, lwork, info)
INTEGER*4          info, lda, ldb, lwork, m, n, p
REAL*8             a(lda, m), b(ldb, p), d(n), work(lwork), x(m), y(p)
CALL DGGGLM(n, m, p, a, lda, b, ldb, d, x, y, work, lwork, info)
INTEGER*4          info, lda, ldb, lwork, m, n, p
COMPLEX*8          a(lda, m), b(ldb, p), d(n), work(lwork), x(m), y(p)
CALL CGGGLM(n, m, p, a, lda, b, ldb, d, x, y, work, lwork, info)
INTEGER*4          info, lda, ldb, lwork, m, n, p
COMPLEX*16         a(lda, m), b(ldb, p), d(n), work(lwork), x(m), y(p)
CALL ZGGGLM(n, m, p, a, lda, b, ldb, d, x, y, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, lda, ldb, lwork, m, n, p
REAL*8             a(lda, m), b(ldb, p), d(n), work(lwork), x(m), y(p)
CALL SGGGLM(n, m, p, a, lda, b, ldb, d, x, y, work, lwork, info)
INTEGER*8          info, lda, ldb, lwork, m, n, p
COMPLEX*16         a(lda, m), b(ldb, p), d(n), work(lwork), x(m), y(p)
CALL CGGGLM(n, m, p, a, lda, b, ldb, d, x, y, work, lwork, info)
```

Input

n The number of rows of the matrices A and B. $\mathbf{n} \geq \mathbf{m}$ and $\mathbf{n} \leq \mathbf{m+p}$.

m The number of columns of the matrix A. $\mathbf{m} \geq 0$.

p The number of columns of the matrix B. $\mathbf{p} \geq 0$.

a The **n**-by-**m** matrix A.

lda The leading dimension of array **a** in the calling program unit. $\mathbf{lda} \geq \max(1,\mathbf{n})$.

b The **n**-by-**p** matrix B.

ldb The leading dimension of array **b** in the calling program unit. $\mathbf{ldb} \geq \max(1,\mathbf{n})$.

d The left hand side vector d of the GLM equation.

lwork The length of array **work**. $\mathbf{lwork} \geq \mathbf{m} + \mathbf{p} + \max(\mathbf{n},\mathbf{m},\mathbf{p})$.

For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work Array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a, b, d Destroyed.

x, y The solution vectors x and y of the GLM problem.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

n < 0,
m < 0,
p < 0,
n < **m**,
n > **m**+**p**,
lda < max(1,**n**),
ldb < max(1,**n**), and
lwork too small.

NAME

SGGLSE/DGGLSE/CGGLSE/ZGGLSE – Linear Equality Constraints

Purpose

These subprograms solve the linear equality constrained least squares (LSE) problem:

$$\min_x ||Ax-c||_2 \qquad \text{subject to} \qquad Bx = d$$

using a generalized RQ factorization of matrices A and B, where A is an m-by-n matrix, B is a p-by-n matrix, and $||\ \ ||_2$ denotes the vector Euclidean norm.

It is assumed that B is of rank p, with $p \le n \le m+p$, and that the null spaces of A and B intersect only trivially:

$$\text{null}(A) \cap \text{null}(B) = \{0\}.$$

The latter condition is equivalent to

$$\text{rank}\left(\begin{bmatrix} A \\ B \end{bmatrix}\right) = n.$$

Usage

LAPACK:

```
INTEGER*4          info, lda, ldb, lwork, m, n, p
REAL*4             a(lda, n), b(ldb, n), c(m), d(p), work(lwork), x(n)
CALL SGGLSE(m, n, p, a, lda, b, ldb, c, d, x, work, lwork, info)
INTEGER*4          info, lda, ldb, lwork, m, n, p
REAL*8             a(lda, n), b(ldb, n), c(m), d(p), work(lwork), x(n)
CALL DGGLSE(m, n, p, a, lda, b, ldb, c, d, x, work, lwork, info)
INTEGER*4          info, lda, ldb, lwork, m, n, p
COMPLEX*8          a(lda, n), b(ldb, n), c(m), d(p), work(lwork), x(n)
CALL CGGLSE(m, n, p, a, lda, b, ldb, c, d, x, work, lwork, info)
INTEGER*4          info, lda, ldb, lwork, m, n, p
COMPLEX*16         a(lda, n), b(ldb, n), c(m), d(p), work(lwork), x(n)
CALL ZGGLSE(m, n, p, a, lda, b, ldb, c, d, x, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, lda, ldb, lwork, m, n, p
REAL*8             a(lda, n), b(ldb, n), c(m), d(p), work(lwork), x(n)
CALL SGGLSE(m, n, p, a, lda, b, ldb, c, d, x, work, lwork, info)
INTEGER*8          info, lda, ldb, lwork, m, n, p
COMPLEX*16         a(lda, n), b(ldb, n), c(m), d(p), work(lwork), x(n)
CALL CGGLSE(m, n, p, a, lda, b, ldb, c, d, x, work, lwork, info)
```

Input

m	The number of rows of the matrix A. $\mathbf{m} \geq 0$.
n	The number of columns of the matrices A and B. $\mathbf{n} \geq 0$.
p	The number of rows of the matrix B. $\mathbf{p} \geq 0$.
a	The **m**-by-**n** matrix A for the least squares part of the LSE problem.
lda	The leading dimension of array **a** in the calling program unit. $\mathbf{lda} \geq \max(1,\mathbf{m})$.
b	The **p**-by-**n** matrix B for the constraint equations part of the LSE problem.
ldb	The leading dimension of array **b** in the calling program unit. $\mathbf{ldb} \geq \max(1,\mathbf{p})$.
c	The right hand side vector c for the least squares part of the LSE problem.
d	The right hand side vector d for the constraint equations part of the LSE problem.
lwork	The length of array **work**. $\mathbf{lwork} \geq \mathbf{n} + \mathbf{p} + \max(\mathbf{m},\mathbf{n},\mathbf{p})$. For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work	Array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a, b	Destroyed.	
c	The Euclidean norm of the residual vector $Ax–c$ is given by the Euclidean norm of elements $n–p+1$ to m of **c**.	
d	Destroyed.	
x	The solution vector x of the LSE problem.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
p < 0,
n < **p**,
n > **m**+**p**,
lda < max(1,**m**),
ldb < max(1,**p**), and
lwork too small.

6 Computational Subprograms for Orthogonal Factorizations

Overview

This chapter describes the computational subprograms to compute several forms of orthogonal factorizations of a matrix, to compute several forms of the generalized orthogonal factorization of a pair of matrices, and to make use of the resulting orthogonal matrix.

This chapter also shows how to use these and other LAPACK subprograms to solve linear least squares problems.

These operations are performed for both real and complex general matrices:

- Compute the QR factorization
- Compute the RQ factorization
- Compute the QL factorization
- Compute the LQ factorization
- Compute the QR factorization using column pivoting
- Compute the generalized QR factorization of a pair of matrices
- Compute the generalized RQ factorization of a pair of matrices
- Multiply another matrix by the Q matrix produced by one of these factorizations
- Generate the Q matrix from the factored form produced during the above computations

The following documents provide supplemental material for this chapter:

- Anderson, E. *et al. LAPACK Users' Guide*, Second Edition. Philadelphia, PA: Society for Industrial and Applied Mathematics. 1995.
- Forsythe, G. and C.B. Moler. *Computer Solution of Linear Algebraic Systems*. Englewood Cliffs, NJ: Prentice-Hall, Inc. 1967.
- Golub, G.H. and C.F. Van Loan. *Matrix Computations*, 2nd Edition. Baltimore, MD: The Johns Hopkins University Press. 1989.

Chapter Objectives

After you read this chapter you will:

- Know how orthogonal and unitary matrices are represented in factored form
- Know how to use the described subprograms

What You Need to Know to Use These Subprograms

The LAPACK subprograms in this chapter are organized so that it is usually necessary to call two or more subprograms to perform the above operations. This division of labor significantly enhances the number of processing options you may form by combining these and other LAPACK subprograms.

Combining Computational Subprograms

When you use the computational subprograms instead of calling the drivers, you usually must put two or more of them together to carry out your entire computation. This section shows how to assemble an algorithm from several computational subprograms. In these examples, assume your matrix is a 10-by-5 real general matrix stored in a single precision array large enough to handle a 20-by-10 problem. The examples do not show how the matrix, or the right hand side, if needed, are generated.

Solving a Full-Rank Linear Least Squares Problem

The following code segment shows how to solve a full-rank linear least squares problem

$$\min_x ||b - Ax||_2$$

SGEQRF computes the QR factorization of the coefficient matrix A. Then SORMQR computes $Q^T b$. Finally, STRTRS, a computational subprogram for linear equations, computes the solution vector $x = R^{-1}(Q^T b)$, overwriting the right hand side vector B with it.

```
      INTEGER*4 INFO, LDA, LDB, M, MMAX, N, NMAX, NRHS
      PARAMETER ( MMAX  = 20 )
      PARAMETER ( NMAX  = 10 )
      PARAMETER ( LDA   = MMAX )
      PARAMETER ( LDB   = MMAX )
      PARAMETER ( LWORK = NMAX )
      REAL*4 A(LDA,NMAX), B(LDB), TAU(NMAX), WORK(LWORK)

      M     = 10
      N     = 5
      NRHS  = 1
      CALL SGEQRF (M, N, A, LDA, TAU, WORK, LWORK, INFO)
      CALL SORMQR ('Left', 'Transposed', M, NRHS, N, A, LDA, TAU, B, LDB,
     &                        WORK, LWORK, INFO)
      CALL STRTRS ('Upper', 'NonTransposed', 'NonUnit', N, NRHS, A, LDA,
     &                        B, LDB, INFO)
```

Determine the Effective Rank of a Matrix

The QR factorization with column pivoting can be used to determine the effective numerical rank of a matrix less expensively than the more robust Singular Value Decomposition. SLANGE is used to compute $\|A\|_1$, from which a tolerance is determined to measure smallness. SGEQPF computes the QR factorization of A with column pivoting. The subsequent loop determines the rank by counting the number of nonsmall diagonal elements of the R matrix.

```
      INTEGER*4 INFO, LDA, M, N, NMAX, RANK
      PARAMETER ( NMAX  = 10 )
      PARAMETER ( LDA   = 20 )
      REAL*4    ANORM, SLAMCH, SLANGE, TOL
      INTEGER*4 JPVT(NMAX), RANK
      REAL*4    A(LDA,NMAX), TAU(NMAX), WORK(3*NMAX)
      M = 10
      N = 5
      ANORM = SLANGE('1', M, N, A, LDA, WORK)
      TOL = MAX(M, N) * ANORM * SLAMCH('Precision')
      DO 10 I = 1, N
         JPVT(I) = 0
10    CONTINUE
      CALL SGEQPF (M, N, A, LDA, JPVT, TAU, WORK, INFO)

      RANK = 0
      DO 20 I = 1, MIN(M, N)
         IF( ABS(A(I,I)) .GT. TOL ) RANK = RANK + 1
20    CONTINUE
```

NAME

SGELQF/DGELQF/.../ZGELQF – *LQ* Factorization of General Matrix

Purpose

These subprograms compute the *LQ* factorization of a general *m*-by-*n* matrix *A*. The factorization has the form $A = LQ$, where *L* is a lower triangular matrix (lower trapezoidal if $m > n$) and *Q* is an orthogonal or unitary matrix. The computed matrix *Q* is represented as a product of elementary reflection matrices

$$Q = H_k H_{k-1} \ldots H_1$$

where $k = min(m,n)$. Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an *n*-dimensional vector whose first $i-1$ components are zero and whose *i*th component is 1.

Additional subprograms are provided to make it easier to use the matrix *Q* in its factored form. The operations furnished are to multiply a general matrix by the *Q* matrix, and to generate (expand) the *Q* matrix into regular, unfactored form. The names of these companion subprograms depend on the data type:

Data Type	*LQ* Factorization	Generate *Q*	Multiply Matrix by *Q*
REAL*4	SGELQF	SORGLQ	SORMLQ
REAL*8	DGELQF	DORGLQ	DORMLQ
COMPLEX*8	CGELQF	CUNGLQ	CUNMLQ
COMPLEX*16	ZGELQF	ZUNGLQ	ZUNMLQ

Usage

LAPACK:

```
INTEGER*4          info, lda, lwork, m, n
REAL*4             a(lda, n), tau(min(m,n)), work(lwork)
CALL SGELQF(m, n, a, lda, tau, work, lwork, info)

INTEGER*4          info, lda, lwork, m, n
REAL*8             a(lda, n), tau(min(m,n)), work(lwork)
CALL DGELQF(m, n, a, lda, tau, work, lwork, info)

INTEGER*4          info, lda, lwork, m, n
COMPLEX*8          a(lda, n), tau(min(m,n)), work(lwork)
CALL CGELQF(m, n, a, lda, tau, work, lwork, info)
```

```
INTEGER*4          info, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(min(m,n)), work(lwork)
CALL ZGELQF(m, n, a, lda, tau, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, lda, lwork, m, n
REAL*8             a(lda, n), tau(min(m,n)), work(lwork)
CALL SGELQF(m, n, a, lda, tau, work, lwork, info)

INTEGER*8          info, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(min(m,n)), work(lwork)
CALL CGELQF(m, n, a, lda, tau, work, lwork, info)
```

Input

m The number of rows of the matrix A. **m** ≥ 0.

n The number of columns of the matrix A. **n** ≥ 0.

a The **m**-by-**n** matrix A to be factored.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**m**).

lwork The length of array **work**. **lwork** ≥ max(1,**m**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the factors L and Q from the factorization $A = LQ$, stored as follows:

If **m** ≤ **n**, the elements on and below the principal diagonal of **a** contain the **m**-by-**m** lower triangular matrix L.

If **m** > **n**, the elements on and below the principal diagonal of **a** contain the **n**-by-**m** lower trapezoidal matrix L.

The elements above the principal diagonal of the ith row of **a**, i = 1, 2, ..., min(**m**,**n**–1), contain components i+1 to **n** of v_i.

tau On successful exit, the scalar factors, τ_i, i = 1, 2, ..., min(**m**,**n**), of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$.

info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
lda < max(1,**m**), and
lwork < max(1,**m**).

NAME

SGEQLF/DGEQLF/.../ZGEQLF – *QL* Factorization of General Matrix

Purpose

These subprograms compute the *QL* factorization of a general *m*-by-*n* matrix *A*. The factorization has the form $A = QL$, where *Q* is an orthogonal or unitary matrix and *L* is a lower triangular matrix (lower trapezoidal if $m < n$). The computed matrix *Q* is represented as a product of elementary reflection matrices

$$Q = H_k H_{k-1} \ldots H_1$$

where $k = min(m,n)$. Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an *m*-dimensional vector whose $)n-k+i)$th component is 1 and whose last $k-i$ components are zero.

Additional subprograms are provided to make it easier to use the matrix *Q* in its factored form. The operations furnished are to multiply a general matrix by the *Q* matrix, and to generate (expand) the *Q* matrix into regular, unfactored form. The names of these companion subprograms depend on the data type:

Data Type	*QL* Factorization	Generate *Q*	Multiply Matrix by *Q*
REAL*4	SGEQLF	SORGQL	SORMQL
REAL*8	DGEQLF	DORGQL	DORMQL
COMPLEX*8	CGEQLF	CUNGQL	CUNMQL
COMPLEX*16	ZGEQLF	ZUNGQL	ZUNMQL

Usage

LAPACK:

```
INTEGER*4          info, lda, lwork, m, n
REAL*4             a(lda, n), tau(min(m,n)), work(lwork)
CALL SGEQLF(m, n, a, lda, tau, work, lwork, info)

INTEGER*4          info, lda, lwork, m, n
REAL*8             a(lda, n), tau(min(m,n)), work(lwork)
CALL DGEQLF(m, n, a, lda, tau, work, lwork, info)

INTEGER*4          info, lda, lwork, m, n
COMPLEX*8          a(lda, n), tau(min(m,n)), work(lwork)
CALL CGEQLF(m, n, a, lda, tau, work, lwork, info)
```

```
INTEGER*4          info, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(min(m,n)), work(lwork)
CALL ZGEQLF(m, n, a, lda, tau, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, lda, lwork, m, n
REAL*8             a(lda, n), tau(min(m,n)), work(lwork)
CALL SGEQLF(m, n, a, lda, tau, work, lwork, info)

INTEGER*8          info, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(min(m,n)), work(lwork)
CALL CGEQLF(m, n, a, lda, tau, work, lwork, info)
```

Input

m — The number of rows of the matrix A. **m** ≥ 0.

n — The number of columns of the matrix A. **n** ≥ 0.

a — The **m**-by-**n** matrix A to be factored.

lda — The leading dimension of array **a** in the calling program unit. **lda** $\geq$ max(1,**m**).

lwork — The length of array **work**. **lwork** $\geq$ max(1,**n**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work — An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a — On successful exit, the factors Q and L from the factorization $A = QL$, stored as follows:

If **m** > **n**, the elements on and below the (**m**–**n**)-th subdiagonal of **a** contain the **n**-by-**n** lower triangular matrix L.

If **m** = **n**, the elements on and below the principal diagonal of **a** contain the **n**-by-**n** lower triangular matrix L.

If **m** < **n**, the elements on and below the (**n**–**m**)-th superdiagonal of **a** contain the **m**-by-**n** lower trapezoidal matrix L.

The remaining elements of **a** contain components of the v vectors:

If $\mathbf{m} \geq \mathbf{n}$, column i of **a**, $i = 1, 2, ..., \mathbf{n}$, contains components 1 to $\mathbf{m}-\mathbf{n}+i-1$ of v_i.

If $\mathbf{m} < \mathbf{n}$, column $\mathbf{n}-\mathbf{m}+i$ of **a**, $i = 2, 3, ..., \mathbf{n}$, contains components 1 to $i-1$ of v_i.

tau On successful exit, the scalar factors, τ_i, $i = 1, 2, ..., \min(\mathbf{m},\mathbf{n})$, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
lda < max(1,**m**), and
lwork < max(1,**n**).

NAME

SGEQPF/DGEQPF/.../ZGEQPF – *QR* Factorization of General Matrix

Purpose

These subprograms compute the *QR* factorization of a general *m*-by-*n* matrix *A* using column pivoting. The factorization has the form $AP = QR$, where *Q* is an orthogonal or unitary matrix, *R* is an upper triangular matrix (upper trapezoidal if $m < n$), and *P* is a permutation matrix chosen so that if *A* is of rank *r* then the first *r* columns of *Q* span the range of *A*.

The computed matrix *Q* is represented as a product of elementary reflection matrices

$$Q = H_1 H_2 \ldots H_k$$

where $k = min(m,n)$. Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an *m*-dimensional vector whose first $i-1$ components are zero and whose *i*th component is 1.

Additional subprograms are provided to make it easier to use the matrix *Q* in its factored form. The operations furnished are to multiply a general matrix by the *Q* matrix, and to generate (expand) the *Q* matrix into regular, unfactored form. The names of these companion subprograms depend on the data type:

Data Type	*QR* Factorization	Generate *Q*	Multiply Matrix by *Q*
REAL*4	SGEQPF	SORGQR	SORMQR
REAL*8	DGEQPF	DORGQR	DORMQR
COMPLEX*8	CGEQPF	CUNGQR	CUNMQR
COMPLEX*16	ZGEQPF	ZUNGQR	ZUNMQR

Usage

LAPACK:

```
INTEGER*4       info, lda, m, n
INTEGER*4       jpvt(n)
REAL*4          a(lda, n), tau(min(m,n)), work(3*n)
CALL SGEQPF(m, n, a, lda, jpvt, tau, work, info)

INTEGER*4       info, lda, m, n
INTEGER*4       jpvt(n)
REAL*8          a(lda, n), tau(min(m,n)), work(3*n)
CALL DGEQPF(m, n, a, lda, jpvt, tau, work, info)
```

```
INTEGER*4          info, lda, m, n
INTEGER*4          jpvt(n)
REAL*4             rwork(2*n)
COMPLEX*8          a(lda, n), tau(min(m,n)), work(n)
CALL CGEQPF(m, n, a, lda, jpvt, tau, work, rwork, info)

INTEGER*4          info, lda, m, n
INTEGER*4          jpvt(n)
REAL*8             rwork(2*n)
COMPLEX*16         a(lda, n), tau(min(m,n)), work(n)
CALL ZGEQPF(m, n, a, lda, jpvt, tau, work, rwork, info)
```

LAPACK8:

```
INTEGER*8          info, lda, m, n
INTEGER*8          jpvt(n)
REAL*8             a(lda, n), tau(min(m,n)), work(3*n)
CALL SGEQPF(m, n, a, lda, jpvt, tau, work, info)

INTEGER*8          info, lda, m, n
INTEGER*8          jpvt(n)
REAL*8             rwork(2*n)
COMPLEX*16         a(lda, n), tau(min(m,n)), work(n)
CALL CGEQPF(m, n, a, lda, jpvt, tau, work, rwork, info)
```

Input

m The number of rows of the matrix A. $\mathbf{m} \geq 0$.

n The number of columns of the matrix A. $\mathbf{n} \geq 0$.

a The **m**-by-**n** matrix A to be factored.

lda The leading dimension of array **a** in the calling program unit. $\mathbf{lda} \geq \max(1,\mathbf{m})$.

jpvt If $\mathbf{jpvt}(j) \neq 0$, column j of A is permuted to the front of matrix AP and will not be subject to further algorithmic pivoting.

If $\mathbf{jpvt}(j) = 0$, column j of A is a free column and will be pivoted as the algorithm determines.

Working Storage

work, rwork Arrays used for work space.

Output

a On successful exit, the factors Q and R from the factorization $AP = QR$, stored as follows:

The elements on and above the diagonal of **a** contain the min(**m**,**n**)-by-**n** upper triangular or upper trapezoidal matrix R.

The elements below the diagonal of the ith column of **a**, $i = 1, 2, ..., \min(\mathbf{m}-1,\mathbf{n})$, contain the last **m**–i components of v_i. See "Purpose" for details.

jpvt If **jpvt**(j) = k, then column k of A was permuted to column j of the matrix AP. Thus, the jth column of P is e_k, the kth canonical unit vector, $(0,0,...,0,1,0,...,0)^T$, where the "1" is in the kth position.

tau On successful exit, the scalar factors, τ_i, $i = 1, 2, ..., \min(\mathbf{m},\mathbf{n})$, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = –k, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0, and
lda < max(1,**m**).

NAME

SGEQRF/DGEQRF/.../ZGEQRF – *QR* Factorization of General Matrix

Purpose

These subprograms compute the *QR* factorization of a general *m*-by-*n* matrix *A*. The factorization has the form $A = QR$, where *Q* is an orthogonal or unitary matrix and *R* is an upper triangular matrix (upper trapezoidal if $m < n$). The computed matrix *Q* is represented as a product of elementary reflection matrices

$$Q = H_1 H_2 \ldots H_k$$

where $k = min(m,n)$. Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an *m*-dimensional vector whose first $i-1$ components are zero and whose *i*th component is 1.

Additional subprograms are provided to make it easier to use the matrix *Q* in its factored form. The operations furnished are to multiply a general matrix by the *Q* matrix, and to generate (expand) the *Q* matrix into regular, unfactored form. The names of these companion subprograms depend on the data type:

Data Type	*QR* Factorization	Generate *Q*	Multiply Matrix by *Q*
REAL*4	SGEQRF	SORGQR	SORMQR
REAL*8	DGEQRF	DORGQR	DORMQR
COMPLEX*8	CGEQRF	CUNGQR	CUNMQR
COMPLEX*16	ZGEQRF	ZUNGQR	ZUNMQR

Usage

LAPACK:

```
INTEGER*4          info, lda, lwork, m, n
REAL*4             a(lda, n), tau(min(m,n)), work(lwork)
CALL SGEQRF(m, n, a, lda, tau, work, lwork, info)

INTEGER*4          info, lda, lwork, m, n
REAL*8             a(lda, n), tau(min(m,n)), work(lwork)
CALL DGEQRF(m, n, a, lda, tau, work, lwork, info)

INTEGER*4          info, lda, lwork, m, n
COMPLEX*8          a(lda, n), tau(min(m,n)), work(lwork)
CALL CGEQRF(m, n, a, lda, tau, work, lwork, info)
```

```
INTEGER*4          info, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(min(m,n)), work(lwork)
CALL ZGEQRF(m, n, a, lda, tau, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, lda, lwork, m, n
REAL*8             a(lda, n), tau(min(m,n)), work(lwork)
CALL SGEQRF(m, n, a, lda, tau, work, lwork, info)

INTEGER*8          info, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(min(m,n)), work(lwork)
CALL CGEQRF(m, n, a, lda, tau, work, lwork, info)
```

Input

m The number of rows of the matrix A. **m** ≥ 0.

n The number of columns of the matrix A. **n** ≥ 0.

a The **m**-by-**n** matrix A to be factored.

lda The leading dimension of array **a** in the calling program unit. **lda** $\geq \max(1,\mathbf{m})$.

lwork The length of array **work**. **lwork** $\geq \max(1,\mathbf{n})$. For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the factors Q and R from the factorization $A = QR$, stored as follows:

If **m** $\geq$ **n**, the elements on and above the principal diagonal of **a** contain the **n**-by-**n** upper triangular matrix R.

If **m** < **n**, the elements on and above the principal diagonal of **a** contain the **m**-by-**n** upper trapezoidal matrix R.

The elements below the principal diagonal of the jth column of **a**, $j = 1, 2, \ldots, \min(\mathbf{m}-1,\mathbf{n})$, contain components $j+1$ to **m** of v_j.

tau On successful exit, the scalar factors, τ_i, $i = 1, 2, \ldots, \min(\mathbf{m},\mathbf{n})$, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$.

info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
lda < max(1,**m**), and
lwork < max(1,**n**).

NAME

SGERQF/DGERQF/.../ZGERQF – *RQ* Factorization of General Matrix

Purpose

These subprograms compute the *RQ* factorization of a general *m*-by-*n* matrix *A*. The factorization has the form $A = RQ$, where *R* is an upper triangular matrix (upper trapezoidal if $m > n$) and *Q* is an orthogonal or unitary matrix. The computed matrix *Q* is represented as a product of elementary reflection matrices

$$Q = H_1 H_2 \ldots H_k$$

where $k = min(m,n)$. Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an *m*-dimensional vector whose $(n-k+i)$th component is 1 and whose last $k-i$ components are zero.

Additional subprograms are provided to make it easier to use the matrix *Q* in its factored form. The operations furnished are to multiply a general matrix by the *Q* matrix, and to generate (expand) the *Q* matrix into regular, unfactored form. The names of these companion subprograms depend on the data type:

Data Type	*RQ* Factorization	Generate *Q*	Multiply Matrix by *Q*
REAL*4	SGERQF	SORGRQ	SORMRQ
REAL*8	DGERQF	DORGRQ	DORMRQ
COMPLEX*8	CGERQF	CUNGRQ	CUNMRQ
COMPLEX*16	ZGERQF	ZUNGRQ	ZUNMRQ

Usage

LAPACK:

```
INTEGER*4          info, lda, lwork, m, n
REAL*4             a(lda, n), tau(min(m,n)), work(lwork)
CALL SGERQF(m, n, a, lda, tau, work, lwork, info)

INTEGER*4          info, lda, lwork, m, n
REAL*8             a(lda, n), tau(min(m,n)), work(lwork)
CALL DGERQF(m, n, a, lda, tau, work, lwork, info)

INTEGER*4          info, lda, lwork, m, n
COMPLEX*8          a(lda, n), tau(min(m,n)), work(lwork)
CALL CGERQF(m, n, a, lda, tau, work, lwork, info)
```

```
INTEGER*4          info, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(min(m,n)), work(lwork)
CALL ZGERQF(m, n, a, lda, tau, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, lda, lwork, m, n
REAL*8             a(lda, n), tau(min(m,n)), work(lwork)
CALL SGERQF(m, n, a, lda, tau, work, lwork, info)

INTEGER*8          info, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(min(m,n)), work(lwork)
CALL CGERQF(m, n, a, lda, tau, work, lwork, info)
```

Input

m The number of rows of the matrix A. **m** ≥ 0.

n The number of columns of the matrix A. **n** ≥ 0.

a The **m**-by-**n** matrix A to be factored.

lda The leading dimension of array **a** in the calling program unit. **lda** $\geq$ max(1,**m**).

lwork The length of array **work**. **lwork** $\geq$ max(1,**m**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the factors R and Q from the factorization $A = RQ$, stored as follows:

If **m** < **n**, the elements on and above the (**n**–**m**)-th superdiagonal of **a** contain the **m**-by-**m** upper triangular matrix R.

If **m** = **n**, the elements on and above the principal diagonal of **a** contain the **m**-by-**m** upper triangular matrix R.

If **m** > **n**, the elements on and above the (**m**–**n**)-th subdiagonal of **a** contain the **m**-by-**n** upper trapezoidal matrix R.

The remaining elements of **a** contain components of the v vectors:

If $\mathbf{m} \leq \mathbf{n}$, row i of **a**, $i = 1, 2, ..., \mathbf{m}$, contains components 1 to $\mathbf{n}-\mathbf{m}+i-1$ of v_i.

If $\mathbf{m} > \mathbf{n}$, row $\mathbf{m}-\mathbf{n}+i$ of **a**, $i = 2, 3, ..., \mathbf{n}$, contains components 1 to $i-1$ of v_i.

tau On successful exit, the scalar factors, τ_i, $i = 1, 2, ..., \min(\mathbf{m},\mathbf{n})$, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
lda < max(1,**m**), and
lwork < max(1,**m**).

NAME

SGGQRF/DGGQRF/CGGQRF/ZGGQRF – Generalized *QR* Factorization

Purpose

These subprograms compute the generalized *QR* (GQR) factorization of an *m*-by-*n* matrix *A* and an *m*-by-*p* matrix *B*. The factorization has the form

$$A = QR, \quad B = QTZ$$

where *Q* is an *m*-by-*m* orthogonal or unitary matrix, *Z* is a *p*-by-*p* orthogonal or unitary matrix, *R* assumes one of the forms:

$$\text{if } m \le n, \ R = [R_{11} \ \ R_{12}], \qquad \text{if } m > n, \ R = \begin{bmatrix} R_{11} \\ 0 \end{bmatrix},$$

where R_{11} is upper triangular, and *T* assumes one of the forms:

$$\text{if } m \le p, \ T = [0 \ \ T_{12}], \qquad \text{if } m > p, \ T = \begin{bmatrix} T_{11} \\ T_{21} \end{bmatrix},$$

where T_{12} or T_{21} is an upper triangular matrix.

If *B* is square and nonsingular, the GQR factorization of *A* and *B* implicitly gives the *QR* factorization of the matrix $B^{-1}A$:

$$B^{-1}A = Z^*(T^{-1}R).$$

The computed matrix *Q* is represented as a product of elementary reflection matrices

$$Q = H_1 H_2 \ldots H_k$$

where $k = min(m,n)$. Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an *m*-dimensional vector whose first $i-1$ components are zero and whose *i*th component is 1.

Z is represented as a product of elementary reflection matrices

$$Z = \overline{H}_1 \overline{H}_2 \ldots \overline{H}_{\bar{k}}$$

where $\bar{k} = min(m,p)$. Each $\overline{H}_i$ has the form

$$\overline{H}_i = I - \bar{\tau}_i \bar{v}_i \bar{v}_i^*$$

where $\bar{\tau}_i$ is a scalar and $\bar{v}_i$ is an m-dimensional vector whose $(p-\bar{k}+i)$th component is 1 and whose last $\bar{k}-i$ components are zero.

Additional subprograms are provided to make it easier to use Q and Z in their factored forms. The operations furnished are to multiply a general matrix by Q or Z, and to generate (expand) Q or Z into regular, unfactored form. The names of these companion subprograms depend on the data type:

Data Type	GQR Factorization	Generate		Multiply Matrix by	
		Q	*Z*	*Q*	*Z*
REAL*4	SGGQRF	SORGQR	SORGRQ	SORMQR	SORMRQ
REAL*8	DGGQRF	DORGQR	DORGRQ	DORMQR	DORMRQ
COMPLEX*8	CGGQRF	CUNGQR	CUNGRQ	CUNMQR	CUNMRQ
COMPLEX*16	ZGGQRF	ZUNGQR	ZUNGRQ	ZUNMQR	ZUNMRQ

Usage

LAPACK:

```
INTEGER*4          info, lda, ldb, lwork, m, n, p
REAL*4             a(lda, n), b(ldb, p), taua(min(m,n)), taub(min(m,p)),
                   work(lwork)
CALL SGGQRF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)

INTEGER*4          info, lda, ldb, lwork, m, n, p
REAL*8             a(lda, n), b(ldb, p), taua(min(m,n)), taub(min(m,p)),
                   work(lwork)
CALL DGGQRF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)

INTEGER*4          info, lda, ldb, lwork, m, n, p
COMPLEX*8          a(lda, n), b(ldb, p), taua(min(m,n)), taub(min(m,p)),
                   work(lwork)
CALL CGGQRF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)

INTEGER*4          info, lda, ldb, lwork, m, n, p
COMPLEX*16         a(lda, n), b(ldb, p), taua(min(m,n)), taub(min(m,p)),
                   work(lwork)
CALL ZGGQRF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, lda, ldb, lwork, m, n, p
REAL*8             a(lda, n), b(ldb, p), taua(min(m,n)), taub(min(m,p)),
                   work(lwork)
CALL SGGQRF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)
INTEGER*8          info, lda, ldb, lwork, m, n, p
COMPLEX*16         a(lda, n), b(ldb, p), taua(min(m,n)), taub(min(m,p)),
                   work(lwork)
CALL CGGQRF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)
```

Input

m The number of rows of the matrices A and B. **m** ≥ 0.

n The number of columns of the matrix A. **n** ≥ 0.

p The number of columns of the matrix B. **p** ≥ 0.

a The **m**-by-**n** matrix A.

lda The leading dimension of array **a** in the calling program unit. **lda** $\geq$ max(1,**m**).

b The **m**-by-**p** matrix B.

ldb The leading dimension of array **b** in the calling program unit. **ldb** $\geq$ max(1,**m**).

lwork The length of array **work**. **lwork** $\geq$ max(1,**m**,**n**,**p**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the factors Q and R from the factorization $A = QR$, stored as follows:

If **m** $\geq$ **n**, the elements on and above the principal diagonal of **a** contain the **n**-by-**n** upper triangular matrix R.

If **m** < **n**, the elements on and above the principal diagonal of **a** contain the **m**-by-**n** upper trapezoidal matrix R.

The elements below the principal diagonal of the jth column of **a**, $j = 1, 2, ...,$ min(**m**–1,**n**), contain components $j+1$ to **m** of v_j.

taua On successful exit, the scalar factors, τ_i, $i = 1, 2, ..., \min(\mathbf{m},\mathbf{n})$, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$.

b On successful exit, the factors T and Z from the factorization $B = QTZ$, stored as follows:

If $\mathbf{m} < \mathbf{p}$, the elements on and above the $(\mathbf{p}-\mathbf{m})$-th superdiagonal of **b** contain the **m**-by-**m** upper triangular matrix T.

If $\mathbf{m} = \mathbf{p}$, the elements on and above the principal diagonal of **b** contain the **m**-by-**m** upper triangular matrix T.

If $\mathbf{m} > \mathbf{p}$, the elements on and above the $(\mathbf{m}-\mathbf{p})$-th subdiagonal of **b** contain the **m**-by-**p** upper trapezoidal matrix R.

The remaining elements of **b** contain components of the $\bar{v}$ vectors:

If $\mathbf{m} \le \mathbf{p}$, row i of **b**, $i = 1, 2, ..., \mathbf{m}$, contains components 1 to $\mathbf{p}-\mathbf{m}+i-1$ of $\bar{v}_i$.

If $\mathbf{m} > \mathbf{p}$, row $\mathbf{m}-\mathbf{p}+i$ of **b**, $i = 2, 3, ..., \mathbf{p}$, contains components 1 to $i-1$ of $\bar{v}_i$.

taub On successful exit, the scalar factors, $\bar{\tau}_i$, $i = 1, 2, ...,$ $\min(\mathbf{m},\mathbf{p})$, of the elementary reflection matrices, $\bar{H}_i = I - \bar{\tau}_i \bar{v}_i \bar{v}_i^*$.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
p < 0,
lda < max(1,**m**),
ldb < max(1,**m**), and
lwork < max(1,**m**,**n**,**p**).

NAME

SGGRQF/DGGRQF/CGGRQF/ZGGRQF – Generalized RQ Factorization

Purpose

These subprograms compute the generalized RQ (GRQ) factorization of an m-by-p matrix A and an n-by-p matrix B. The factorization has the form

$$A = RQ, \quad B = ZTQ$$

where Q is an m-by-m orthogonal or unitary matrix, Z is a p-by-p orthogonal or unitary matrix, R assumes one of the forms:

$$\text{if } m \le p, \quad R = [0 \quad R_{12}], \qquad \text{if } m > p, \quad R = \begin{bmatrix} R_{11} \\ R_{21} \end{bmatrix},$$

where R_{12} or R_{21} is an upper triangular matrix, and T assumes one of the forms:

$$\text{if } n < p, \quad T = [T_{11} \quad T_{12}], \qquad \text{if } n \ge p, \quad T = \begin{bmatrix} T_{11} \\ 0 \end{bmatrix},$$

where T_{11} is upper triangular.

If B is square and nonsingular, the GRQ factorization of A and B implicitly gives the RQ factorization of the matrix AB^{-1}:

$$AB^{-1} = (RT^{-1})Z^*.$$

The computed matrix Q is represented as a product of elementary reflection matrices

$$Q = H_1 H_2 \ldots H_k$$

where $k = min(m,p)$. Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is a p-dimensional vector whose $(i-k+i)$th component is 1 and whose last $k-i$ components are zero.

Z is represented as a product of elementary reflection matrices

$$Z = \bar{H}_1 \bar{H}_2 \ldots \bar{H}_{\bar{k}}$$

where $\bar{k} = min(n,p)$. Each $\bar{H}_i$ has the form

$$\bar{H}_i = I - \bar{\tau}_i \bar{v}_i \bar{v}_i^*$$

where $\bar{\tau}_i$ is a scalar and $\bar{v}_i$ is an m-dimensional vector whose first $i-i$ components are zero and whose ith component is 1.

Additional subprograms are provided to make it easier to use Q and Z in their factored forms. The operations furnished are to multiply a general matrix by Q or Z, and to generate (expand) Q or Z into regular, unfactored form. The names of these companion subprograms depend on the data type:

Data Type	GRQ Factorization	Generate		Multiply Matrix by	
		Q	*Z*	*Q*	*Z*
REAL*4	SGGRQF	SORGRQ	SORGQR	SORMRQ	SORMQR
REAL*8	DGGRQF	DORGRQ	DORGQR	DORMRQ	DORMQR
COMPLEX*8	CGGRQF	CUNGRQ	CUNGQR	CUNMRQ	CUNMQR
COMPLEX*16	ZGGRQF	ZUNGRQ	ZUNGQR	ZUNMRQ	ZUNMQR

Usage

LAPACK:

```
INTEGER*4          info, lda, ldb, lwork, m, n, p
REAL*4             a(lda, p), b(ldb, p), taua(min(m,p)), taub(min(n,p)),
                   work(lwork)
CALL SGGRQF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)

INTEGER*4          info, lda, ldb, lwork, m, n, p
REAL*8             a(lda, p), b(ldb, p), taua(min(m,p)), taub(min(n,p)),
                   work(lwork)
CALL DGGRQF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)

INTEGER*4          info, lda, ldb, lwork, m, n, p
COMPLEX*8          a(lda, p), b(ldb, p), taua(min(m,p)), taub(min(n,p)),
                   work(lwork)
CALL CGGRQF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)

INTEGER*4          info, lda, ldb, lwork, m, n, p
COMPLEX*16         a(lda, p), b(ldb, p), taua(min(m,p)), taub(min(n,p)),
                   work(lwork)
CALL ZGGRQF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, lda, ldb, lwork, m, n, p
REAL*8             a(lda, p), b(ldb, p), taua(min(m,p)), taub(min(n,p)),
                   work(lwork)
CALL SGGRQF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)
INTEGER*8          info, lda, ldb, lwork, m, n, p
COMPLEX*16         a(lda, p), b(ldb, p), taua(min(m,p)), taub(min(n,p)),
                   work(lwork)
CALL CGGRQF(m, n, p, a, lda, taua, b, ldb, taub, work, lwork, info)
```

Input

m The number of rows of the matrix A. **m** ≥ 0.

n The number of rows of the matrix B. **n** ≥ 0.

p The number of columns of the matrices A and B. **p** ≥ 0.

a The **m**-by-**p** matrix A.

lda The leading dimension of array **a** in the calling program unit. **lda** $\geq$ max(1,**m**).

b The **n**-by-**p** matrix B.

ldb The leading dimension of array **b** in the calling program unit. **ldb** $\geq$ max(1,**n**).

lwork The length of array **work**. **lwork** $\geq$ max(1,**m**,**n**,**p**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the factors R and Q from the factorization $A = RQ$, stored as follows:

If **m** < **p**, the elements on and above the (**p**–**m**)-th superdiagonal of **a** contain the **m**-by-**m** upper triangular matrix R.

If **m** = **p**, the elements on and above the principal diagonal of **a** contain the **m**-by-**m** upper triangular matrix R.

If **m** > **p**, the elements on and above the (**m**–**p**)-th subdiagonal of **a** contain the **m**-by-**p** upper trapezoidal matrix R.

The remaining elements of **a** contain components of the v vectors:

If **m** ≤ **p**, row i of **a**, i = 1, 2, ..., **m**, contains components 1 to **p**–**m**+i-1 of v_i.

If **m** > **p**, row **m**–**p**+i of **a**, i = 2, 3, ..., **p**, contains components 1 to i–1 of v_i.

taua On successful exit, the scalar factors, τ_i, i = 1, 2, ..., min(**m**,**p**), of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$.

b On successful exit, the factors T and Z from the factorization $B = ZTQ$, stored as follows:

If **n** ≥ **p**, the elements on and above the principal diagonal of **b** contain the **p**-by-**p** upper triangular matrix T.

If **n** < **p**, the elements on and above the principal diagonal of **b** contain the **n**-by-**p** upper trapezoidal matrix T.

The elements below the principal diagonal of the jth column of **b**, j = 1, 2, ..., min(**n**–1,**p**), contain components j+1 to **n** of $\bar{v}_j$.

taub On successful exit, the scalar factors, $\bar{\tau}_i$, i = 1, 2, ..., min(**n**,**p**), of the elementary reflection matrices, $\bar{H}_i = I - \bar{\tau}_i \bar{v}_i \bar{v}_i^*$.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = –k, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
p < 0,
lda < max(1,**m**),
ldb < max(1,**n**), and
lwork < max(1,**m**,**n**,**p**).

NAME

SORGLQ/.../ZUNGLQ – Generate Unfactored Q from an LQ Factorization

Purpose

Given an orthogonal or unitary matrix represented as a product of elementary reflection matrices

$$Q = H_k H_{k-1} \ldots H_1$$

as computed by _GELQF, these subprograms generate (expand) the matrix Q into regular, unfactored form.

Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an m-dimensional vector whose first $i-1$ components are zero and whose ith component is 1.

The unfactored form of Q overwrites the input factored form of Q.

Usage

LAPACK:

```
INTEGER*4          info, k, lda, lwork, m, n
REAL*4             a(lda, n), tau(k), work(lwork)
CALL SORGLQ(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
REAL*8             a(lda, n), tau(k), work(lwork)
CALL DORGLQ(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
COMPLEX*8          a(lda, n), tau(k), work(lwork)
CALL CUNGLQ(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(k), work(lwork)
CALL ZUNGLQ(m, n, k, a, lda, tau, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, k, lda, lwork, m, n
REAL*8             a(lda, n), tau(k), work(lwork)
CALL SORGLQ(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*8          info, k, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(k), work(lwork)
CALL CUNGLQ(m, n, k, a, lda, tau, work, lwork, info)
```

Input

m The number of rows of the matrix Q. **m** ≥ 0.

n The number of columns of the matrix Q. **n** ≥ **m**.

k The number of elementary reflection matrices whose product defines the matrix Q. **k** ≥ 0 and **k** ≤ **m**.

a The matrix Q, represented as a product of **k** elementary reflection matrices, as computed by _GELQF.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**m**).

tau The scalar factors, τ_i, i = 1, 2, ..., **k**, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$, as computed by _GELQF.

lwork The length of array **work**. **lwork** ≥ max(1,**m**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the input is overwritten by the **m**-by-**n** matrix Q, in unfactored form.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < **m**,
k < 0,
k > **m**,
lda < max(1,**m**), and
lwork < max(1,**m**).

NAME

SORGQL/.../ZUNGQL – Generate Unfactored Q from a QL Factorization

Purpose

Given an orthogonal or unitary matrix represented as a product of elementary reflection matrices

$$Q = H_k H_{k-1} \ldots H_1$$

as computed by _GEQLF, these subprograms generate (expand) the matrix Q into regular, unfactored form.

Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an m-dimensional vector whose first i–1 components are zero and whose ith component is 1.

The unfactored form of Q overwrites the input factored form of Q.

Usage

LAPACK:

```
INTEGER*4          info, k, lda, lwork, m, n
REAL*4             a(lda, n), tau(k), work(lwork)
CALL SORGQL(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
REAL*8             a(lda, n), tau(k), work(lwork)
CALL DORGQL(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
COMPLEX*8          a(lda, n), tau(k), work(lwork)
CALL CUNGQL(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(k), work(lwork)
CALL ZUNGQL(m, n, k, a, lda, tau, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, k, lda, lwork, m, n
REAL*8             a(lda, n), tau(k), work(lwork)
CALL SORGQL(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*8          info, k, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(k), work(lwork)
CALL CUNGQL(m, n, k, a, lda, tau, work, lwork, info)
```

Input

m	The number of rows of the matrix Q. **m** ≥ 0.
n	The number of columns of the matrix Q. **n** ≥ 0 and **n** $\leq$ **m**.
k	The number of elementary reflection matrices whose product defines the matrix Q. **k** ≥ 0 and **k** $\leq$ **n**.
a	The matrix Q, represented as a product of **k** elementary reflection matrices, as computed by _GEQLF.
lda	The leading dimension of array **a** in the calling program unit. **lda** $\geq$ max(1,**m**).
tau	The scalar factors, τ_i, i = 1, 2, ..., **k**, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$, as computed by _GEQLF.
lwork	The length of array **work**. **lwork** $\geq$ max(1,**n**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work	An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a	On successful exit, the input is overwritten by the **m**-by-**n** matrix Q, in unfactored form.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
n > **m**,
k < 0,
k > **n**,
lda < max(1,**m**), and
lwork < max(1,**n**).

NAME

SORGQR/.../ZUNGQR – Generate Unfactored Q from a QR Factorization

Purpose

Given an orthogonal or unitary matrix represented as a product of elementary reflection matrices

$$Q = H_1 H_2 \ldots H_k$$

as computed by _GEQRF, _GGQRF, or _GGRQF, these subprograms generate (expand) the matrix Q into regular, unfactored form.

Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an m-dimensional vector whose first i–1 components are zero and whose ith component is 1.

The unfactored form of Q overwrites the input factored form of Q.

Usage

LAPACK:

```
INTEGER*4          info, k, lda, lwork, m, n
REAL*4             a(lda, k), tau(k), work(lwork)
CALL SORGQR(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
REAL*8             a(lda, k), tau(k), work(lwork)
CALL DORGQR(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
COMPLEX*8          a(lda, k), tau(k), work(lwork)
CALL CUNGQR(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
COMPLEX*16         a(lda, k), tau(k), work(lwork)
CALL ZUNGQR(m, n, k, a, lda, tau, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, k, lda, lwork, m, n
REAL*8             a(lda, k), tau(k), work(lwork)
CALL SORGQR(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*8          info, k, lda, lwork, m, n
COMPLEX*16         a(lda, k), tau(k), work(lwork)
CALL CUNGQR(m, n, k, a, lda, tau, work, lwork, info)
```

Input

m The number of rows of the matrix Q. $\mathbf{m} \geq 0$.

n The number of columns of the matrix Q. $\mathbf{n} \geq 0$ and $\mathbf{n} \leq \mathbf{m}$.

k The number of elementary reflection matrices whose product defines the matrix Q. $\mathbf{k} \geq 0$ and $\mathbf{k} \leq \mathbf{n}$.

a The matrix Q, represented as a product of **k** elementary reflection matrices, as computed by _GEQRF, _GGQRF, or _GGRQF.

lda The leading dimension of array **a** in the calling program unit. $\mathbf{lda} \geq \max(1,\mathbf{m})$.

tau The scalar factors, τ_i, $i = 1, 2, ..., \mathbf{k}$, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$, as computed by _GEQRF, _GGQRF, or _GGRQF.

lwork The length of array **work**. $\mathbf{lwork} \geq \max(1,\mathbf{n})$. For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the input is overwritten by the **m**-by-**n** matrix Q, in unfactored form.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < 0,
n > **m**,
k < 0,
k > **n**,
lda < max(1,**m**), and
lwork < max(1,**n**).

NAME

SORGRQ/.../ZUNGRQ – Generate Unfactored Q from an RQ Factorization

Purpose

Given an orthogonal or unitary matrix represented as a product of elementary reflection matrices

$$Q = H_1 H_2 \ldots H_k$$

as computed by _GERQF, _GGQRF, or _GGRQF, these subprograms generate (expand) the matrix Q into regular, unfactored form.

Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an m-dimensional vector whose first i–1 components are zero and whose ith component is 1.

The unfactored form of Q overwrites the input factored form of Q.

Usage

LAPACK:

```
INTEGER*4          info, k, lda, lwork, m, n
REAL*4             a(lda, n), tau(k), work(lwork)
CALL SORGRQ(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
REAL*8             a(lda, n), tau(k), work(lwork)
CALL DORGRQ(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
COMPLEX*8          a(lda, n), tau(k), work(lwork)
CALL CUNGRQ(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*4          info, k, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(k), work(lwork)
CALL ZUNGRQ(m, n, k, a, lda, tau, work, lwork, info)
```

LAPACK8:

```
INTEGER*8          info, k, lda, lwork, m, n
REAL*8             a(lda, n), tau(k), work(lwork)
CALL SORGRQ(m, n, k, a, lda, tau, work, lwork, info)

INTEGER*8          info, k, lda, lwork, m, n
COMPLEX*16         a(lda, n), tau(k), work(lwork)
CALL CUNGRQ(m, n, k, a, lda, tau, work, lwork, info)
```

Input

m	The number of rows of the matrix Q. **m** ≥ 0.
n	The number of columns of the matrix Q. **n** ≥ **m**.
k	The number of elementary reflection matrices whose product defines the matrix Q. **k** ≥ 0 and **k** ≤ **m**.
a	The matrix Q, represented as a product of **k** elementary reflection matrices, as computed by _GERQF, _GGQRF, or _GGRQF.
lda	The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**m**).
tau	The scalar factors, τ_i, i = 1, 2, ..., **k**, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$, as computed by _GERQF, _GGQRF, or _GGRQF.
lwork	The length of array **work**. **lwork** ≥ max(1,**m**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work	An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a	On successful exit, the input is overwritten by the **m**-by-**n** matrix Q, in unfactored form.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n < **m**,
k < 0,
k > **m**,
lda < max(1,**m**), and
lwork < max(1,**m**).

NAME

SORMLQ/.../ZUNMLQ – Multiply Matrix by Q from an LQ Factorization

Purpose

Given an m-by-n matrix C, these subprograms compute one of the matrix products QC, Q^*C, CQ, or CQ^*, where Q is an orthogonal or unitary matrix computed by _GELQF, and Q^* is the conjugate transpose of Q (ordinary transpose if the matrices are real). The matrix product overwrites the input C matrix.

The matrix Q is represented as a product of elementary reflection matrices

$$Q = H_k H_{k-1} \ldots H_1.$$

Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an m-dimensional vector if QC or Q^*C is requested, or an n-dimensional vector if CQ or CQ^* is requested. The first $i-1$ components of v_i are zero and the ith component is 1.

Usage

LAPACK:

```
CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
REAL*4          a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL SORMLQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
REAL*8          a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL DORMLQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
COMPLEX*8       a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL CUNMLQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
COMPLEX*16      a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL ZUNMLQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

LAPACK8:

```
CHARACTER*1     side, trans
INTEGER*8       info, k, lda, ldc, lwork, m, n
REAL*8          a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL SORMLQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

```
CHARACTER*1     side, trans
INTEGER*8       info, k, lda, ldc, lwork, m, n
COMPLEX*16      a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL CUNMLQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

Input

side Specifies whether orthogonal or unitary matrix Q is the left or right matrix operand:

side = 'L' or 'l'	Q is the left matrix operand.
side = 'R' or 'r'	Q is the right matrix operand.

trans Transposition option for Q:

trans = 'N' or 'n'	Use matrix Q directly
trans = 'T' or 't'	Use Q^T, the transpose of Q
trans = 'C' or 'c'	Use Q*, the conjugate transpose of Q

In SORMLQ and DORMLQ, only 'N' and 'n' and 'T' and 't' are valid.

In CUNMLQ and ZUNMLQ, only 'N' and 'n' and 'C' and 'c' are valid.

m The number of rows of the matrix C. **m** ≥ 0.

n The number of columns of the matrix C. **n** ≥ 0.

k The number of elementary reflection matrices whose product defines the matrix Q. **k** ≥ 0. If **side** = 'L' or 'l', **k** ≤ **m**. If **side** = 'R' or 'r', **k** ≤ **n**.

a The orthogonal or unitary matrix Q, represented as a product of elementary reflection matrices as computed by _GELQF. If **side** = 'L' or 'l', Q is an **m**-by-**m** matrix. If **side** = 'R' or 'r', Q is an **n**-by-**n** matrix. **a** is modified by the subprogram but is restored to its input value on exit.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**k**).

tau The scalar factors, τ_i, i = 1, 2, ..., **k**, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i$*, as computed by _GELQF.

c The **m**-by-**n** input matrix C.

ldc The leading dimension of array **c** in the calling program unit. **ldc** ≥ max(1,**m**).

lwork The length of array **work**. If **side** = 'L' or 'l', **lwork** ≥ max(1,**n**). If **side** = 'R' or 'r', **lwork** ≥ max(1,**m**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

c On successful exit, the input is overwritten by the requested matrix product.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

side ≠ 'L' or 'l' or 'R' or 'r',
trans invalid,
m < 0,
n < 0,
k < 0,
k too large,
lda < max(1,**k**),
ldc < max(1,**m**), and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **side** argument as 'Left' for 'L' or 'Right' for 'R'.

NAME

SORMQL/.../ZUNMQL – Multiply Matrix by Q from a QL Factorization

Purpose

Given an m-by-n matrix C, these subprograms compute one of the matrix products QC, Q^*C, CQ, or CQ^*, where Q is an orthogonal or unitary matrix computed by _GEQLF, and Q^* is the conjugate transpose of Q (ordinary transpose if the matrices are real). The matrix product overwrites the input C matrix.

The matrix Q is represented as a product of elementary reflection matrices

$$Q = H_k H_{k-1} \ldots H_1.$$

Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an m-dimensional vector whose first i–1 components are zero and whose ith component is 1.

Usage

LAPACK:

```
CHARACTER*1      side, trans
INTEGER*4        info, k, lda, ldc, lwork, m, n
REAL*4           a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL SORMQL(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1      side, trans
INTEGER*4        info, k, lda, ldc, lwork, m, n
REAL*8           a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL DORMQL(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1      side, trans
INTEGER*4        info, k, lda, ldc, lwork, m, n
COMPLEX*8        a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL CUNMQL(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1      side, trans
INTEGER*4        info, k, lda, ldc, lwork, m, n
COMPLEX*16       a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL ZUNMQL(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

LAPACK8:

```
CHARACTER*1      side, trans
INTEGER*8        info, k, lda, ldc, lwork, m, n
REAL*8           a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL SORMQL(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

```
CHARACTER*1     side, trans
INTEGER*8       info, k, lda, ldc, lwork, m, n
COMPLEX*16      a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL CUNMQL(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

Input

side Specifies whether orthogonal or unitary matrix Q is the left or right matrix operand:

side = 'L' or 'l'	Q is the left matrix operand.
side = 'R' or 'r'	Q is the right matrix operand.

trans Transposition option for Q:

trans = 'N' or 'n'	Use matrix Q directly
trans = 'T' or 't'	Use Q^T, the transpose of Q
trans = 'C' or 'c'	Use Q*, the conjugate transpose of Q

In SORMQL and DORMQL, only 'N' and 'n' and 'T' and 't' are valid.

In CUNMQL and ZUNMQL, only 'N' and 'n' and 'C' and 'c' are valid.

m The number of rows of the matrix C. **m** ≥ 0.

n The number of columns of the matrix C. **n** ≥ 0.

k The number of elementary reflection matrices whose product defines the matrix Q. **k** ≥ 0. If **side** = 'L' or 'l', **k** ≤ **m**. If **side** = 'R' or 'r', **k** ≤ **n**.

a The orthogonal or unitary matrix Q, represented as a product of elementary reflection matrices as computed by _GEQLF. If **side** = 'L' or 'l', Q is an **m**-by-**m** matrix. If **side** = 'R' or 'r', Q is an **n**-by-**n** matrix. **a** is modified by the subprogram but is restored to its input value on exit.

lda The leading dimension of array **a** in the calling program unit. If **side** = 'L' or 'l', **lda** ≥ max(1,**m**). If **side** = 'R' or 'r', **lda** ≥ max(1,**n**).

tau The scalar factors, τ_i, i = 1, 2, ..., **k**, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i$*, as computed by _GEQLF.

c The **m**-by-**n** input matrix C.

ldc The leading dimension of array **c** in the calling program unit. **ldc** ≥ max(1,**m**).

lwork The length of array **work**. If **side** = 'L' or 'l', **lwork** ≥ max(1,**n**). If **side** = 'R' or 'r', **lwork** ≥ max(1,**m**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

c On successful exit, the input is overwritten by the requested matrix product.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

side ≠ 'L' or 'l' or 'R' or 'r',
trans invalid,
m < 0,
n < 0,
k < 0,
k too large,
lda too small,
ldc < max(1,**m**), and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **side** argument as 'Left' for 'L' or 'Right' for 'R'.

NAME

SORMQR/.../ZUNMQR – Multiply Matrix by Q from a QR Factorization

Purpose

Given an m-by-n matrix C, these subprograms compute one of the matrix products QC, Q^*C, CQ, or CQ^*, where Q is an orthogonal or unitary matrix computed by _GEQRF, _GGQRF, or _GGRQF, and Q^* is the conjugate transpose of Q (ordinary transpose if the matrices are real). The matrix product overwrites the input C matrix.

The matrix Q is represented as a product of elementary reflection matrices

$$Q = H_1 H_2 \ldots H_k.$$

Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an m-dimensional vector whose first i–1 components are zero and whose ith component is 1.

Usage

LAPACK:

```
CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
REAL*4          a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL SORMQR(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
REAL*8          a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL DORMQR(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
COMPLEX*8       a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL CUNMQR(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
COMPLEX*16      a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL ZUNMQR(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

LAPACK8:

```
CHARACTER*1     side, trans
INTEGER*8       info, k, lda, ldc, lwork, m, n
REAL*8          a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL SORMQR(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

```
CHARACTER*1     side, trans
INTEGER*8       info, k, lda, ldc, lwork, m, n
COMPLEX*16      a(lda, k), c(ldc, n), tau(k), work(lwork)
CALL CUNMQR(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

Input

side Specifies whether orthogonal or unitary matrix Q is the left or right matrix operand:

side = 'L' or 'l'	Q is the left matrix operand.
side = 'R' or 'r'	Q is the right matrix operand.

trans Transposition option for Q:

trans = 'N' or 'n'	Use matrix Q directly
trans = 'T' or 't'	Use Q^T, the transpose of Q
trans = 'C' or 'c'	Use Q^*, the conjugate transpose of Q

In SORMQR and DORMQR, only 'N' and 'n' and 'T' and 't' are valid.

In CUNMQR and ZUNMQR, only 'N' and 'n' and 'C' and 'c' are valid.

m The number of rows of the matrix C. **m** ≥ 0.

n The number of columns of the matrix C. **n** ≥ 0.

k The number of elementary reflection matrices whose product defines the matrix Q. **k** ≥ 0. If **side** = 'L' or 'l', **k** ≤ **m**. If **side** = 'R' or 'r', **k** ≤ **n**.

a The orthogonal or unitary matrix Q, represented as a product of elementary reflection matrices as computed by _GEQRF, _GGQRF, or _GGRQF. If **side** = 'L' or 'l', Q is an **m**-by-**m** matrix. If **side** = 'R' or 'r', Q is an **n**-by-**n** matrix. **a** is modified by the subprogram but is restored to its input value on exit.

lda The leading dimension of array **a** in the calling program unit. If **side** = 'L' or 'l', **lda** ≥ max(1,**m**). If **side** = 'R' or 'r', **lda** ≥ max(1,**n**).

tau The scalar factors, τ_i, i = 1, 2, ..., **k**, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$, as computed by _GEQRF, _GGQRF, or _GGRQF.

c The **m**-by-**n** input matrix C.

ldc The leading dimension of array **c** in the calling program unit. **ldc** ≥ max(1,**m**).

lwork The length of array **work**. If **side** = 'L' or 'l', **lwork** ≥ max(1,**n**). If **side** = 'R' or 'r', **lwork** ≥ max(1,**m**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

c On successful exit, the input is overwritten by the requested matrix product.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

side ≠ 'L' or 'l' or 'R' or 'r',
trans invalid,
m < 0,
n < 0,
k < 0,
k too large,
lda too small,
ldc < max(1,**m**), and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **side** argument as 'Left' for 'L' or 'Right' for 'R'.

NAME

SORMRQ/.../ZUNMRQ – Multiply Matrix by Q from an RQ Factorization

Purpose

Given an m-by-n matrix C, these subprograms compute one of the matrix products QC, Q^*C, CQ, or CQ^*, where Q is an orthogonal or unitary matrix computed by _GERQF, _GGQRF, or _GGRQF, and Q^* is the conjugate transpose of Q (ordinary transpose if the matrices are real). The matrix product overwrites the input C matrix.

The matrix Q is represented as a product of elementary reflection matrices

$$Q = H_1 H_2 \ldots H_k.$$

Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an m-dimensional vector if QC or Q^*C is requested, or an n-dimensional vector if CQ or CQ^* is requested. The first i–1 components of v_i are zero and the ith component is 1.

Usage

LAPACK:

```
CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
REAL*4          a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL SORMRQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
REAL*8          a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL DORMRQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
COMPLEX*8       a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL CUNMRQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)

CHARACTER*1     side, trans
INTEGER*4       info, k, lda, ldc, lwork, m, n
COMPLEX*16      a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL ZUNMRQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

LAPACK8:

```
CHARACTER*1     side, trans
INTEGER*8       info, k, lda, ldc, lwork, m, n
REAL*8          a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL SORMRQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

```
CHARACTER*1     side, trans
INTEGER*8       info, k, lda, ldc, lwork, m, n
COMPLEX*16      a(lda, *), c(ldc, n), tau(k), work(lwork)
CALL CUNMRQ(side, trans, m, n, k, a, lda, tau, c, ldc, work, lwork, info)
```

Input

side Specifies whether orthogonal or unitary matrix Q is the left or right matrix operand:

side = 'L' or 'l'	Q is the left matrix operand.
side = 'R' or 'r'	Q is the right matrix operand.

trans Transposition option for Q:

trans = 'N' or 'n'	Use matrix Q directly
trans = 'T' or 't'	Use Q^T, the transpose of Q
trans = 'C' or 'c'	Use Q*, the conjugate transpose of Q

In SORMRQ and DORMRQ, only 'N' and 'n' and 'T' and 't' are valid.

In CUNMRQ and ZUNMRQ, only 'N' and 'n' and 'C' and 'c' are valid.

m The number of rows of the matrix C. **m** ≥ 0.

n The number of columns of the matrix C. **n** ≥ 0.

k The number of elementary reflection matrices whose product defines the matrix Q. **k** ≥ 0. If **side** = 'L' or 'l', **k** ≤ **m**. If **side** = 'R' or 'r', **k** ≤ **n**.

a The orthogonal or unitary matrix Q, represented as a product of elementary reflection matrices as computed by _GERQF, _GGQRF, or _GGRQF. If **side** = 'L' or 'l', Q is an **m**-by-**m** matrix. If **side** = 'R' or 'r', Q is an **n**-by-**n** matrix. **a** is modified by the subprogram but is restored to its input value on exit.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**k**).

tau The scalar factors, τ_i, i = 1, 2, ..., **k**, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i$*, as computed by _GERQF, _GGQRF, or _GGRQF.

c The **m**-by-**n** input matrix C.

ldc The leading dimension of array **c** in the calling program unit. **ldc** ≥ max(1,**m**).

lwork The length of array **work**. If **side** = 'L' or 'l', **lwork** ≥ max(1,**n**). If **side** = 'R' or 'r', **lwork** ≥ max(1,**m**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

c On successful exit, the input is overwritten by the requested matrix product.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

side ≠ 'L' or 'l' or 'R' or 'r',
trans invalid,
m < 0,
n < 0,
k < 0,
k too large,
lda < max(1,**k**),
ldc < max(1,**m**), and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **side** argument as 'Left' for 'L' or 'Right' for 'R'.

NAME

STZRQF/.../ZTZRQF – *RQ* Factorization of Upper Trapezoidal Matrix

Purpose

Given an m-by-n matrix A of the form $A = [U \quad X]$, where $m \leq n$, U is an m-by-m upper triangular matrix, and $X$is an m-by-$(n-m)$ general matrix, these subprograms compute the RQ factorization of A.

The factorization has the form $A = [R \quad 0]\, Q$, where R is an m-by-m upper triangular matrix, 0 is an m-by-$(n-m)$ zero matrix, and Q is an n-by-n orthogonal or unitary matrix. The computed matrix Q is represented as a product of elementary reflection matrices

$$Q = H_m H_{m-1} \ldots H_1$$

Each H_i has the form

$$H_i = I - \tau_i v_i v_i^*$$

where τ_i is a scalar and v_i is an n-dimensional vector all of whose components are zero except the ith, which is 1, and the last $n-m$ components, which are computed.

Usage

LAPACK:

```
INTEGER*4          info, lda, m, n
REAL*4             a(lda, n), tau(m)
CALL STZRQF(m, n, a, lda, tau, info)

INTEGER*4          info, lda, m, n
REAL*8             a(lda, n), tau(m)
CALL DTZRQF(m, n, a, lda, tau, info)

INTEGER*4          info, lda, m, n
COMPLEX*8          a(lda, n), tau(m)
CALL CTZRQF(m, n, a, lda, tau, info)

INTEGER*4          info, lda, m, n
COMPLEX*16         a(lda, n), tau(m)
CALL ZTZRQF(m, n, a, lda, tau, info)
```

LAPACK8:

```
INTEGER*8          info, lda, m, n
REAL*8             a(lda, n), tau(m)
CALL STZRQF(m, n, a, lda, tau, info)

INTEGER*8          info, lda, m, n
COMPLEX*16         a(lda, n), tau(m)
CALL CTZRQF(m, n, a, lda, tau, info)
```

Input

m	The number of rows of the matrix A. **m** ≥ 0.
n	The number of columns of the matrix A. **n** $\geq$ **m**.
a	The **m**-by-**n** upper trapezoidal matrix A to be factored. The strictly lower triangular part of **a** is not used as input.
lda	The leading dimension of array **a** in the calling program unit. **lda** $\geq$ max(1,**m**).

Output

a	On successful exit, the factors R and Q from the factorization $A = [R \quad 0]\, Q$, stored as follows: The **m**-by-**m** upper triangular part of **a** contains the upper triangular matrix R. Columns **m**+1 to **n** of row i, $i = 1, 2, ..., \mathbf{m}$, of **a** contain components **m**+1 to **n** of v_i.
tau	On successful exit, the scalar factors, τ_i, $i = 1, 2, ..., \mathbf{m}$, of the elementary reflection matrices, $H_i = I - \tau_i v_i v_i^*$.
info	Status response: **info** = 0: Successful exit. **info** < 0: If **info** = $-k$, the k-th argument had an invalid value.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

m < 0,
n <**M** 0, and
lda < max(1,**m**).

7 Simple Drivers for Ordinary Eigenvalue Problems

Overview

This chapter explains how to use LAPACK simple drivers to compute the Schur form, Schur vectors, eigenvalues, or eigenvalues and eigenvectors of matrices. The operations covered are:

- General dense eigenproblems, $Ax = \lambda x$, for arbitrary A
- Symmetric and Hermitian dense eigenproblems, $Ax = \lambda x$
- Symmetric and Hermitian banded eigenproblems, $Ax = \lambda x$
- Symmetric tridiagonal eigenproblems, $Ax = \lambda x$

Chapter 8 describes the LAPACK expert drivers for ordinary eigenvalue problems. Refer to Chapter 9 for software to compute the eigenvalues or eigenvalues and eigenvectors of generalized eigenproblems.

Refer to Chapter 7 of the *HP MLIB VECLIB User's Guide* for software to compute the eigenvalues or eigenvalues and eigenvectors of a real symmetric, sparse, ordinary or generalized eigenproblem.

The following documents provide supplemental material for this chapter:

- Golub, G.H. and C.F. Van Loan. *Matrix Computations*, 2nd Edition. Baltimore, MD: The Johns Hopkins University Press. 1989.
- Parlett, B.N. *The Symmetric Eigenproblem*. Englewood Cliffs, NJ: Prentice-Hall, Inc. 1980.
- Wilkinson, J.H. *The Algebraic Eigenproblem*. New York, NY: Oxford University Press. 1965.

Chapter Objectives

After reading this chapter you will know how to use the described subprograms.

What You Need to Know to Use These Subprograms

To use these subprograms, it is helpful to know some basic theory of eigensystems and the Schur Form, especially as they relate to your particular application. A few facts discussed in basic textbooks are given here.

If A is an n-by-n matrix, $det(\lambda I - A)$ is an n-th degree polynomial in λ, called the *characteristic polynomial*. This equation has n zeros, counting algebraic multiplicity, although some or all of them may be complex (with nonzero imaginary part) even if A is real. If λ is one of these zeros, there exists a nonzero vector x such that $Ax = \lambda x$. λ is called an *eigenvalue* of A, and x is called an *eigenvector* belonging to λ.

Alternatively, the definitions can be made without resorting to the characteristic polynomial, as follows: if λ is a scalar for which there exists a nonzero vector x such that $Ax = \lambda x$, then λ is called an *eigenvalue* of A, and x is called an *eigenvector* belonging to λ.

If A is a real symmetric or complex Hermitian matrix, the eigenvalues of A are real, and there exists a complete orthonormal set of eigenvectors, that is, appropriately chosen and scaled eigenvectors form an orthogonal unit-vector basis for n-dimensional Euclidean space. In the real nonsymmetric case, any non-real eigenvalues occur in complex conjugate pairs. In the nonsymmetric, non-Hermitian case, n linearly independent eigenvectors may or may not exist.

When a complete set of eigenvectors does exist, say, the columns of the n-by-n matrix X, then $AX = X\Lambda$, where Λ is the diagonal matrix of eigenvalues of A. X is invertible since its columns are linearly independent. It follows that $X^{-1}AX = \Lambda$, so X is said to *diagonalize* A. In the real symmetric case, X can be made orthogonal, while if A is a complex Hermitian matrix, X can be made unitary.

Even when a complete set of eigenvectors does not exist, a basic theorem due to Schur states that any matrix is unitarily similar to a triangular matrix; that is, there exists a unitary matrix Q and an upper triangular matrix R such that $Q^*AQ = R$. Such an R is called the Schur Form of A, and the columns of Q are called the Schur vectors. Even if A is a real matrix, Q and R may be complex. However, real matrices Q and R do exist, with Q orthogonal and R block-triangular with 1-by-1 and 2-by-2 diagonal blocks, such that $Q^TAQ = R$. It is common to call the block upper triangular R matrix the Schur Form and the real vectors that are the columns of the Q matrix the Schur vectors.

NAME

SGEES/DGEES/CGEES/ZGEES – Schur Form of a General Matrix

Purpose

These subprograms compute the eigenvalues and the Schur Form of an n-by-n general matrix A, and optionally compute the Schur vectors of A and order the eigenvalues on the diagonal of the Schur Form so that selected eigenvalues are at the upper left.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

A real matrix is in Schur Form if it is block upper triangular with 1-by-1 and 2-by-2 diagonal blocks. 1-by-1 blocks correspond to real eigenvalues, and 2-by-2 blocks correspond to complex conjugate eigenpairs. 2-by-2 blocks are standardized in the form

$$\begin{bmatrix} a & b \\ c & a \end{bmatrix}$$

where $bc < 0$. The eigenvalues of such a block are $a \pm i\sqrt{|bc|}$.

A complex matrix is in Schur Form if it upper triangular.

If T is the Schur Form of A, then the columns of unitary matrix Q such that

$$A = QTQ^*$$

are known as the Schur vectors of A.

Usage

LAPACK:

CHARACTER*1	**jobvs, sort**
INTEGER*4	**info, lda, ldvs, lwork, n, sdim**
LOGICAL*4	**bwork(n)**
REAL*4	**a(lda, n), vs(ldvs, n), wi(n), work(lwork), wr(n)**
LOGICAL*4	**select**
EXTERNAL	**select**

CALL SGEES(jobvs, sort, select, n, a, lda, sdim, wr, wi, vs, ldvs, work, lwork, bwork, info)

```
CHARACTER*1     jobvs, sort
INTEGER*4       info, lda, ldvs, lwork, n, sdim
LOGICAL*4       bwork(n)
REAL*8          a(lda, n), vs(ldvs, n), wi(n), work(lwork), wr(n)
LOGICAL*4       select
EXTERNAL        select
CALL DGEES(jobvs, sort, select, n, a, lda, sdim, wr, wi, vs, ldvs, work,
  lwork, bwork, info)
```

```
CHARACTER*1     jobvs, sort
INTEGER*4       info, lda, ldvs, lwork, n, sdim
LOGICAL*4       bwork(n)
REAL*4          rwork(n)
COMPLEX*8       a(lda, n), vs(ldvs, n), w(n), work(lwork)
LOGICAL*4       select
EXTERNAL        select
CALL CGEES(jobvs, sort, select, n, a, lda, sdim, w, vs, ldvs, work, lwork,
  rwork, bwork, info)
```

```
CHARACTER*1     jobvs, sort
INTEGER*4       info, lda, ldvs, lwork, n, sdim
LOGICAL*4       bwork(n)
REAL*8          rwork(n)
COMPLEX*16      a(lda, n), vs(ldvs, n), w(n), work(lwork)
LOGICAL*4       select
EXTERNAL        select
CALL ZGEES(jobvs, sort, select, n, a, lda, sdim, w, vs, ldvs, work, lwork,
  rwork, bwork, info)
```

LAPACK8:

```
CHARACTER*1     jobvs, sort
INTEGER*8       info, lda, ldvs, lwork, n, sdim
LOGICAL*8       bwork(n)
REAL*8          a(lda, n), vs(ldvs, n), wi(n), work(lwork), wr(n)
LOGICAL*8       select
EXTERNAL        select
CALL SGEES(jobvs, sort, select, n, a, lda, sdim, wr, wi, vs, ldvs, work,
  lwork, bwork, info)
```

```
CHARACTER*1     jobvs, sort
INTEGER*8       info, lda, ldvs, lwork, n, sdim
LOGICAL*8       bwork(n)
REAL*8          rwork(n)
COMPLEX*16      a(lda, n), vs(ldvs, n), w(n), work(lwork)
LOGICAL*8       select
EXTERNAL        select
CALL CGEES(jobvs, sort, select, n, a, lda, sdim, w, vs, ldvs, work, lwork,
  rwork, bwork, info)
```

Input

jobvs Specifies whether the Schur vectors are to be computed, as follows:

- **jobvs** = 'N' or 'n': Schur vectors are not computed.
- **jobvs** = 'V' or 'v': Schur vectors are computed.

sort Specifies whether the eigenvalues on the diagonal of the Schur Form are to be reordered, as follows:

- **sort** = 'N' or 'n': The eigenvalues are not specially ordered.
- **sort** = 'S' or 's': The eigenvalues are ordered so that the eigenvalues λ_j for which the LOGICAL function **select**(**wr**(j),**wi**(j)) (in SGEES and DGEES) or **select**(**w**(j)) (in CGEES and ZGEES) is true will appear at the top left corner of the Schur Form. (In SGEES and DGEES, if an eigenvalue is complex and either **select**(**wr**(j),**wi**(j)) or **select**(**wr**(j),–**wi**(j)) is true, both eigenvalues are selected.)

select The name of a user-defined function subprogram used if **sort** = 'S' or 's' to select eigenvalues to reorder to the upper left of the Schur Form. For SGEES and DGEES, **select** requires two arguments of the same type as **wr** and **wi**, while for CGEES and ZGEES, **select** requires one argument of the same type as **w**. The eigenvalue λ_j is selected if **select**(**wr**(j),**wi**(j)) or **select**(**w**(j)) is true. Note that a selected complex eigenvalue may no longer satisfy **select**(λ_j) = .TRUE. after ordering, since ordering may perturb the value of complex eigenvalues, and especially ill-conditioned ones; in this case **info** may be set to a positive value (see **info** below). **select** must be declared EXTERNAL in the calling subroutine. **select** is not referenced if **sort** = 'N' or 'n'.

n The order of the matrix A. **n** ≥ 0.

a The **n**-by-**n** matrix A.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

ldvs The leading dimension of array **vs** in the calling program unit. **ldvs** ≥ 1, and if **jobvs** = 'V' or 'v', then **ldvs** ≥ **n**.

lwork The length of array **work**. **lwork** ≥ max(1,3**n**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

rwork An array used for work space.

bwork An array used for work space. Not referenced if **sort** = 'N' or 'n'.

Output

a On successful exit, the Schur Form of A overwrites the input. If **sort** = 'S' or 's', the output Schur Form is

$$\begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}$$

where A_{11} is **sdim**-by-**sdim**, A_{12} is **sdim**-by-(**n**–**sdim**), and A_{22} is (**n**–**sdim**)-by-(**n**–**sdim**), and where the eigenvalues $\lambda_j, j = 1, 2, ..., \mathbf{sdim}$, of A_{11} satisfy **select**(λ_j) = .TRUE. and the eigenvalues $\lambda_j, j = \mathbf{sdim}+1, \mathbf{sdim}+2, ..., \mathbf{n}$, of A_{22} satisfy **select**(λ_j) = .FALSE.

sdim If **sort** = 'N' or 'n', **sdim** = 0.

If **sort** = 'S' or 's', **sdim** is the number of eigenvalues (after reordering) for which **select** is true. In SGEES and DGEES, complex conjugate pairs for which **select** is true for either eigenvalue count as 2.

wr, wi On successful exit from SGEES and DGEES, **wr**(j) and **wi**(j) contain the real and imaginary parts, respectively, of the computed eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are in the same order in which they appear as the eigenvalues of the diagonal 1-by-1 and 2-by-2 blocks of the Schur Form. Complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having the positive imaginary part first.

w	On successful exit from CGEES and ZGEES, **w**(j) contains the computed eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are in the same order in which they appear on the diagonal of the Schur Form.	
vs	On successful exit, if **jobvs** = 'V' or 'v', the Schur vectors of A. Not referenced if **jobvs** = 'N' or 'n'.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	The algorithm terminated before completing the requested computation.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobvs ≠ 'N' or 'n' or 'V' or 'v',
sort ≠ 'N' or 'n' or 'S' or 's',
n < 0,
lda < max(1,**n**),
ldvs too small, and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobvs** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SGEEV/DGEEV/CGEEV/ZGEEV – General Matrix Eigenproblem

Purpose

These subprograms compute all eigenvalues and, optionally, all left and right eigenvectors of an n-by-n nonsymmetric matrix A.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Optionally, the z_i, which are called right eigenvectors, also may be computed. In addition, these subprograms also can compute the left eigenvectors, which satisfy

$$y_i{}^*A = \lambda_i y_i{}^*.$$

Usage

LAPACK:

CHARACTER*1 **jobvl, jobvr**
INTEGER*4 **info, lda, ldvl, ldvr, lwork, n**
REAL*4 **a(lda, n), vl(ldvl, n), vr(ldvr, n), wi(n), work(lwork), wr(n)**
CALL SGEEV(jobvl, jobvr, n, a, lda, wr, wi, vl, ldvl, vr, ldvr, work, lwork, info)

CHARACTER*1 **jobvl, jobvr**
INTEGER*4 **info, lda, ldvl, ldvr, lwork, n**
REAL*8 **a(lda, n), vl(ldvl, n), vr(ldvr, n), wi(n), work(lwork), wr(n)**
CALL DGEEV(jobvl, jobvr, n, a, lda, wr, wi, vl, ldvl, vr, ldvr, work, lwork, info)

CHARACTER*1 **jobvl, jobvr**
INTEGER*4 **info, lda, ldvl, ldvr, lwork, n**
REAL*4 **rwork(2*n)**
COMPLEX*8 **a(lda, n), vl(ldvl, n), vr(ldvr, n), w(n), work(lwork)**
CALL CGEEV(jobvl, jobvr, n, a, lda, w, vl, ldvl, vr, ldvr, work, lwork, rwork, info)

CHARACTER*1 **jobvl, jobvr**
INTEGER*4 **info, lda, ldvl, ldvr, lwork, n**
REAL*8 **rwork(2*n)**
COMPLEX*16 **a(lda, n), vl(ldvl, n), vr(ldvr, n), w(n), work(lwork)**
CALL ZGEEV(jobvl, jobvr, n, a, lda, w, vl, ldvl, vr, ldvr, work, lwork, rwork, info)

LAPACK8:

```
CHARACTER*1     jobvl, jobvr
INTEGER*8       info, lda, ldvl, ldvr, lwork, n
REAL*8          a(lda, n), vl(ldvl, n), vr(ldvr, n), wi(n), work(lwork),
                wr(n)
CALL SGEEV(jobvl, jobvr, n, a, lda, wr, wi, vl, ldvl, vr, ldvr, work, lwork,
  info)
CHARACTER*1     jobvl, jobvr
INTEGER*8       info, lda, ldvl, ldvr, lwork, n
REAL*8          rwork(2*n)
COMPLEX*16      a(lda, n), vl(ldvl, n), vr(ldvr, n), w(n), work(lwork)
CALL CGEEV(jobvl, jobvr, n, a, lda, w, vl, ldvl, vr, ldvr, work, lwork,
  rwork, info)
```

Input

jobvl Specifies whether the left eigenvectors of A are to be computed, as follows:

- **jobvl** = 'N' or 'n': Do not compute the left eigenvectors.
- **jobvl** = 'V' or 'v': Compute the left eigenvectors.

jobvr Specifies whether the right eigenvectors of A are to be computed, as follows:

- **jobvr** = 'N' or 'n': Do not compute the right eigenvectors.
- **jobvr** = 'V' or 'v': Compute the right eigenvectors.

n The order of the matrix A. **n** ≥ 0.

a The **n**-by-**n** matrix whose eigenvalues and eigenvectors are desired.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

ldvl The leading dimension of array **vl** in the calling program unit. **ldvl** ≥ 1, and if **jobvl** = 'V' or 'v', then **ldvl** ≥ **n**.

ldvr The leading dimension of array **vr** in the calling program unit. **ldvr** ≥ 1, and if **jobvr** = 'V' or 'v', then **ldvr** ≥ **n**.

lwork The length of array **work**. **lwork** ≥ max(1,3**n**) if **jobvl** = 'N' or 'n' and **jobvr** = 'N' or 'n', and **lwork** ≥ max(1,4**n**) otherwise. For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work, rwork Arrays used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a Destroyed.

wr, wi On successful exit from SGEEV and DGEEV, **wr**(j) and **wi**(j) contain the real and imaginary parts, respectively, of the computed eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are not in any particular order, except that complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having the positive imaginary part first.

w On successful exit from CGEEV and ZGEEV, **w**(j) contains the computed eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are not in any particular order.

vl On successful exit, if **jobvl** = 'V' or 'v', the left eigenvectors, $y_j, j = 1, 2, ..., \mathbf{n}$, stored one after another in the columns of **vl**, in the same order as the eigenvalues. The eigenvectors are normalized to have Euclidean norm equal to 1, and to have the largest component real.

In SGEEV and DGEEV, a left eigenvector corresponding to a real eigenvalue is real and takes up one column. An eigenvector pair corresponding to a complex conjugate pair of eigenvalues is complex and takes up two columns: the first column holds the real part and the second column holds the imaginary part of the eigenvector corresponding to the eigenvalue with positive imaginary part.

Therefore, if **wi**(j) > 0, the left eigenvector corresponding to **wr**(j) + i**wi**(j) is **vl**(j) + i**vl**(j+1), and if **wi**(j) < 0, the left eigenvector corresponding to **wr**(j) + i**wi**(j) is **vl**(j–1) – i**vl**(j), where $i = \sqrt{-1}$.

In CGEEV and ZGEEV, each left eigenvector takes up one column.

Not referenced if **jobvl** = 'N' or 'n'.

vr On successful exit, if **jobvr** = 'V' or 'v', the right eigenvectors, $z_j, j = 1, 2, ..., \mathbf{n}$, stored one after another in the columns of **vr**, in the same order as their eigenvalues.

The eigenvectors are normalized to have Euclidean norm equal to 1, and to have the largest component real.

In SGEEV and DGEEV, a right eigenvector corresponding to a real eigenvalue is real and takes up one column. An eigenvector pair corresponding to a complex conjugate pair of eigenvalues is complex and takes up two columns: the first column holds the real part and the second column holds the imaginary part of the eigenvector corresponding to the eigenvalue with positive imaginary part.

Therefore, if **wi**(j) > 0, the right eigenvector corresponding to **wr**(j) + i**wi**(j) is **vr**(j) + i**vr**(j+1), and if **wi**(j) < 0, the right eigenvector corresponding to **wr**(j) + i**wi**(j) is **vr**(j–1) – i**vr**(j), where $i = \sqrt{-1}$.

In CGEEV and ZGEEV, each right eigenvector takes up one column.

Not referenced if **jobvr** = 'N' or 'n'.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	The algorithm terminated before completing the requested computation.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobvl ≠ 'N' or 'n' or 'V' or 'v',
jobvr ≠ 'N' or 'n' or 'V' or 'v',
n < 0,
lda < max(1,**n**),
ldvl too small,
ldvr too small, and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **jobvl** and **jobvr** arguments as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSBEV/DSBEV/CHBEV/ZHBEV – Symmetric or Hermitian Band Matrix

Purpose

These subprograms compute all eigenvalues and, optionally, all eigenvectors of a real symmetric or complex Hermitian band matrix.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

A matrix is banded if its nonzero elements all lie fairly near the principal diagonal. Specifically, $a_{ij} = 0$ if $|i-j| > kd$ for some integer kd. The smallest such kd for a given matrix is called the half bandwidth, and $2kd+1$ is called the total bandwidth.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Optionally, the eigenvectors z_i also may be computed.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, and since either triangle of A may be obtained from the other, you need only provide the band within one triangle of A. Compared to storing the entire matrix, this can save memory in two ways: only the elements within the band are stored, and of them, only the upper or the lower triangle.

The following examples illustrate the storage of real symmetric band matrices. Consider the following matrix A of order $n = 7$ and half bandwidth $kd = 2$:

11	12	13	0	0	0	0
12	22	23	24	0	0	0
13	23	33	34	35	0	0
0	24	34	44	45	46	0
0	0	35	45	55	56	57
0	0	0	46	56	66	67
0	0	0	0	57	67	77

Upper triangular storage. The upper triangle of the matrix A is stored in an array **ab** with at least $kd+1 = 3$ rows and 7 columns as follows:

```
 *   *  13  24  35  46  57
 *  12  23  34  45  56  67
11  22  33  44  55  66  77
```

The asterisks represent elements in the kd-by-kd triangle at the upper left corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the upper triangle of A, it is stored in **ab**($kd+1+i-j,j$). Therefore, the columns of the upper triangle of A are stored in the columns of **ab**, and the diagonals of the upper triangle of A are stored in the rows of **ab**.

Lower triangular storage. The lower triangle of A is stored in the array **ab** as follows:

```
11  22  33  44  55  66  77
12  23  34  45  56  67   *
13  24  35  46  57   *   *
```

The asterisks represent elements in the kd-by-kd triangle at the lower right corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the lower triangle of A, it is stored in **ab**($1+i-j,j$). Therefore, the columns of the lower triangle of A are stored in the columns of **ab**, and the diagonals of the lower triangle of A are stored in the rows of **ab**.

Usage

LAPACK:

```
CHARACTER*1        jobz, uplo
INTEGER*4          info, kd, ldab, ldz, n
REAL*4             ab(ldab, n), w(n), work(max(1,3*n-2)), z(ldz, n)
CALL SSBEV(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, info)

CHARACTER*1        jobz, uplo
INTEGER*4          info, kd, ldab, ldz, n
REAL*8             ab(ldab, n), w(n), work(max(1,3*n-2)), z(ldz, n)
CALL DSBEV(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, info)

CHARACTER*1        jobz, uplo
INTEGER*4          info, kd, ldab, ldz, n
REAL*4             rwork(max(1,3*n-2)), w(n)
COMPLEX*8          ab(ldab, n), work(n), z(ldz, n)
CALL CHBEV(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, rwork, info)
```

```
CHARACTER*1     jobz, uplo
INTEGER*4       info, kd, ldab, ldz, n
REAL*8          rwork(max(1,3*n–2)), w(n)
COMPLEX*16      ab(ldab, n), work(n), z(ldz, n)
CALL ZHBEV(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1     jobz, uplo
INTEGER*8       info, kd, ldab, ldz, n
REAL*8          ab(ldab, n), w(n), work(max(1,3*n–2)), z(ldz, n)
CALL SSBEV(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, info)
```

```
CHARACTER*1     jobz, uplo
INTEGER*8       info, kd, ldab, ldz, n
REAL*8          rwork(max(1,3*n–2)), w(n)
COMPLEX*16      ab(ldab, n), work(n), z(ldz, n)
CALL CHBEV(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, rwork, info)
```

Input

jobz Specifies whether the eigenvectors are to be computed, as follows:

- **jobz** = 'N' or 'n': Compute eigenvalues only.
- **jobz** = 'V' or 'v': Compute eigenvectors as well.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or '1': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

kd The number of super-diagonals of the matrix A if **uplo** = 'U' or 'u', or the number of subdiagonals if **uplo** = 'L' or '1'. $\mathbf{kd} \geq 0$.

ab The upper or lower triangle of the symmetric or Hermitian band matrix, stored in the first **kd**+1 rows of array **ab**. The j-th column of A is stored in the j-th column of array **ab** as follows:

If **uplo** = 'U' or 'u', $\mathbf{ab}(\mathbf{kd}+1+i-j,j) = A(i,j)$ for $\max(1,j-\mathbf{kd}) \leq i \leq j$;

If **uplo** = 'L' or '1', $\mathbf{ab}(1+i-j,j) = A(i,j)$ for $j \leq i \leq \min(\mathbf{n},j+\mathbf{kd})$.

ldab The leading dimension of array **ab** in the calling program unit. **ldab** ≥ **kd**+1.

ldz The leading dimension of array **z** in the calling program unit. **ldz** ≥ 1, and if **jobz** = 'V' or 'v', then **ldz** ≥ **n**.

Working Storage

work, rwork Arrays used for work space.

Output

ab Destroyed.

w On successful exit, the eigenvalues in ascending order. If an error exit is made, the eigenvalues are correct for indices 1, 2, ..., **info**–1, but they are unordered and may not be the smallest eigenvalues of the matrix.

z On successful exit, if **jobz** = 'V' or 'v', the orthonormal eigenvectors of the matrix. If an error exit is made, **z** contains the eigenvectors associated with the stored eigenvalues.

Not referenced if **jobz** = 'N' or 'n'.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = –k, the k-th argument had an invalid value.
info > 0:	If **info** = k, the algorithm terminated before finding the k-th eigenvalue.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
kd < 0,
ldab < **kd**+1, and
ldz too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSBEVD/DSBEVD/.../ZHBEVD – Symmetric or Hermitian Band Matrix

Purpose

These subprograms compute all eigenvalues and, optionally, all eigenvectors of a real symmetric or complex Hermitian band matrix. If the eigenvectors are desired, the subroutines use a divide-and-conquer algorithm.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

A matrix is banded if its nonzero elements all lie fairly near the principal diagonal. Specifically, $a_{ij} = 0$ if $|i-j| > kd$ for some integer kd. The smallest such kd for a given matrix is called the half bandwidth, and $2kd+1$ is called the total bandwidth.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Optionally, the eigenvectors z_i also may be computed.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, and since either triangle of A may be obtained from the other, you need only provide the band within one triangle of A. Compared to storing the entire matrix, this can save memory in two ways: only the elements within the band are stored, and of them, only the upper or the lower triangle.

The following examples illustrate the storage of real symmetric band matrices. Consider the following matrix A of order $n = 7$ and half bandwidth $kd = 2$:

11	12	13	0	0	0	0
12	22	23	24	0	0	0
13	23	33	34	35	0	0
0	24	34	44	45	46	0
0	0	35	45	55	56	57
0	0	0	46	56	66	67
0	0	0	0	57	67	77

Upper triangular storage. The upper triangle of the matrix A is stored in an array **ab** with at least $kd+1 = 3$ rows and 7 columns as follows:

*	*	13	24	35	46	57
*	12	23	34	45	56	67
11	22	33	44	55	66	77

The asterisks represent elements in the kd-by-kd triangle at the upper left corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the upper triangle of A, it is stored in **ab**($kd+1+i-j,j$). Therefore, the columns of the upper triangle of A are stored in the columns of **ab**, and the diagonals of the upper triangle of A are stored in the rows of **ab**.

Lower triangular storage. The lower triangle of A is stored in the array **ab** as follows:

11	22	33	44	55	66	77
12	23	34	45	56	67	*
13	24	35	46	57	*	*

The asterisks represent elements in the kd-by-kd triangle at the lower right corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the lower triangle of A, it is stored in **ab**($1+i-j,j$). Therefore, the columns of the lower triangle of A are stored in the columns of **ab**, and the diagonals of the lower triangle of A are stored in the rows of **ab**.

Usage

LAPACK:

```
CHARACTER*1        jobz, uplo
INTEGER*4          info, kd, ldab, ldz, liwork, lwork, n
INTEGER*4          iwork(liwork)
REAL*4             ab(ldab, n), w(n), work(lwork), z(ldz, n)
CALL SSBEVD(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, lwork, iwork,
  liwork, info)

CHARACTER*1        jobz, uplo
INTEGER*4          info, kd, ldab, ldz, liwork, lwork, n
INTEGER*4          iwork(liwork)
REAL*8             ab(ldab, n), w(n), work(lwork), z(ldz, n)
CALL DSBEVD(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, lwork, iwork,
  liwork, info)
```

```
CHARACTER*1     jobz, uplo
INTEGER*4       info, kd, ldab, ldz, liwork, lrwork, lwork, n
INTEGER*4       iwork(liwork)
REAL*4          rwork(lrwork), w(n)
COMPLEX*8       ab(ldab, n), work(n), z(ldz, n)
CALL CHBEVD(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, lwork, rwork,
  lrwork, iwork, liwork, info)

CHARACTER*1     jobz, uplo
INTEGER*4       info, kd, ldab, ldz, liwork, lrwork, lwork, n
INTEGER*4       iwork(liwork)
REAL*8          rwork(lrwork), w(n)
COMPLEX*16      ab(ldab, n), work(n), z(ldz, n)
CALL ZHBEVD(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, lwork, rwork,
  lrwork, iwork, liwork, info)
```

LAPACK8:

```
CHARACTER*1     jobz, uplo
INTEGER*8       info, kd, ldab, ldz, liwork, lwork, n
INTEGER*8       iwork(liwork)
REAL*8          ab(ldab, n), w(n), work(lwork), z(ldz, n)
CALL SSBEVD(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, lwork, iwork,
  liwork, info)

CHARACTER*1     jobz, uplo
INTEGER*8       info, kd, ldab, ldz, liwork, lrwork, lwork, n
INTEGER*8       iwork(liwork)
REAL*8          rwork(lrwork), w(n)
COMPLEX*16      ab(ldab, n), work(n), z(ldz, n)
CALL CHBEVD(jobz, uplo, n, kd, ab, ldab, w, z, ldz, work, lwork, rwork,
  lrwork, iwork, liwork, info)
```

Input

jobz Specifies whether the eigenvectors are to be computed, as follows:

- **jobz** = 'N' or 'n': Compute eigenvalues only.
- **jobz** = 'V' or 'v': Compute eigenvectors as well.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or 'l': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

kd The number of super-diagonals of the matrix A if **uplo** = 'U' or 'u', or the number of subdiagonals if **uplo** = 'L' or 'l'. **kd** ≥ 0.

ab The upper or lower triangle of the symmetric or Hermitian band matrix, stored in the first **kd**+1 rows of array **ab**. The j-th column of A is stored in the j-th column of array **ab** as follows:

If **uplo** = 'U' or 'u', **ab**(**kd**+1+i–j,j) = $A(i,j)$ for max(1,j–**kd**) ≤ i ≤ j;

If **uplo** = 'L' or 'l', **ab**(1+i–j,j) = $A(i,j)$ for j ≤ i ≤ min(**n**,j+**kd**).

ldab The leading dimension of array **ab** in the calling program unit. **ldab** ≥ **kd**+1.

ldz The leading dimension of array **z** in the calling program unit. **ldz** ≥ 1, and if **jobz** = 'V' or 'v', then **ldz** ≥ **n**.

lwork The length of array **work**.

For SSBEVD and DSBEVD, **lwork** ≥ max(1,2*__n__) if **jobz** = 'N' or 'n', and **lwork** ≥ 3*__n__**2+4*__n__+2*__n__*lg(__n__)+1 if **jobz** = 'V' or 'v', where lg(__n__) is the smallest integer k ≥ 0 such that 2^k ≥ **n**.

For CHBEVD and ZHBEVD, **lwork** ≥ max(1,__n__) if **jobz** = 'N' or 'n', and **lwork** ≥ max(1,2*__n__**2) if **jobz** = 'V' or 'v'.

For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

lrwork The length of array **rwork**. **lrwork** ≥ max(1,__n__) if **jobz** = 'N' or 'n', and **lrwork** ≥ 3*__n__**2+4*__n__+2*__n__*lg(__n__)+1 if **jobz** = 'V' or 'v', where lg(__n__) is the smallest integer k ≥ 0 such that 2^k ≥ **n**. For good performance, **lrwork** must generally be larger. The optimum value of **lrwork** for high performance is returned in **rwork**(1).

liwork The length of array **iwork**. **liwork** ≥ 1 if **jobz** = 'N' or 'n', and **liwork** ≥ 5*__n__+2 if **jobz** = 'V' or 'v'. For good performance, **liwork** must generally be larger. The optimum value of **liwork** for high performance is returned in **iwork**(1).

Working Storage

work Array used for work space. On successful exit, if **lwork** > 0, **work**(1) contains the optimal work space length **lwork** for high performance.

rwork Array used for work space. On successful exit, **rwork**(1) contains the optimal work space length **lrwork** for high performance.

iwork Array used for work space. On successful exit, if **liwork** > 0, **iwork**(1) contains the optimal work space length **liwork** for high performance.

Output

ab Destroyed.

w On successful exit, the eigenvalues in ascending order.

z On successful exit, if **jobz** = 'V' or 'v', the orthonormal eigenvectors of the matrix.

Not referenced if **jobz** = 'N' or 'n'.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, the algorithm failed to converge; k off-diagonal elements of an intermediate tridiagonal form did not converge to zero.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
kd < 0,
ldab < **kd**+1,
ldz too small,
lwork too small,
lrwork too small, and
liwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSPEV/DSPEV/CHPEV/ZHPEV – Symmetric or Hermitian Packed Matrix

Purpose

These subprograms compute all eigenvalues and, optionally, all eigenvectors of a real symmetric or complex Hermitian matrix in packed storage.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Optionally, the eigenvectors z_i also may be computed.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A, either the upper or the lower triangle. Compared to storing the entire matrix, you save memory by supplying that triangle stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular storage. If the lower triangle of A is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**(i+(j–1)×(2n–j)/2).

Usage

LAPACK:

```
CHARACTER*1        jobz, uplo
INTEGER*4          info, ldz, n
REAL*4             ap((n*(n+1))/2), w(n), work(max(1,3*n)), z(ldz, n)
CALL SSPEV(jobz, uplo, n, ap, w, z, ldz, work, info)

CHARACTER*1        jobz, uplo
INTEGER*4          info, ldz, n
REAL*8             ap((n*(n+1))/2), w(n), work(max(1,3*n)), z(ldz, n)
CALL DSPEV(jobz, uplo, n, ap, w, z, ldz, work, info)

CHARACTER*1        jobz, uplo
INTEGER*4          info, ldz, n
REAL*4             rwork(max(1,3*n–1)), w(n)
COMPLEX*8          ap((n*(n+1))/2), work(max(1,2*n–1)), z(ldz, n)
CALL CHPEV(jobz, uplo, n, ap, w, z, ldz, work, rwork, info)

CHARACTER*1        jobz, uplo
INTEGER*4          info, ldz, n
REAL*8             rwork(max(1,3*n–1)), w(n)
COMPLEX*16         ap((n*(n+1))/2), work(max(1,2*n–1)), z(ldz, n)
CALL ZHPEV(jobz, uplo, n, ap, w, z, ldz, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1        jobz, uplo
INTEGER*8          info, ldz, n
REAL*8             ap((n*(n+1))/2), w(n), work(max(1,3*n)), z(ldz, n)
CALL SSPEV(jobz, uplo, n, ap, w, z, ldz, work, info)
```

```
CHARACTER*1     jobz, uplo
INTEGER*8       info, ldz, n
REAL*8          rwork(max(1,3*n–1)), w(n)
COMPLEX*16      ap((n*(n+1))/2), work(max(1,2*n–1)), z(ldz, n)
CALL CHPEV(jobz, uplo, n, ap, w, z, ldz, work, rwork, info)
```

Input

jobz Specifies whether eigenvectors are to be computed, as follows:

jobz = 'N' or 'n': Compute eigenvalues only.

jobz = 'V' or 'v': Compute eigenvectors as well.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored in array **ap**, as follows:

uplo = 'U' or 'u': The upper triangular part of A is stored.

uplo = 'L' or '1': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

ap The upper or lower triangular part of the symmetric or Hermitian matrix A, packed columnwise in a linear array as follows:

If **uplo** = 'U' or 'u', $\mathbf{ap}(i + (j-1) \times j/2) = A(i,j)$ for $1 \leq i \leq j$;

If **uplo** = 'L' or '1', $\mathbf{ap}(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \leq i \leq \mathbf{n}$.

ldz The leading dimension of array **z** in the calling program unit. $\mathbf{ldz} \geq 1$. If eigenvectors are desired, then $\mathbf{ldz} \geq \max(1,\mathbf{n})$.

Working Storage

work, rwork Arrays used for work space.

Output

ap Destroyed.

w On successful exit, the eigenvalues in ascending order. If an error exit is made, the eigenvalues are correct for indices 1, 2, ..., **info**–1, but they are unordered and may not be the smallest eigenvalues of the matrix.

z	On successful exit, if **jobz** = 'V' or 'v', the orthonormal eigenvectors of the matrix. If an error exit is made, **z** contains the eigenvectors associated with the stored eigenvalues. Not referenced if **jobz** = 'N' or 'n'.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k, the algorithm terminated before finding the k-th eigenvalue.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
ldz too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSPEVD/DSPEVD/.../ZHPEVD – Symmetric or Hermitian Packed Matrix

Purpose

These subprograms compute all eigenvalues and, optionally, all eigenvectors of a real symmetric or complex Hermitian matrix in packed storage. If the eigenvectors are desired, the subroutines use a divide-and-conquer algorithm.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Optionally, the eigenvectors z_i also may be computed.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A, either the upper or the lower triangle. Compared to storing the entire matrix, you save memory by supplying that triangle stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular storage. If the lower triangle of A is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**($i+(j-1)\times(2n-j)/2$).

Usage

LAPACK:

```
CHARACTER*1          jobz, uplo
INTEGER*4            info, ldz, liwork, lwork, n
INTEGER*4            iwork(liwork)
REAL*4               ap((n*(n+1))/2), w(n), work(lwork), z(ldz, n)
CALL SSPEVD(jobz, uplo, n, ap, w, z, ldz, work, lwork, iwork, liwork,
  info)

CHARACTER*1          jobz, uplo
INTEGER*4            info, ldz, liwork, lwork, n
INTEGER*4            iwork(liwork)
REAL*8               ap((n*(n+1))/2), w(n), work(lwork), z(ldz, n)
CALL DSPEVD(jobz, uplo, n, ap, w, z, ldz, work, lwork, iwork, liwork,
  info)

CHARACTER*1          jobz, uplo
INTEGER*4            info, ldz, liwork, lrwork, lwork, n
INTEGER*4            iwork(liwork)
REAL*4               rwork(lrwork), w(n)
COMPLEX*8            ap((n*(n+1))/2), work(lwork), z(ldz, n)
CALL CHPEVD(jobz, uplo, n, ap, w, z, ldz, work, lwork, rwork, lrwork,
  iwork, liwork, info)
```

```
CHARACTER*1     jobz, uplo
INTEGER*4       info, ldz, liwork, lrwork, lwork, n
INTEGER*4       iwork(liwork)
REAL*8          rwork(lrwork), w(n)
COMPLEX*16      ap((n*(n+1))/2), work(lwork), z(ldz, n)
CALL ZHPEVD(jobz, uplo, n, ap, w, z, ldz, work, lwork, rwork, lrwork,
  iwork, liwork, info)
```

LAPACK8:

```
CHARACTER*1     jobz, uplo
INTEGER*8       info, ldz, liwork, lwork, n
INTEGER*8       iwork(liwork)
REAL*8          ap((n*(n+1))/2), w(n), work(lwork), z(ldz, n)
CALL SSPEVD(jobz, uplo, n, ap, w, z, ldz, work, lwork, iwork, liwork,
  info)
CHARACTER*1     jobz, uplo
INTEGER*8       info, ldz, liwork, lrwork, lwork, n
INTEGER*8       iwork(liwork)
REAL*8          rwork(lrwork), w(n)
COMPLEX*16      ap((n*(n+1))/2), work(lwork), z(ldz, n)
CALL CHPEVD(jobz, uplo, n, ap, w, z, ldz, work, lwork, rwork, lrwork,
  iwork, liwork, info)
```

Input

jobz Specifies whether eigenvectors are to be computed, as follows:

jobz = 'N' or 'n':	Compute eigenvalues only.
jobz = 'V' or 'v':	Compute eigenvectors as well.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored in array **ap**, as follows:

uplo = 'U' or 'u':	The upper triangular part of A is stored.
uplo = 'L' or '1':	The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

ap The upper or lower triangular part of the symmetric or Hermitian matrix A, packed columnwise in a linear array as follows:

If **uplo** = 'U' or 'u', $\mathbf{ap}(i + (j-1) \times j/2) = A(i,j)$ for $1 \leq i \leq j$;

If **uplo** = 'L' or '1', $\mathbf{ap}(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \leq i \leq \mathbf{n}$.

ldz The leading dimension of array **z** in the calling program unit. **ldz** ≥ 1. If eigenvectors are desired, then **ldz** ≥ max(1,**n**).

lwork The length of array **work**.

For SSPEVD and DSPEVD, **lwork** ≥ max(1,2*n) if **jobz** = 'N' or 'n', and **lwork** ≥ 2*n**2+5*n+2*n*lg(n)+1 if **jobz** = 'V' or 'v', where lg(**n**) is the smallest integer $k \geq 0$ such that $2^k \geq$ **n**.

For CHPEVD and ZHPEVD, **lwork** ≥ max(1,**n**) if **jobz** = 'N' or 'n', and **lwork** ≥ max(1,2*n**2) if **jobz** = 'V' or 'v'.

For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

lrwork The length of array **rwork**. **lrwork** ≥ max(1,**n**) if **jobz** = 'N' or 'n', and **lrwork** ≥ 3*n**2+4*n+2*n*lg(n)+1 if **jobz** = 'V' or 'v', where lg(**n**) is the smallest integer $k \geq 0$ such that $2^k \geq$ **n**. For good performance, **lrwork** must generally be larger. The optimum value of **lrwork** for high performance is returned in **rwork**(1).

liwork The length of array **iwork**. **liwork** ≥ 1 if **jobz** = 'N' or 'n', and **liwork** ≥ 5*n+2 if **jobz** = 'V' or 'v'. For good performance, **liwork** must generally be larger. The optimum value of **liwork** for high performance is returned in **iwork**(1).

Working Storage

work Array used for work space. On successful exit, if **lwork** > 0, **work**(1) contains the optimal work space length **lwork** for high performance.

rwork Array used for work space. On successful exit, **rwork**(1) contains the optimal work space length **lrwork** for high performance.

iwork Array used for work space. On successful exit, if **liwork** > 0, **iwork**(1) contains the optimal work space length **liwork** for high performance.

Output

ap	Destroyed.	
w	On successful exit, the eigenvalues in ascending order.	
z	On successful exit, if **jobz** = 'V' or 'v', the orthonormal eigenvectors of the matrix.	
	Not referenced if **jobz** = 'N' or 'n'.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k, the algorithm failed to converge; k off-diagonal elements of an intermediate tridiagonal form did not converge to zero.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
ldz too small,
lwork too small,
lrwork too small, and
liwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSTEV/DSTEV – Real Symmetric Tridiagonal Matrix

Purpose

These subprograms compute all eigenvalues and, optionally, all eigenvectors of a real symmetric tridiagonal matrix.

A matrix is symmetric if $A = A^T$, its transpose.

A matrix $A = (a_{ij})$ is tridiagonal if its nonzero elements lie only on the principal diagonal ($i = j$), the subdiagonal ($i = j+1$), and the superdiagonal ($i = j-1$) of the matrix.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Optionally, the eigenvectors z_i also may be computed.

Matrix Storage

The following example illustrates the storage of symmetric tridiagonal matrices. Consider the following symmetric tridiagonal matrix of order $n = 7$:

11	21	0	0	0	0	0
21	22	32	0	0	0	0
0	32	33	43	0	0	0
0	0	43	44	54	0	0
0	0	0	54	55	65	0
0	0	0	0	65	66	76
0	0	0	0	0	76	77

The subdiagonal is stored in array **e** and the principal diagonal is stored in array **d**, as follows:

i	**e**(i)	**d**(i)
1	21	11
2	32	22
3	43	33
4	54	44
5	65	55
6	76	66
7		77

Usage

LAPACK:

```
CHARACTER*1     jobz
INTEGER*4       info, ldz, n
REAL*4          d(n), e(n–1), work(max(1,2*n–2)), z(ldz, n)
CALL SSTEV(jobz, n, d, e, z, ldz, work, info)
```

```
CHARACTER*1     jobz
INTEGER*4       info, ldz, n
REAL*8          d(n), e(n–1), work(max(1,2*n–2)), z(ldz, n)
CALL DSTEV(jobz, n, d, e, z, ldz, work, info)
```

LAPACK8:

```
CHARACTER*1     jobz
INTEGER*8       info, ldz, n
REAL*8          d(n), e(n–1), work(max(1,2*n–2)), z(ldz, n)
CALL SSTEV(jobz, n, d, e, z, ldz, work, info)
```

Input

jobz Specifies whether eigenvectors are to be computed, as follows:

jobz = 'N' or 'n': Compute eigenvalues only.

jobz = 'V' or 'v': Compute eigenvectors as well.

n The order in the matrix A. $\mathbf{n} \geq 0$.

d The **n** diagonal elements of the tridiagonal matrix.

e The **n**–1 subdiagonal elements of the tridiagonal matrix.

ldz The leading dimension of array **z** in the calling program unit. $\mathbf{ldz} \geq 1$, and if **jobz** = 'V' or 'v', then $\mathbf{ldz} \geq \mathbf{n}$.

Working Storage

work An array used for work space. Not referenced if **jobz** = 'N' or 'n'.

Output

d On successful exit, the eigenvalues, in ascending order. If an error exit is made, the eigenvalues are correct for indices 1, 2, ..., **info**–1, but they are unordered and may not be the smallest eigenvalues of the matrix.

e Destroyed.

z On successful exit, if **jobz** = 'V' or 'v', the orthonormal eigenvectors of the matrix. If an error exit is made, **z** contains the eigenvectors associated with the stored eigenvalues.

Not referenced if **jobz** = 'N' or 'n'.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, the algorithm terminated before finding the k-th eigenvalue.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
n < 0,
ldz too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSTEVD/DSTEVD – Real Symmetric Tridiagonal Matrix

Purpose

These subprograms compute all eigenvalues and, optionally, all eigenvectors of a real symmetric tridiagonal matrix. If the eigenvectors are desired, the subroutines use a divide-and-conquer algorithm.

A matrix is symmetric if $A = A^T$, its transpose.

A matrix $A = (a_{ij})$ is tridiagonal if its nonzero elements lie only on the principal diagonal ($i = j$), the subdiagonal ($i = j+1$), and the superdiagonal ($i = j-1$) of the matrix.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Optionally, the eigenvectors z_i also may be computed.

Matrix Storage

The following example illustrates the storage of symmetric tridiagonal matrices. Consider the following symmetric tridiagonal matrix of order $n = 7$:

11	21	0	0	0	0	0
21	22	32	0	0	0	0
0	32	33	43	0	0	0
0	0	43	44	54	0	0
0	0	0	54	55	65	0
0	0	0	0	65	66	76
0	0	0	0	0	76	77

The subdiagonal is stored in array **e** and the principal diagonal is stored in array **d**, as follows:

i	**e**(i)	**d**(i)
1	21	11
2	32	22
3	43	33
4	54	44
5	65	55
6	76	66
7		77

Usage

LAPACK:

```
CHARACTER*1     jobz
INTEGER*4       info, ldz, liwork, lwork, n
INTEGER*4       iwork(liwork)
REAL*4          d(n), e(n–1), work(lwork), z(ldz, n)
CALL SSTEVD(jobz, n, d, e, z, ldz, work, lwork, iwork, liwork, info)

CHARACTER*1     jobz
INTEGER*4       info, ldz, liwork, lwork, n
INTEGER*4       iwork(liwork)
REAL*8          d(n), e(n–1), work(lwork), z(ldz, n)
CALL DSTEVD(jobz, n, d, e, z, ldz, work, lwork, iwork, liwork, info)
```

LAPACK8:

```
CHARACTER*1     jobz
INTEGER*8       info, ldz, liwork, lwork, n
INTEGER*8       iwork(liwork)
REAL*8          d(n), e(n–1), work(lwork), z(ldz, n)
CALL SSTEVD(jobz, n, d, e, z, ldz, work, lwork, iwork, liwork, info)
```

Input

jobz Specifies whether eigenvectors are to be computed, as follows:

- **jobz** = 'N' or 'n': Compute eigenvalues only.
- **jobz** = 'V' or 'v': Compute eigenvectors as well.

n The order in the matrix A. $\mathbf{n} \geq 0$.

d The **n** diagonal elements of the tridiagonal matrix.

e The **n**–1 subdiagonal elements of the tridiagonal matrix.

ldz The leading dimension of array **z** in the calling program unit. **ldz** ≥ 1, and if **jobz** = 'V' or 'v', then **ldz** ≥ **n**.

lwork The length of array **work**. **lwork** ≥ 1 if **jobz** = 'N' or 'n', and **lwork** ≥ 2*n**2+3*n+2*n*lg(n)+1 if **jobz** = 'V' or 'v', where lg(**n**) is the smallest integer $k \geq 0$ such that $2^k \geq$ **n**. The optimal value of **lwork** is returned in **work**(1).

liwork The length of array **iwork**. **liwork** ≥ 1 if **jobz** = 'N' or 'n', and **liwork** ≥ 5*n+2 if **jobz** = 'V' or 'v'. The optimal value of **liwork** is returned in **iwork**(1).

Working Storage

work Array used for work space. On successful exit, if **lwork** > 0, **work**(1) contains the optimal work space length **lwork**.

iwork Array used for work space. On successful exit, if **liwork** > 0, **iwork**(1) contains the optimal work space length **liwork**.

Output

d On successful exit, the eigenvalues, in ascending order.

e Destroyed.

z On successful exit, if **jobz** = 'V' or 'v', the orthonormal eigenvectors of the matrix.

Not referenced if **jobz** = 'N' or 'n'.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = –k, the k-th argument had an invalid value.
info > 0:	If **info** = k, the algorithm failed to converge; k off-diagonal elements of **e** did not converge to zero.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
n < 0,
ldz too small,
lwork too small, and
liwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSYEV/DSYEV/CHEEV/ZHEEV – Symmetric or Hermitian Matrix

Purpose

These subprograms compute all eigenvalues and, optionally, all eigenvectors of a real symmetric or complex Hermitian matrix.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Optionally, the eigenvectors z_i also may be computed.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A. You may supply either the upper or the lower triangle of A, in a two-dimensional array large enough to hold the entire matrix. The other triangle of the array is not referenced.

Usage

LAPACK:

```
CHARACTER*1     jobz, uplo
INTEGER*4       info, lda, lwork, n
REAL*4          a(lda, n), w(n), work(lwork)
CALL SSYEV(jobz, uplo, n, a, lda, w, work, lwork, info)

CHARACTER*1     jobz, uplo
INTEGER*4       info, lda, lwork, n
REAL*8          a(lda, n), w(n), work(lwork)
CALL DSYEV(jobz, uplo, n, a, lda, w, work, lwork, info)

CHARACTER*1     jobz, uplo
INTEGER*4       info, lda, lwork, n
REAL*4          rwork(max(1,3*n–2)), w(n)
COMPLEX*8       a(lda, n), work(lwork)
CALL CHEEV(jobz, uplo, n, a, lda, w, work, lwork, rwork, info)

CHARACTER*1     jobz, uplo
INTEGER*4       info, lda, lwork, n
REAL*8          rwork(max(1,3*n–2)), w(n)
COMPLEX*16      a(lda, n), work(lwork)
CALL ZHEEV(jobz, uplo, n, a, lda, w, work, lwork, rwork, info)
```

LAPACK8:

```
CHARACTER*1        jobz, uplo
INTEGER*8          info, lda, lwork, n
REAL*8             a(lda, n), w(n), work(lwork)
CALL SSYEV(jobz, uplo, n, a, lda, w, work, lwork, info)

CHARACTER*1        jobz, uplo
INTEGER*8          info, lda, lwork, n
REAL*8             rwork(max(1,3*n-2)), w(n)
COMPLEX*16         a(lda, n), work(lwork)
CALL CHEEV(jobz, uplo, n, a, lda, w, work, lwork, rwork, info)
```

Input

jobz Specifies whether eigenvectors are to be computed, as follows:

- **jobz** = 'N' or 'n': Compute eigenvalues only.
- **jobz** = 'V' or 'v': Compute eigenvectors as well.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or '1': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

a The symmetric or Hermitian matrix A.

If **uplo** = 'U' or 'u', only the upper triangular part of **a** is used to define the elements of the matrix and the strict lower triangular part of **a** is not used for input.

If **uplo** = 'L' or '1', only the lower triangular part of **a** is used to define the elements of the matrix and the strict upper triangular part of **a** is not used for input.

lda The leading dimension of array **a** in the calling program unit. $\mathbf{lda} \geq \max(1,\mathbf{n})$.

lwork The length of array **work**. $\mathbf{lwork} \geq \max(1,3\mathbf{n}-1)$. For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work, rwork Arrays used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, if **jobz** = 'V' or 'v', the orthonormal eigenvectors of the matrix. If an error exit is made, **a** contains the eigenvectors associated with the stored eigenvalues.

If **jobz** = 'N' or 'n', then the triangle of **a** specified by **uplo**, including the diagonal, has been destroyed.

w On successful exit, the eigenvalues in ascending order. If an error exit is made, the eigenvalues are correct for indices 1, 2, ..., **info**–1, but they are unordered and may not be the smallest eigenvalues of the matrix.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, the algorithm terminated before finding the k-th eigenvalue.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
lda < max(1,**n**), and
lwork < max(1,3**n**–1).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSYEVD/DSYEVD/CHEEVD/ZHEEVD – Symmetric or Hermitian Matrix

Purpose

These subprograms compute all eigenvalues and, optionally, all eigenvectors of a real symmetric or complex Hermitian matrix. If the eigenvectors are desired, the subroutines use a divide-and-conquer algorithm.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Optionally, the eigenvectors z_i also may be computed.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A. You may supply either the upper or the lower triangle of A, in a two-dimensional array large enough to hold the entire matrix. The other triangle of the array is not referenced.

Usage

LAPACK:

```
CHARACTER*1     jobz, uplo
INTEGER*4       info, lda, liwork, lwork, n
INTEGER*4       iwork(liwork)
REAL*4          a(lda, n), w(n), work(lwork)
CALL SSYEVD(jobz, uplo, n, a, lda, w, work, lwork, iwork, liwork, info)

CHARACTER*1     jobz, uplo
INTEGER*4       info, lda, liwork, lwork, n
INTEGER*4       iwork(liwork)
REAL*8          a(lda, n), w(n), work(lwork)
CALL DSYEVD(jobz, uplo, n, a, lda, w, work, lwork, iwork, liwork, info)

CHARACTER*1     jobz, uplo
INTEGER*4       info, lda, liwork, lrwork, lwork, n
INTEGER*4       iwork(liwork)
REAL*4          rwork(lrwork), w(n)
COMPLEX*8       a(lda, n), work(lwork)
CALL CHEEVD(jobz, uplo, n, a, lda, w, work, lwork, rwork, lrwork,
  iwork, liwork, info)
```

```
CHARACTER*1     jobz, uplo
INTEGER*4       info, lda, liwork, lrwork, lwork, n
INTEGER*4       iwork(liwork)
REAL*8          rwork(lrwork), w(n)
COMPLEX*16      a(lda, n), work(lwork)
CALL ZHEEVD(jobz, uplo, n, a, lda, w, work, lwork, rwork, lrwork, iwork,
  liwork, info)
```

LAPACK8:

```
CHARACTER*1     jobz, uplo
INTEGER*8       info, lda, liwork, lwork, n
INTEGER*8       iwork(liwork)
REAL*8          a(lda, n), w(n), work(lwork)
CALL SSYEVD(jobz, uplo, n, a, lda, w, work, lwork, iwork, liwork, info)
```

```
CHARACTER*1     jobz, uplo
INTEGER*8       info, lda, liwork, lrwork, lwork, n
INTEGER*8       iwork(liwork)
REAL*8          rwork(lrwork), w(n)
COMPLEX*16      a(lda, n), work(lwork)
CALL CHEEVD(jobz, uplo, n, a, lda, w, work, lwork, rwork, lrwork,
  iwork, liwork, info)
```

Input

jobz Specifies whether eigenvectors are to be computed, as follows:

- **jobz** = 'N' or 'n': Compute eigenvalues only.
- **jobz** = 'V' or 'v': Compute eigenvectors as well.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or 'l': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

a The symmetric or Hermitian matrix A.

If **uplo** = 'U' or 'u', only the upper triangular part of **a** is used to define the elements of the matrix and the strict lower triangular part of **a** is not used for input.

If **uplo** = 'L' or 'l', only the lower triangular part of **a** is used to define the elements of the matrix and the strict upper triangular part of **a** is not used for input.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

lwork The length of array **work**.

For SSYEVD and DSYEVD, **lwork** ≥ 2***n**+1 if **jobz** = 'N' or 'n', and **lwork** ≥ 3***n****2+5***n**+2***n***lg(**n**)+1 if **jobz** = 'V' or 'v', where lg(**n**) is the smallest integer $k \geq 0$ such that $2^k \geq \mathbf{n}$.

For CHEEVD and ZHEEVD, **lwork** ≥ **n**+1 if **jobz** = 'N' or 'n', and **lwork** ≥ max(1,2***n**+**n****2) if **jobz** = 'V' or 'v'.

For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

lrwork The length of array **rwork**. **lrwork** ≥ max(1,**n**) if **jobz** = 'N' or 'n', and **lrwork** ≥ 3***n****2+4***n**+2***n***lg(**n**)+1 if **jobz** = 'V' or 'v', where lg(**n**) is the smallest integer $k \geq 0$ such that $2^k \geq \mathbf{n}$. For good performance, **lrwork** must generally be larger. The optimum value of **lrwork** for high performance is returned in **rwork**(1).

liwork The length of array **iwork**. **liwork** ≥ 1 if **jobz** = 'N' or 'n', and **liwork** ≥ 5***n**+2 if **jobz** = 'V' or 'v'. For good performance, **liwork** must generally be larger. The optimum value of **liwork** for high performance is returned in **iwork**(1).

Working Storage

work Array used for work space. On successful exit, if **lwork** > 0, **work**(1) contains the optimal work space length **lwork** for high performance.

rwork Array used for work space. On successful exit, **rwork**(1) contains the optimal work space length **lrwork** for high performance.

iwork Array used for work space. On successful exit, if **liwork** > 0, **iwork**(1) contains the optimal work space length **liwork** for high performance.

Output

a On successful exit, if **jobz** = 'V' or 'v', the orthonormal eigenvectors of the matrix.

If **jobz** = 'N' or 'n', then the triangle of **a** specified by **uplo**, including the diagonal, has been destroyed.

w	On successful exit, the eigenvalues in ascending order.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k, the algorithm failed to converge; k off-diagonal elements of an intermediate tridiagonal form did not converge to zero.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
lda < max(1,**n**),
lwork too small,
lrwork too small, and
liwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

8 Expert Drivers for Ordinary Eigenvalue Problems

Overview

This chapter explains how to use LAPACK expert drivers to compute the Schur form, Schur vectors, eigenvalues, or eigenvalues and eigenvectors of matrices. The problems covered are:

- General dense eigenproblems, $Ax = \lambda x$, for arbitrary A
- Symmetric and Hermitian dense eigenproblems, $Ax = \lambda x$, with $A = A^T$ or $A = A^*$
- Symmetric and Hermitian banded eigenproblems, $Ax = \lambda x$, with $A = A^T$ or $A = A^*$
- Symmetric tridiagonal eigenproblems, $Ax = \lambda x$, with $A = A^T$

Chapter 7 describes the LAPACK simple drivers for ordinary eigenvalue problems. Use the simple drivers when you want to compute all of the eigenvalues of a matrix, instead of only some of them. Refer to Chapter 9 for software to compute the eigenvalues or eigenvalues and eigenvectors of generalized eigenproblems.

Refer to Chapter 7 of the *HP MLIB VECLIB User's Guide* for software to compute the eigenvalues or eigenvalues and eigenvectors of a real symmetric, sparse, ordinary or generalized eigenproblem.

The following documents provide supplemental material for this chapter:

- Anderson, E. *et al. LAPACK Users' Guide*, Second Edition. Philadelphia, PA: Society for Industrial and Applied Mathematics. 1995.
- Golub, G.H. and C.F. Van Loan. *Matrix Computations*, 2nd Edition. Baltimore, MD: The Johns Hopkins University Press. 1989.
- Parlett, B.N. *The Symmetric Eigenproblem*. Englewood Cliffs, NJ: Prentice-Hall, Inc. 1980.
- Wilkinson, J.H. *The Algebraic Eigenproblem*. New York, NY: Oxford University Press. 1965.

Chapter Objectives

After reading this chapter you will know how to use the described subprograms.

What You Need to Know to Use These Subprograms

To use these subprograms, it is helpful to know some basic theory of eigensystems and the Schur Form, especially as they relate to your particular application. A few facts discussed in basic textbooks are given in the introduction to Chapter 7.

The eigenvalues for real symmetric or complex Hermitian matrices are real. The subprograms in this chapter that deal with this type of matrix allow you to select only some of the eigenvalues. For example, you can select all the eigenvalues in a half-open interval $a < \lambda_j \leq b$, or you can choose a range of indices of ordered eigenvalues, such as the five smallest, the seven largest, or the twelfth smallest through the seventeenth smallest.

The eigenvalues of a general nonsymmetric matrix may change radically as a result of small perturbations in the elements of the matrix. The subprograms in this chapter that solve the eigenproblem for a general matrix optionally compute a condition number that measures the sensitivity of eigenvalues. An estimate of a condition number for the eigenvectors also can be computed.

Since real symmetric and complex Hermitian eigenvalues are always well conditioned, no condition numbers are estimated by the subprograms for these types of matrices.

NAME

SGEESX/DGEESX/CGEESX/ZGEESX – Schur Form of a General Matrix

Purpose

These subprograms compute the eigenvalues and the Schur Form of an n-by-n general matrix A, and optionally compute the Schur vectors of A and order the eigenvalues on the diagonal of the Schur Form so that selected eigenvalues are at the upper left.

Given a general matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

A real matrix is in Schur Form if it is block upper triangular with 1-by-1 and 2-by-2 blocks. 1-by-1 blocks correspond to real eigenvalues, and 2-by-2 blocks correspond to complex conjugate eigenpairs. 2-by-2 blocks are standardized in the form

$$\begin{bmatrix} a & b \\ c & a \end{bmatrix}$$

where $bc < 0$. The eigenvalues of such a block are $a \pm i\sqrt{|bc|}$.

A complex matrix is in Schur Form if it upper triangular.

If T is the Schur Form of A, then the columns of unitary matrix Q such that

$$A = QTQ^*$$

are known as the Schur vectors of A.

Also, optionally, two condition numbers may be estimated; one measures the sensitivity of the average of the eigenvalues to errors in the matrix or to small roundoff errors introduced during the computation, and the other estimates the conditioning of the right invariant subspace corresponding to the selected eigenvalues.

Usage

LAPACK:

```
CHARACTER*1     jobvs, sense, sort
INTEGER*4       info, lda, ldvs, liwork, lwork, n, sdim
REAL*4          rconde, rcondv
LOGICAL*4       bwork(n)
INTEGER*4       iwork(liwork)
REAL*4          a(lda, n), vs(ldvs, n), wi(n), work(lwork), wr(n)
LOGICAL*4       select
EXTERNAL        select
CALL SGEESX(jobvs, sort, select, sense, n, a, lda, sdim, wr, wi, vs, ldvs,
   rconde, rcondv, work, lwork, iwork, liwork, bwork, info)

CHARACTER*1     jobvs, sense, sort
INTEGER*4       info, lda, ldvs, liwork, lwork, n, sdim
REAL*8          rconde, rcondv
LOGICAL*4       bwork(n)
INTEGER*4       iwork(liwork)
REAL*8          a(lda, n), vs(ldvs, n), wi(n), work(lwork), wr(n)
LOGICAL*4       select
EXTERNAL        select
CALL DGEESX(jobvs, sort, select, sense, n, a, lda, sdim, wr, wi, vs, ldvs,
   rconde, rcondv, work, lwork, iwork, liwork, bwork, info)

CHARACTER*1     jobvs, sense, sort
INTEGER*4       info, lda, ldvs, lwork, n, sdim
REAL*4          rconde, rcondv
LOGICAL*4       bwork(n)
REAL*4          rwork(n)
COMPLEX*8       a(lda, n), vs(ldvs, n), w(n), work(lwork)
LOGICAL*4       select
EXTERNAL        select
CALL CGEESX(jobvs, sort, select, sense, n, a, lda, sdim, w, vs, ldvs,
   rconde, rcondv, work, lwork, rwork, bwork, info)

CHARACTER*1     jobvs, sense, sort
INTEGER*4       info, lda, ldvs, lwork, n, sdim
REAL*8          rconde, rcondv
LOGICAL*4       bwork(n)
REAL*8          rwork(n)
COMPLEX*16      a(lda, n), vs(ldvs, n), w(n), work(lwork)
LOGICAL*4       select
EXTERNAL        select
CALL ZGEESX(jobvs, sort, select, sense, n, a, lda, sdim, w, vs, ldvs,
   rconde, rcondv, work, lwork, rwork, bwork, info)
```

LAPACK8:

```
CHARACTER*1     jobvs, sense, sort
INTEGER*8       info, lda, ldvs, liwork, lwork, n, sdim
REAL*8          rconde, rcondv
LOGICAL*8       bwork(n)
INTEGER*4       iwork(liwork)
REAL*8          a(lda, n), vs(ldvs, n), wi(n), work(lwork), wr(n)
LOGICAL*8       select
EXTERNAL        select
CALL SGEESX(jobvs, sort, select, sense, n, a, lda, sdim, wr, wi, vs, ldvs,
  rconde, rcondv, work, lwork, iwork, liwork, bwork, info)

CHARACTER*1     jobvs, sense, sort
INTEGER*8       info, lda, ldvs, lwork, n, sdim
REAL*8          rconde, rcondv
LOGICAL*8       bwork(n)
REAL*8          rwork(n)
COMPLEX*16      a(lda, n), vs(ldvs, n), w(n), work(lwork)
LOGICAL*8       select
EXTERNAL        select
CALL CGEESX(jobvs, sort, select, sense, n, a, lda, sdim, w, vs, ldvs,
  rconde, rcondv, work, lwork, rwork, bwork, info)
```

Input

jobvs Specifies whether the Schur vectors are to be computed, as follows:

jobvs 'N' or 'n':	Schur vectors are not computed.
jobvs = 'V' or 'v':	Schur vectors are computed.

sort Specifies whether the eigenvalues on the diagonal of the Schur Form are to be reordered, as follows:

sort = 'N' or 'n':	The eigenvalues are not specially ordered.

sort = 'S' or 's': The eigenvalues are ordered so that the eigenvalues λ_j for which the LOGICAL function **select**(**wr**(j),**wi**(j)) (in SGEESX and DGEESX) or **select**(**w**(j)) (in CGEESX and ZGEESX) is true will appear at the top left corner of the Schur Form. (In SGEESX and DGEESX, if an eigenvalue is complex and either **select**(**wr**(j),**wi**(j)) or **select**(**wr**(j),–**wi**(j)) is true, both eigenvalues are selected.)

select The name of a user-defined function subprogram used if **sort** = 'S' or 's' to select eigenvalues to reorder to the upper left of the Schur Form. For SGEESX and DGEESX, **select** requires two arguments of the same type as **wr** and **wi**, while for CGEESX and ZGEESX, **select** requires one argument of the same type as **w**. The eigenvalue λ_j is selected if **select**(**wr**(j),**wi**(j)) or **select**(**w**(j)) is true. Note that a selected complex eigenvalue may no longer satisfy **select**(λ_j) = .TRUE. after ordering, since ordering may perturb the value of complex eigenvalues, and especially ill-conditioned ones; in this case **info** may be set to a positive value (see **info** below). **select** must be declared EXTERNAL in the calling subroutine. **select** is not referenced if **sort** = 'N' or 'n'.

sense Specifies which reciprocal condition numbers are to be computed, as follows:

sense = 'N' or 'n': None.

sense = 'E' or 'e': Compute **rconde** only.

sense = 'V' or 'v': Compute **rcondv** only.

sense = 'B' or 'b': Compute both **rconde** and **rcondv**.

If **sense** = 'E' or 'e' or 'V' or 'v' or 'B' or 'b', then **sort** must be 'S' or 's'.

n The order of the matrix A. **n** ≥ 0.

a The **n**-by-**n** matrix A.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

ldvs The leading dimension of array **vs** in the calling program unit. **ldvs** ≥ 1, and if **jobvs** = 'V' or 'v', then **ldvs** ≥ **n**.

lwork The length of array **work**. **lwork** ≥ max(1,3**n**). If **sense** = 'E' or 'e' or 'V' or 'v' or 'B' or 'b', then **lwork** ≥ **n** + 2**sdim**×(**n**–**sdim**) where **sdim** is the total number of eigenvalues selected. Note that **n** + 2**sdim**×(**n**–**sdim**) ≤ **n**×(1+**n**/2). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

liwork The length of array **iwork**. If **sense** = 'V' or 'v' or 'B' or 'b', then **lwork** ≥ **sdim**×(**n**–**sdim**) where **sdim** is the total number of eigenvalues selected.

Not referenced if **sense** = 'N' or 'n' or 'E' or 'e'.

Working Storage

work An array used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

iwork An array used for work space. Not referenced if **sense** = 'N' or 'n' or 'E' or 'e'.

rwork An array used for work space.

bwork An array used for work space. Not referenced if **sort** = 'N' or 'n'.

Output

a On successful exit, the Schur Form of A overwrites the input. If **sort** = 'S' or 's', the output Schur Form is

$$\begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}$$

where A_{11} is **sdim**-by-**sdim**, A_{12} is **sdim**-by-(**n**–**sdim**), and A_{22} is (**n**–**sdim**)-by-(**n**–**sdim**), and where the eigenvalues $\lambda_j, j = 1, 2, ...,$ **sdim**, of A_{11} satisfy **select**(λ_j) = .TRUE. and the eigenvalues $\lambda_j, j =$ **sdim**+1, **sdim**+2, ..., **n**, of A_{22} satisfy **select**(λ_j) = .FALSE.

sdim If **sort** = 'N' or 'n', **sdim** = 0.

If **sort** = 'S' or 's', **sdim** is the number of eigenvalues (after reordering) for which **select** is true. In SGEESX and DGEESX, complex conjugate pairs for which **select** is true for either eigenvalue count as 2.

wr, wi On successful exit from SGEESX and DGEESX, **wr**(j) and **wi**(j) contain the real and imaginary parts, respectively, of the computed eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are in the same order in which they appear as the eigenvalues of the diagonal 1-by-1 and 2-by-2 blocks of the Schur Form. Complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having the positive imaginary part first.

w On successful exit from CGEESX and ZGEESX, **w**(j) contains the computed eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are in the same order in which they appear on the diagonal of the Schur Form.

vs On successful exit, if **jobvs** = 'V' or 'v', the Schur vectors of A. Not referenced if **jobvs** = 'N' or 'n'.

rconde On successful exit, if **sense** = 'E' or 'e' or 'B' or 'b', the reciprocal condition number for the average of the selected eigenvalues. **rconde** measures the sensitivity of the average of the eigenvalues of A_{11}:

$$(\lambda_1 + \lambda_2 + ... + \lambda_{\mathbf{sdim}})/\mathbf{sdim}$$

$0 \le$ **rconde** ≤ 1, with **rconde** [απε] 0 indicating very poor conditioning, and **rconde** [απε] 1 indicating very good conditioning. **rconde** is computed as follows. First, we compute R so that

$$P = \begin{bmatrix} I & R \\ 0 & 0 \end{bmatrix}$$

is the projector on the invariant subspace associated with A_{11}. R is the solution of the Sylvester equation

$$A_{11}R - RA_{22} = A_{12}.$$

Then **rconde** = $(1+\|R\|_F^2)^{-1/2}$, where $\|\ \ \|_F$ is the Frobenius norm. **rconde** underestimates the true reciprocal condition number, but not by more than a factor of $\sqrt{n}$.

An approximate bound on the error between the computed average of the eigenvalues of A_{11} is $\epsilon\|A\|$/**rconde**, where ϵ is the machine precision.

rcondv On successful exit, if **sense** = 'V' or 'v' or 'B' or 'b', the reciprocal condition number for the average of the selected right invariant subspace, that is, the subspace spanned by A_{11}. **rcondv** is defined as the separation of A_{11} and A_{22}:

$$\text{sep}(A_{11}, A_{22}) = \sigma_{min}(K)$$

where σ_{min} is the smallest singular value of the **sdim**×(**n**–**sdim**)-by-**sdim**×(**n**–**sdim**) matrix

$$K = I_{\mathbf{n-sdim}} \otimes A_{11} - A_{22}^T \otimes I_{\mathbf{sdim}}$$

where I_m is an m-by-m identity matrix and ⊗denotes the Kronecker product. The smallest singular value is approximated by the reciprocal of an estimate of $\|K^{-1}\|_1$. **rconde** cannot differ from the true reciprocal condition number by more than a factor of (**sdim**×(**n**–**sdim**))$^{1/2}$. When **rcondv** is small, small changes in A can cause large changes in the invariant subspace spanned by A_{11}. An approximate bound on the maximum angular error in the computed invariant subspace is $\epsilon\|A\|$/**rcondv**, where ϵ is the machine precision.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = –k, the k-th argument had an invalid value.
info > 0:	The algorithm terminated before completing the requested computation.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobvs ≠ 'N' or 'n' or 'V' or 'v',
sort ≠ 'N' or 'n' or 'S' or 's',
sense ≠ 'N' or 'n' or 'E' or 'e' or 'V' or 'v' or 'B' or 'b',
sense = 'E' or 'e' or 'V' or 'v' or 'B' or 'b' and **sort** ≠ 'S' or 's',
n < 0,
lda < max(1,**n**),
ldvs too small, and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobvs** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SGEEVX/DGEEVX/CGEEVX/ZGEEVX – General Matrix Eigenproblem

Purpose

These subprograms compute all eigenvalues and, optionally, all left and right eigenvectors of an n-by-n nonsymmetric matrix A. Optionally, A may be balanced to improve the conditioning of its eigenvalues and eigenvectors. Balancing a matrix means permuting its rows and columns into a more nearly upper triangular form, and computing a similar matrix DAD^{-1}, where D is a diagonal scaling matrix, to make its rows and columns closer in norm and the condition numbers of its eigenvalues and eigenvectors smaller.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Optionally, the z_i, which are called right eigenvectors, also may be computed. In addition, these subprograms also can compute the left eigenvectors, which satisfy

$$y_i{}^*A = \lambda_i y_i{}^*.$$

Also optionally, two sets of condition numbers may be estimated; one set measures the sensitivity of the eigenvalues to errors in the matrix or to small roundoff errors introduced during the computation, and the other set estimates the conditioning of the eigenvectors.

Usage

LAPACK:

```
CHARACTER*1     balanc, jobvl, jobvr, sense
INTEGER*4       ihi, ilo, info, lda, ldvl, ldvr, lwork, n
REAL*4          abnrm
INTEGER*4       iwork(max(1,2*n-2))
REAL*4          a(lda, n), rconde(n), rcondv(n), scale(n), vl(ldvl, n),
                vr(ldvr, n), wi(n), work(lwork), wr(n)
CALL SGEEVX(balanc, jobvl, jobvr, sense, n, a, lda, wr, wi, vl, ldvl, vr,
  ldvr, ilo, ihi, scale, abnrm, rconde, rcondv, work, lwork, iwork, info)

CHARACTER*1     balanc, jobvl, jobvr, sense
INTEGER*4       ihi, ilo, info, lda, ldvl, ldvr, lwork, n
REAL*8          abnrm
INTEGER*4       iwork(max(1,2*n-2))
REAL*8          a(lda, n), rconde(n), rcondv(n), scale(n), vl(ldvl, n),
                vr(ldvr, n), wi(n), work(lwork), wr(n)
CALL DGEEVX(balanc, jobvl, jobvr, sense, n, a, lda, wr, wi, vl, ldvl, vr,
  ldvr, ilo, ihi, scale, abnrm, rconde, rcondv, work, lwork, iwork, info)
```

```
CHARACTER*1     balanc, jobvl, jobvr, sense
INTEGER*4       ihi, ilo, info, lda, ldvl, ldvr, lwork, n
REAL*4          abnrm
REAL*4          rconde(n), rcondv(n), rwork(2*n), scale(n)
COMPLEX*8       a(lda, n), vl(ldvl, n), vr(ldvr, n), w(n), work(lwork)
CALL CGEEVX(balanc, jobvl, jobvr, sense, n, a, lda, w, vl, ldvl, vr, ldvr,
  ilo, ihi, scale, abnrm, rconde, rcondv, work, lwork, rwork, info)

CHARACTER*1     balanc, jobvl, jobvr, sense
INTEGER*4       ihi, ilo, info, lda, ldvl, ldvr, lwork, n
REAL*8          abnrm
REAL*8          rconde(n), rcondv(n), rwork(2*n), scale(n)
COMPLEX*16      a(lda, n), vl(ldvl, n), vr(ldvr, n), w(n), work(lwork)
CALL ZGEEVX(balanc, jobvl, jobvr, sense, n, a, lda, w, vl, ldvl, vr, ldvr,
  ilo, ihi, scale, abnrm, rconde, rcondv, work, lwork, rwork, info)
```

LAPACK8:

```
CHARACTER*1     balanc, jobvl, jobvr, sense
INTEGER*8       ihi, ilo, info, lda, ldvl, ldvr, lwork, n
REAL*8          abnrm
INTEGER*8       iwork(max(1,2*n–2))
REAL*8          a(lda, n), rconde(n), rcondv(n), scale(n), vl(ldvl, n),
                vr(ldvr, n), wi(n), work(lwork), wr(n)
CALL SGEEVX(balanc, jobvl, jobvr, sense, n, a, lda, wr, wi, vl, ldvl, vr,
  ldvr, ilo, ihi, scale, abnrm, rconde, rcondv, work, lwork, iwork, info)

CHARACTER*1     balanc, jobvl, jobvr, sense
INTEGER*8       ihi, ilo, info, lda, ldvl, ldvr, lwork, n
REAL*8          abnrm
REAL*8          rconde(n), rcondv(n), rwork(2*n), scale(n)
COMPLEX*16      a(lda, n), vl(ldvl, n), vr(ldvr, n), w(n), work(lwork)
CALL CGEEVX(balanc, jobvl, jobvr, sense, n, a, lda, w, vl, ldvl, vr, ldvr,
  ilo, ihi, scale, abnrm, rconde, rcondv, work, lwork, rwork, info)
```

Input

balanc Specifies how A should be permuted and diagonally scaled to improve the conditioning of its eigenvalues and eigenvectors, as follows:

- **balanc** = 'N' or 'n': Do not permute or diagonally scale A.
- **balanc** = 'P' or 'p': Permute A into a more nearly upper triangular form, but do not diagonally scale A.

balanc = 'S' or 's': Scale A, that is, replace A by DAD^{-1} where D is a diagonal scaling matrix chosen to make the rows and columns of DAD^{-1}more equal in norm, but do not permute A.

balanc = 'B' or 'b': Both permute and diagonally scale A.

jobvl Specifies whether the left eigenvectors of A are to be computed, as follows:

jobvl = 'N' or 'n': Do not compute the left eigenvectors.

jobvl = 'V' or 'v': Compute the left eigenvectors.

jobvr Specifies whether the right eigenvectors of A are to be computed, as follows:

jobvr = 'N' or 'n': Do not compute the right eigenvectors.

jobvr = 'V' or 'v': Compute the right eigenvectors.

sense Specifies which reciprocal condition numbers are to be computed, as follows:

sense = 'N' or 'n': None.

sense = 'E' or 'e': Compute **rconde** only.

sense = 'V' or 'v': Compute **rcondv** only.

sense = 'B' or 'b': Compute both **rconde** and **rcondv**.

If **sense** = 'E' or 'e' or 'B' or 'b', both the left and right eigenvectors must also be computed, that is, **jobvl** = 'V' or 'v' and **jobvr** = 'V' or 'v'.

n The order of the matrix A. $\mathbf{n} \geq 0$.

a The **n**-by-**n** matrix whose eigenvalues and eigenvectors are desired.

lda The leading dimension of array **a** in the calling program unit. $\mathbf{lda} \geq \max(1,\mathbf{n})$.

ldvl The leading dimension of array **vl** in the calling program unit. $\mathbf{ldvl} \geq 1$, and if **jobvl** = 'V' or 'v', then $\mathbf{ldvl} \geq \mathbf{n}$.

ldvr The leading dimension of array **vr** in the calling program unit. $\mathbf{ldvr} \geq 1$, and if **jobvr** = 'V' or 'v', then $\mathbf{ldvr} \geq \mathbf{n}$.

lwork The length of array **work**. For SGEEVX and DGEEVX, if **sense** = 'N' or 'n' or 'E' or 'e', $\mathbf{lwork} \geq \max(1,2\mathbf{n})$, and if **jobvl** = 'V' or 'v' or **jobvr** = 'V' or 'v', $\mathbf{lwork} \geq \max(1,3\mathbf{n})$. If **sense** = 'V' or 'v' or 'B' or 'b', $\mathbf{lwork} \geq \mathbf{n}\times(\mathbf{n}+6)$.

For CGEEVX and ZGEEVX, if **sense** = 'N' or 'n' or 'E' or 'e', **lwork** ≥ max(1,2**n**). If **sense** = 'V' or 'v' or 'B' or 'b', **lwork** ≥ **n**×(**n**+2).

For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work, iwork, rwork — Arrays used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance. **iwork** is not referenced if **sense** = 'N' or 'n' or 'E' or 'e'.

Output

a — Destroyed.

wr, wi — On successful exit from SGEEVX and DGEEVX, **wr**(j) and **wi**(j) contain the real and imaginary parts, respectively, of the computed eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are not in any particular order, except that complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having the positive imaginary part first.

w — On successful exit from CGEEVX and ZGEEVX, **w**(j) contains the computed eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are not in any particular order.

vl — On successful exit, if **jobvl** = 'V' or 'v', the left eigenvectors, $y_j, j = 1, 2, ..., \mathbf{n}$, stored one after another in the columns of **vl**, in the same order as the eigenvalues. The eigenvectors are normalized to have Euclidean norm equal to 1, and to have the largest component real.

In SGEEVX and DGEEVX, a left eigenvector corresponding to a real eigenvalue is real and takes up one column. An eigenvector pair corresponding to a complex conjugate pair of eigenvalues is complex and takes up two columns: the first column holds the real part and the second column holds the imaginary part of the eigenvector corresponding to the eigenvalue with positive imaginary part.

Therefore, if **wi**(j) > 0, the left eigenvector corresponding to **wr**(j) + i**wi**(j) is **vl**(j) + i**vl**(j+1), and if **wi**(j) < 0, the left eigenvector corresponding to **wr**(j) + i**wi**(j) is **vl**(j–1) – i**vl**(j), where $i = \sqrt{-1}$.

In CGEEVX and ZGEEVX, each left eigenvector takes up one column.

Not referenced if **jobvl** = 'N' or 'n'.

vr On successful exit, if **jobvr** = 'V' or 'v', the right eigenvectors, $z_j, j = 1, 2, ..., \mathbf{n}$, stored one after another in the columns of **vr**, in the same order as their eigenvalues. The eigenvectors are normalized to have Euclidean norm equal to 1, and to have the largest component real.

In SGEEVX and DGEEVX, a right eigenvector corresponding to a real eigenvalue is real and takes up one column. An eigenvector pair corresponding to a complex conjugate pair of eigenvalues is complex and takes up two columns: the first column holds the real part and the second column holds the imaginary part of the eigenvector corresponding to the eigenvalue with positive imaginary part.

Therefore, if **wi**(j) > 0, the right eigenvector corresponding to **wr**(j) + i**wi**(j) is **vr**(j) + i**vr**(j+1), and if **wi**(j) < 0, the right eigenvector corresponding to **wr**(j) + i**wi**(j) is **vr**(j–1) – i**vr**(j), where $i = \sqrt{-1}$.

In CGEEVX and ZGEEVX, each right eigenvector takes up one column.

Not referenced if **jobvr** = 'N' or 'n'.

ilo, ihi, scale On successful exit, information about the permutations and diagonal scaling factors used in balancing. The permutations consist of row and column interchanges which put the matrix in the form

$$PAP = \begin{bmatrix} T_{11} & X & Y \\ 0 & B & Z \\ 0 & 0 & T_{33} \end{bmatrix}$$

where T_{11} and T_{33} are upper triangular matrices. The indices **ilo** and **ihi** are the beginning and ending rows and columns of submatrix B. P is a product of transpositions:

$$P = (\mathbf{ilo}-1,\ P_{\mathbf{ilo}-1}) \ldots (2,\ P_2)\ (1,\ P_1)\ (\mathbf{ihi}+1,\ P_{\mathbf{ihi}+1}) \ldots (\mathbf{n}-1,\ P_{\mathbf{n}-1})\ (\mathbf{n},\ P_{\mathbf{n}})$$

where $(j,\ P_j)$ denotes the transposition that interchanges j with P_j.

Scaling consists of applying a diagonal similarity transformation, $D^{-1}BD$ to make the 1-norms of each row of B and its corresponding column nearly equal.

The contents of **scale** is as follows:

$$\mathbf{scale}(j) = \begin{cases} P_j & \text{for } j = 1,\ 2,\ \ldots,\ \mathbf{ilo}-1 \\ D_{jj} & \text{for } j = \mathbf{ilo},\ \mathbf{ilo}+1,\ \ldots,\ \mathbf{ihi} \\ P_j & \text{for } j = \mathbf{ihi}+1,\ \mathbf{ihi}+2,\ \ldots,\ \mathbf{n}. \end{cases}$$

abnrm On successful exit, the one-norm of the balanced matrix.

rconde On successful exit, **rconde**(j) is the reciprocal condition number of eigenvalue λ_j with respect to the balanced matrix, defined as

$$\mathbf{rconde}(j) = |y_j{}^* z_j|$$

where y_j and z_j are left and right unit eigenvectors, respectively, corresponding to λ_j. $0 \le \mathbf{rconde}(j) \le 1$, with **rconde**($j$) ≈ 0 indicating that λ_j is very poorly conditioned, and **rconde**(j) ≈ 1 indicating that λ_j is very well conditioned.

An approximate bound on the error between the computed eigenvalue $\tilde{\lambda}_j$ and the correct eigenvalue λ_j is given by

$$|\tilde{\lambda}_j - \lambda_j| <\approx \varepsilon ||A||_1 / \mathbf{rconde}(j)$$

where ϵ is the machine precision.

rcondv On successful exit, **rcondv**(j) is an approximation to the reciprocal condition number of the right eigenvector z_j corresponding to λ_j, defined as follows. Suppose T is the Schur Form of A (see SGEESX) with $T_{11} = \lambda_j$:

$$Q^*AQ = \begin{bmatrix} \lambda_j & T_{12} \\ 0 & T_{22} \end{bmatrix}$$

where T_{12} is 1-by-(**n**–1) and T_{22} is (**n**–1)-by-(**n**–1). Then

$$\mathbf{rcondv}(j) = \sigma_{min}(T_{22} - \lambda_j I)$$

where σ_{min} denotes the smallest singular value. The smallest singular value is approximated by the reciprocal of an estimate of $\|(T_{22} - \lambda_j I)^{-1}\|_1$.

When **rcondv**(j) is small, small changes in the matrix can cause large changes in z_j. If **balanc** = 'N' or 'n' or 'P' or 'p', an approximate bound for a computed right eigenvector z_j is given by

$$\theta(\tilde{z}_j, z_j) <\approx \varepsilon \, \mathbf{abnrm} / \mathbf{rcondv}(j$$

where $\theta(x,y)$ is the angle between vectors x and y, and where ϵ is the machine precision.

The interpretation of **rcondv**(j) is more complicated when **balanc** = 'S' or 's' or 'B' or 'b'. See (Anderson, *et al*

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

info > 0:	The *QR* algorithm failed to converge on all the eigenvalues; if **info** = k, elements 1, 2, ..., **ilo**–1 and k+1, k+2, ..., **n** of **wr** and **wi** or **w** contain eigenvalues which have converged. No eigenvectors have been computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

balanc ≠ 'N' or 'n' or 'P' or 'p' or 'S' or 's' or 'B' or 'b',
jobvl ≠ 'N' or 'n' or 'V' or 'v',
jobvr ≠ 'N' or 'n' or 'V' or 'v',
sense ≠ 'N' or 'n' or 'E' or 'e' or 'V' or 'v' or 'B' or 'b',
sense = 'E' or 'e' or 'B' or 'b' and **jobvl** ≠ 'V' or 'v',
sense = 'E' or 'e' or 'B' or 'b' and **jobvr** ≠ 'V' or 'v',
n < 0,
lda < max(1,**n**),
ldvl too small,
ldvr too small, and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobvl** and **jobvr** arguments as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSBEVX/DSBEVX/.../ZHBEVX – Symmetric or Hermitian Band Matrix

Purpose

These subprograms compute selected eigenvalues and, optionally, corresponding eigenvectors of a real symmetric or complex Hermitian matrix band matrix. The desired eigenvalues can be selected by specifying either a range of values or a range of indices.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, and since either triangle of A may be obtained from the other, you need only provide the band within one triangle of A. Compared to storing the entire matrix, this can save memory in two ways: only the elements within the band are stored, and of them, only the upper or the lower triangle.

The following examples illustrate the storage of real symmetric band matrices. Consider the following matrix A of order $n = 7$ and half bandwidth $kd = 2$:

11	12	13	0	0	0	0
12	22	23	24	0	0	0
13	23	33	34	35	0	0
0	24	34	44	45	46	0
0	0	35	45	55	56	57
0	0	0	46	56	66	67
0	0	0	0	57	67	77

Upper triangular storage. The upper triangle of the matrix A is stored in an array **ab** with at least $kd+1 = 3$ rows and 7 columns as follows:

*	*	13	24	35	46	57
*	12	23	34	45	56	67
11	22	33	44	55	66	77

The asterisks represent elements in the *kd*-by-*kd* triangle at the upper left corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the upper triangle of *A*, it is stored in **ab**(*kd*+1+*i*–*j*,*j*). Therefore, the columns of the upper triangle of *A* are stored in the columns of **ab**, and the diagonals of the upper triangle of *A* are stored in the rows of **ab**.

Lower triangular storage. The lower triangle of A is stored in the array **ab** as follows:

11	22	33	44	55	66	77
12	23	34	45	56	67	*
13	24	35	46	57	*	*

The asterisks represent elements in the *kd*-by-*kd* triangle at the lower right corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the lower triangle of *A*, it is stored in **ab**(1+*i*–*j*,*j*). Therefore, the columns of the lower triangle of *A* are stored in the columns of **ab**, and the diagonals of the lower triangle of *A* are stored in the rows of **ab**.

Usage

LAPACK:

CHARACTER*1 **jobz, range, uplo**
INTEGER*4 **il, info, iu, kd, ldab, ldq, ldz, m, n**
REAL*4 **abstol, vl, vu**
INTEGER*4 **ifail(n), iwork(5*n)**
REAL*4 **ab(ldab, n), q(ldq, n), w(n), work(6*n), z(ldz, n)**
CALL SSBEVX(jobz, range, uplo, n, kd, ab, ldab, q, ldq, vl, vu, il, iu, abstol, m, w, z, ldz, work, iwork, ifail, info)

CHARACTER*1 **jobz, range, uplo**
INTEGER*4 **il, info, iu, kd, ldab, ldq, ldz, m, n**
REAL*8 **abstol, vl, vu**
INTEGER*4 **ifail(n), iwork(5*n)**
REAL*8 **ab(ldab, n), q(ldq, n), w(n), work(6*n), z(ldz, n)**
CALL DSBEVX(jobz, range, uplo, n, kd, ab, ldab, q, ldq, vl, vu, il, iu, abstol, m, w, z, ldz, work, iwork, ifail, info)

CHARACTER*1 **jobz, range, uplo**
INTEGER*4 **il, info, iu, kd, ldab, ldq, ldz, m, n**
REAL*4 **abstol, vl, vu**
INTEGER*4 **ifail(n), iwork(5*n)**
REAL*4 **rwork(6*n), w(n)**
COMPLEX*8 **ab(ldab, n), q(ldq, n), work(n), z(ldz, n)**
CALL CHBEVX(jobz, range, uplo, n, kd, ab, ldab, q, ldq, vl, vu, il, iu, abstol, m, w, z, ldz, work, rwork, iwork, ifail, info)

```
CHARACTER*1     jobz, range, uplo
INTEGER*4       il, info, iu, kd, ldab, ldq, ldz, m, n
REAL*8          abstol, vl, vu
INTEGER*4       ifail(n), iwork(5*n)
REAL*8          rwork(6*n), w(n)
COMPLEX*16      ab(ldab, n), q(ldq, n), work(n), z(ldz, n)
CALL ZHBEVX(jobz, range, uplo, n, kd, ab, ldab, q, ldq, vl, vu, il, iu,
  abstol, m, w, z, ldz, work, rwork, iwork, ifail, info)
```

LAPACK8:

```
CHARACTER*1     jobz, range, uplo
INTEGER*8       il, info, iu, kd, ldab, ldq, ldz, m, n
REAL*8          abstol, vl, vu
INTEGER*8       ifail(n), iwork(5*n)
REAL*8          ab(ldab, n), q(ldq, n), w(n), work(6*n), z(ldz, n)
CALL SSBEVX(jobz, range, uplo, n, kd, ab, ldab, q, ldq, vl, vu, il, iu, abstol,
  m, w, z, ldz, work, iwork, ifail, info)
```

```
CHARACTER*1     jobz, range, uplo
INTEGER*8       il, info, iu, kd, ldab, ldq, ldz, m, n
REAL*8          abstol, vl, vu
INTEGER*8       ifail(n), iwork(5*n)
REAL*8          rwork(6*n), w(n)
COMPLEX*16      ab(ldab, n), q(ldq, n), work(n), z(ldz, n)
CALL CHBEVX(jobz, range, uplo, n, kd, ab, ldab, q, ldq, vl, vu, il, iu,
  abstol, m, w, z, ldz, work, rwork, iwork, ifail, info)
```

Input

jobz Specifies whether eigenvectors are to be computed, as follows:

- **jobz** = 'N' or 'n': Compute eigenvalues only.
- **jobz** = 'V' or 'v': Compute eigenvectors as well.

range Specifies which eigenvalues are to be computed, as follows:

- **range** = 'A' or 'a': All eigenvalues are to be computed.
- **range** = 'V' or 'v': Eigenvalues λ with $\mathbf{vl} < \lambda \leq \mathbf{vu}$ are to be computed.
- **range** = 'I' or 'i': Eigenvalues $\lambda_{\mathbf{il}}$ through $\lambda_{\mathbf{iu}}$ are to be computed.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.

uplo = 'L' or '1': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

kd The number of super-diagonals of the matrix A if **uplo** = 'U' or 'u', or the number of subdiagonals if **uplo** = 'L' or '1'. $\mathbf{kd} \geq 0$.

ab The upper or lower triangle of the symmetric or Hermitian band matrix, stored in the first **kd**+1 rows of array **ab**. The j-th column of A is stored in the j-th column of array **ab** as follows:

If **uplo** = 'U' or 'u', $\mathbf{ab}(\mathbf{kd}+1+i-j,j) = A(i,j)$ for $\max(1,j-\mathbf{kd}) \leq i \leq j$;

If **uplo** = 'L' or '1', $\mathbf{ab}(1+i-j,j) = A(i,j)$ for $j \leq i \leq \min(\mathbf{n},j+\mathbf{kd})$.

ldab The leading dimension of array **ab** in the calling program unit. $\mathbf{ldab} \geq \max(1,\mathbf{n})$.

ldq The leading dimension of array **q** in the calling program unit. If **jobz** = 'V' or 'v', then $\mathbf{ldq} \geq \max(1,\mathbf{n})$.

vl If **range** = 'V' or 'v', the left endpoint of the interval of selected eigenvalues. Only eigenvalues $\lambda > \mathbf{vl}$ are returned. $\mathbf{vl} < \mathbf{vu}$.

Not referenced if **range** = 'A' or 'a' or 'I' or 'i'.

vu If **range** = 'V' or 'v', the right endpoint of the interval of selected eigenvalues. Only eigenvalues $\lambda \leq \mathbf{vu}$ are returned. $\mathbf{vu} > \mathbf{vl}$.

Not referenced if **range** = 'A' or 'a' or 'I' or 'i'.

il If **range** = 'I' or 'i', the index of the smallest eigenvalue to be computed. If the eigenvalues are ordered so that $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n$, only eigenvalues λ_i with $i \geq \mathbf{il}$ are returned. $\mathbf{il} \geq 1$.

Not referenced if **range** = 'A' or 'a' or 'V' or 'v'.

iu If **range** = 'I' or 'i', the index of the largest eigenvalue to be computed. If the eigenvalues are ordered so that $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n$, only eigenvalues λ_i with $i \leq \mathbf{iu}$ are returned. $\min(\mathbf{il},\mathbf{n}) \leq \mathbf{iu} \leq \mathbf{n}$.

Not referenced if **range** = 'A' or 'a' or 'V' or 'v'.

abstol The absolute error tolerance for the eigenvalues. An approximate eigenvalue is accepted as converged when it is determined to lie in an interval $[a,b]$ of width

$$b-a \leq \textbf{abstol} + \varepsilon \, max(|a|,|b|),$$

where ϵ is the machine precision. If **abstol** ≤ 0, then $\varepsilon\|T\|_1$ is used in its place, where T is the 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**('Safe minimum'), not zero. If this subprogram returns with **info** > 0, indicating that some eigenvectors did not converge, try setting **abstol** to 2**slamch**('Safe minimum').

ldz The leading dimension of array **z** in the calling program unit. **ldz** ≥ max(1,**n**).

Working Storage

work, iwork, rwork Arrays used for work space.

Output

ab Destroyed.

q If **jobz** = 'V' or 'v', the **n**-by-**n** orthogonal or unitary matrix that reduces A to tridiagonal form.

m The total number of selected eigenvalues found. $0 \leq \textbf{m} \leq \textbf{n}$.

w On successful exit, the first **m** elements contain the selected eigenvalues in ascending order.

z On successful exit, if **jobz** = 'V' or 'v', the first **m** columns of **z** contain the orthonormal eigenvectors of the matrix, corresponding to the selected eigenvalues. 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**.

Not referenced if **jobz** = 'N' or 'n'.

ifail Eigenvector convergence status response. On successful exit, if **jobz** = 'V' or 'v', the first **m** elements are zero. If **info** = k > 0, then the first k elements of **ifail** contain the indices of the eigenvectors that failed to converge.

Not referenced if **jobz** = 'N' or 'n'.

info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k, then k eigenvectors failed to converge. Their indices are stored in the first k elements of **ifail**.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
range ≠ 'A' or 'a' or 'V' or 'v' or 'I' or 'i',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
ldab < **kd**+1,
range = 'V' or 'v' and **vu** ≤ **vl**,
range = 'I' or 'i' and **il** < 1,
range = 'I' or 'i' and **iu** < min(**il**,**n**) or **iu** > **n**, and
ldz < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSPEVX/DSPEVX/.../ZHPEVX – Symmetric or Hermitian Packed Matrix

Purpose

These subprograms compute selected eigenvalues and, optionally, corresponding eigenvectors of a real symmetric or complex Hermitian matrix in packed storage. The desired eigenvalues can be selected by specifying either a range of values or a range of indices.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A, either the upper or the lower triangle. Compared to storing the entire matrix, you save memory by supplying that triangle stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular storage. If the lower triangle of A is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**($i+(j-1)\times(2n-j)/2$).

Usage

LAPACK:

```
CHARACTER*1        jobz, range, uplo
INTEGER*4          il, info, iu, ldz, m, n
REAL*4             abstol, vl, vu
INTEGER*4          ifail(n), iwork(5*n)
REAL*4             ap((n*(n+1))/2), w(n), work(7*n), z(ldz, n)
CALL SSPEVX(jobz, range, uplo, n, ap, vl, vu, il, iu, abstol, m, w, z, ldz,
   work, iwork, ifail, info)

CHARACTER*1        jobz, range, uplo
INTEGER*4          il, info, iu, ldz, m, n
REAL*8             abstol, vl, vu
INTEGER*4          ifail(n), iwork(5*n)
REAL*8             ap((n*(n+1))/2), w(n), work(7*n), z(ldz, n)
CALL DSPEVX(jobz, range, uplo, n, ap, vl, vu, il, iu, abstol, m, w, z, ldz,
   work, iwork, ifail, info)

CHARACTER*1        jobz, range, uplo
INTEGER*4          il, info, iu, ldz, m, n
REAL*4             abstol, vl, vu
INTEGER*4          ifail(n), iwork(5*n)
REAL*4             rwork(6*n), w(n)
COMPLEX*8          ap((n*(n+1))/2), work(2*n), z(ldz, n)
CALL CHPEVX(jobz, range, uplo, n, ap, vl, vu, il, iu, abstol, m, w, z, ldz,
   work, rwork, iwork, ifail, info)
```

```
CHARACTER*1     jobz, range, uplo
INTEGER*4       il, info, iu, ldz, m, n
REAL*8          abstol, vl, vu
INTEGER*4       ifail(n), iwork(5*n)
REAL*8          rwork(6*n), w(n)
COMPLEX*16      ap((n*(n+1))/2), work(2*n), z(ldz, n)
CALL ZHPEVX(jobz, range, uplo, n, ap, vl, vu, il, iu, abstol, m, w, z, ldz,
  work, rwork, iwork, ifail, info)
```

LAPACK8:

```
CHARACTER*1     jobz, range, uplo
INTEGER*8       il, info, iu, ldz, m, n
REAL*8          abstol, vl, vu
INTEGER*8       ifail(n), iwork(5*n)
REAL*8          ap((n*(n+1))/2), w(n), work(7*n), z(ldz, n)
CALL SSPEVX(jobz, range, uplo, n, ap, vl, vu, il, iu, abstol, m, w, z, ldz,
  work, iwork, ifail, info)
```

```
CHARACTER*1     jobz, range, uplo
INTEGER*8       il, info, iu, ldz, m, n
REAL*8          abstol, vl, vu
INTEGER*8       ifail(n), iwork(5*n)
REAL*8          rwork(6*n), w(n)
COMPLEX*16      ap((n*(n+1))/2), work(2*n), z(ldz, n)
CALL CHPEVX(jobz, range, uplo, n, ap, vl, vu, il, iu, abstol, m, w, z, ldz,
  work, rwork, iwork, ifail, info)
```

Input

jobz Specifies whether eigenvectors are to be computed, as follows:

- **jobz** = 'N' or 'n': Compute eigenvalues only.
- **jobz** = 'V' or 'v': Compute eigenvectors as well.

range Specifies which eigenvalues are to be computed, as follows:

- **range** = 'A' or 'a': All eigenvalues are to be computed.
- **range** = 'V' or 'v': Eigenvalues λ with $\mathbf{vl} < \lambda \leq \mathbf{vu}$ are to be computed.
- **range** = 'I' or 'i': Eigenvalues $\lambda_{\mathbf{il}}$ through $\lambda_{\mathbf{iu}}$ are to be computed.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.

uplo = 'L' or '1': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

ap The upper or lower triangular part of the symmetric or Hermitian matrix A, packed columnwise in a linear array as follows:

If **uplo** = 'U' or 'u', $\mathbf{ap}(i + (j-1) \times j/2) = A(i,j)$ for $1 \leq i \leq j$;

If **uplo** = 'L' or '1', $\mathbf{ap}(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \leq i \leq \mathbf{n}$.

vl If **range** = 'V' or 'v', the left endpoint of the interval of selected eigenvalues. Only eigenvalues $\lambda > \mathbf{vl}$ are returned. $\mathbf{vl} < \mathbf{vu}$.

Not referenced if **range** = 'A' or 'a' or 'I' or 'i'.

vu If **range** = 'V' or 'v', the right endpoint of the interval of selected eigenvalues. Only eigenvalues $\lambda \leq \mathbf{vu}$ are returned. $\mathbf{vu} > \mathbf{vl}$.

Not referenced if **range** = 'A' or 'a' or 'I' or 'i'.

il If **range** = 'I' or 'i', the index of the smallest eigenvalue to be computed. If the eigenvalues are ordered so that $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n$, only eigenvalues λ_i with $i \geq \mathbf{il}$ are returned. $\mathbf{il} \geq 1$.

Not referenced if **range** = 'A' or 'a' or 'V' or 'v'.

iu If **range** = 'I' or 'i', the index of the largest eigenvalue to be computed. If the eigenvalues are ordered so that $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n$, only eigenvalues λ_i with $i \leq \mathbf{iu}$ are returned. $\min(\mathbf{il},\mathbf{n}) \leq \mathbf{iu} \leq \mathbf{n}$.

Not referenced if **range** = 'A' or 'a' or 'V' or 'v'.

abstol The absolute error tolerance for the eigenvalues. An approximate eigenvalue is accepted as converged when it is determined to lie in an interval $[a,b]$ of width

$$b-a \leq \mathbf{abstol} + \epsilon \, max(|a|,|b|),$$

where ϵ is the machine precision. If $\mathbf{abstol} \leq 0$, then $\epsilon \|T\|_1$ is used in its place, where T is the 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**('Safe minimum'), not zero. If this subprogram returns with **info** > 0, indicating that some eigenvectors did not converge, try setting **abstol** to 2**slamch**('Safe minimum').

ldz — The leading dimension of array **z** in the calling program unit. **ldz** ≥ max(1,**n**).

Working Storage

work, iwork, rwork — Arrays used for work space.

Output

ap — Destroyed.

m — The total number of selected eigenvalues found. 0 ≤ **m** ≤ **n**.

w — On successful exit, the first **m** elements contain the selected eigenvalues in ascending order.

z — On successful exit, if **jobz** = 'V' or 'v', the first **m** columns of **z** contain the orthonormal eigenvectors of the matrix, corresponding to the selected eigenvalues. 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**.

Not referenced if **jobz** = 'N' or 'n'.

ifail — Eigenvector convergence status response. On successful exit, if **jobz** = 'V' or 'v', the first **m** elements are zero. If **info** = k > 0, then the first k elements of **ifail** contain the indices of the eigenvectors that failed to converge.

Not referenced if **jobz** = 'N' or 'n'.

info — Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, then k eigenvectors failed to converge. Their indices are stored in the first k elements of **ifail**.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
range ≠ 'A' or 'a' or 'V' or 'v' or 'I' or 'i',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
range = 'V' or 'v' and **vu** ≤ **vl**,
range = 'I' or 'i' and **il** < 1,
range = 'I' or 'i' and **iu** < min(**il**,**n**) or **iu** > **n**, and
ldz < max(1,**n**).

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSTEVX/DSTEVX – Real Symmetric Tridiagonal Matrix

Purpose

These subprograms compute selected eigenvalues and, optionally, corresponding eigenvectors of a real symmetric tridiagonal matrix. The desired eigenvalues can be selected by specifying either a range of values or a range of indices.

A matrix is symmetric if $A = A^T$, its transpose.

A matrix $A = (a_{ij})$ is tridiagonal if its nonzero elements lie only on the principal diagonal ($i = j$), the subdiagonal ($i = j+1$), and the superdiagonal ($i = j-1$) of the matrix.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i z_i.$$

Matrix Storage

The following example illustrates the storage of symmetric tridiagonal matrices. Consider the following symmetric tridiagonal matrix of order $n = 7$:

11	21	0	0	0	0	0
21	22	32	0	0	0	0
0	32	33	43	0	0	0
0	0	43	44	54	0	0
0	0	0	54	55	65	0
0	0	0	0	65	66	76
0	0	0	0	0	76	77

The subdiagonal is stored in array **e** and the principal diagonal is stored in array **d**, as follows:

i	**e**(i)	**d**(i)
1	21	11
2	32	22
3	43	33
4	54	44
5	65	55
6	76	66
7		77

Usage

LAPACK:

```
CHARACTER*1        jobz, range
INTEGER*4          il, info, iu, ldz, m, n
REAL*4             abstol, vl, vu
INTEGER*4          ifail(n), iwork(5*n)
REAL*4             d(n), e(n–1), w(n), work(4*n), z(ldz, n)
CALL SSTEVX(jobz, range, n, d, e, vl, vu, il, iu, abstol, m, w, z, ldz, work,
   iwork, ifail, info)

CHARACTER*1        jobz, range
INTEGER*4          il, info, iu, ldz, m, n
REAL*8             abstol, vl, vu
INTEGER*4          ifail(n), iwork(5*n)
REAL*8             d(n), e(n–1), w(n), work(4*n), z(ldz, n)
CALL DSTEVX(jobz, range, n, d, e, vl, vu, il, iu, abstol, m, w, z, ldz, work,
   iwork, ifail, info)
```

LAPACK8:

```
CHARACTER*1        jobz, range
INTEGER*8          il, info, iu, ldz, m, n
REAL*8             abstol, vl, vu
INTEGER*8          ifail(n), iwork(5*n)
REAL*8             d(n), e(n–1), w(n), work(4*n), z(ldz, n)
CALL SSTEVX(jobz, range, n, d, e, vl, vu, il, iu, abstol, m, w, z, ldz, work,
   iwork, ifail, info)
```

Input

jobz Specifies whether eigenvectors are to be computed, as follows:

- **jobz** = 'N' or 'n': Compute eigenvalues only.
- **jobz** = 'V' or 'v': Compute eigenvectors as well.

range Specifies which eigenvalues are to be computed, as follows:

- **range** = 'A' or 'a': All eigenvalues are to be computed.
- **range** = 'V' or 'v': Eigenvalues λ with $\mathbf{vl} < \lambda \leq \mathbf{vu}$ are to be computed.
- **range** = 'I' or 'i': Eigenvalues $\lambda_{\mathbf{il}}$ through $\lambda_{\mathbf{iu}}$ are to be computed.

n The order in the matrix A. $\mathbf{n} \geq 0$.

d The **n** diagonal elements of the tridiagonal matrix.

e The **n**–1 subdiagonal elements of the tridiagonal matrix.

vl If **range** = 'V' or 'v', the left endpoint of the interval of selected eigenvalues. Only eigenvalues $\lambda > \mathbf{vl}$ are returned. $\mathbf{vl} < \mathbf{vu}$.

Not referenced if **range** = 'A' or 'a' or 'I' or 'i'.

vu If **range** = 'V' or 'v', the right endpoint of the interval of selected eigenvalues. Only eigenvalues $\lambda \leq \mathbf{vu}$ are returned. $\mathbf{vu} > \mathbf{vl}$.

Not referenced if **range** = 'A' or 'a' or 'I' or 'i'.

il If **range** = 'I' or 'i', the index of the smallest eigenvalue to be computed. If the eigenvalues are ordered so that $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n$, only eigenvalues λ_i with $i \geq \mathbf{il}$ are returned. $\mathbf{il} \geq 1$.

Not referenced if **range** = 'A' or 'a' or 'V' or 'v'.

iu If **range** = 'I' or 'i', the index of the largest eigenvalue to be computed. If the eigenvalues are ordered so that $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n$, only eigenvalues λ_i with $i \leq \mathbf{iu}$ are returned. $\min(\mathbf{il},\mathbf{n}) \leq \mathbf{iu} \leq \mathbf{n}$.

abstol The absolute error tolerance for the eigenvalues. An approximate eigenvalue is accepted as converged when it is determined to lie in an interval $[a,b]$ of width

$$b-a \leq \textbf{abstol} + \epsilon \, max(|a|,|b|),$$

where ϵ is the machine precision. If **abstol** ≤ 0, then $\epsilon \|A\|_1$ is used in its place.

Eigenvalues will be computed most accurately when **abstol** is set to twice the underflow threshold 2**slamch**('Safe minimum'), not zero. If this subprogram returns with **info** > 0, indicating that some eigenvectors did not converge, try setting **abstol** to 2**slamch**('Safe minimum').

ldz The leading dimension of array **z** in the calling program unit. **ldz** ≥ 1, and if **jobz** = 'V' or 'v', then **ldz** $\geq$ **n**.

Working Storage

work, iwork Arrays used for work space.

Output

d Destroyed.

e Destroyed.

m The total number of selected eigenvalues found. $0 \leq$ **m** $\leq$ **n**.

w On successful exit, the first **m** elements contain the selected eigenvalues in ascending order.

z On successful exit, if **jobz** = 'V' or 'v', the orthonormal eigenvectors of the matrix. If an error exit is made, **z** contains the eigenvectors associated with the stored eigenvalues.

Not referenced if **jobz** = 'N' or 'n'.

ifail Eigenvector convergence status response. On successful exit, if **jobz** = 'V' or 'v', the first **m** elements are zero. If **info** = k > 0, then the first k elements of **ifail** contain the indices of the eigenvectors that failed to converge.

Not referenced if **jobz** = 'N' or 'n'.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

info > 0:	If **info** = k, then k eigenvectors failed to converge. Their indices are stored in the first k elements of **ifail**.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
range ≠ 'A' or 'a' or 'V' or 'v' or 'I' or 'i',
n < 0,
range = 'V' or 'v' and **vu** ≤ **vl**,
range = 'I' or 'i' and **il** < 1,
range = 'I' or 'i' and **iu** < min(**il**,**n**) or **iu** > **n**,
ldz too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSYEVX/DSYEVX/CHEEVX/ZHEEVX – Symmetric or Hermitian Matrix

Purpose

These subprograms compute selected eigenvalues and, optionally, corresponding eigenvectors of a real symmetric or complex Hermitian matrix. The desired eigenvalues can be selected by specifying either a range of values or a range of indices.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

Given such a matrix A, the eigenvalues of A are scalars λ_i, $i = 1, 2, \ldots, n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, \ldots, n$, such that

$$Az_i = \lambda_i z_i.$$

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A. You may supply either the upper or the lower triangle of A, in a two-dimensional array large enough to hold the entire matrix. The other triangle of the array is not referenced.

Usage

LAPACK:

```
CHARACTER*1     jobz, range, uplo
INTEGER*4       il, info, iu, lda, ldz, lwork, m, n
REAL*4          abstol, vl, vu
INTEGER*4       ifail(n), iwork(5*n)
REAL*4          a(lda, n), w(n), work(lwork), z(ldz, n)
CALL SSYEVX(jobz, range, uplo, n, a, lda, vl, vu, il, iu, abstol, m, w, z, ldz,
   work, lwork, iwork, ifail, info)

CHARACTER*1     jobz, range, uplo
INTEGER*4       il, info, iu, lda, ldz, lwork, m, n
REAL*8          abstol, vl, vu
INTEGER*4       ifail(n), iwork(5*n)
REAL*8          a(lda, n), w(n), work(lwork), z(ldz, n)
CALL DSYEVX(jobz, range, uplo, n, a, lda, vl, vu, il, iu, abstol, m, w, z, ldz,
   work, lwork, iwork, ifail, info)
```

```
CHARACTER*1     jobz, range, uplo
INTEGER*4       il, info, iu, lda, ldz, lwork, m, n
REAL*4          abstol, vl, vu
INTEGER*4       ifail(n), iwork(5*n)
REAL*4          rwork(6*n), w(n)
COMPLEX*8       a(lda, n), work(lwork), z(ldz, n)
CALL CHEEVX(jobz, range, uplo, n, a, lda, vl, vu, il, iu, abstol, m, w, z, ldz,
  work, lwork, rwork, iwork, ifail, info)
```

```
CHARACTER*1     jobz, range, uplo
INTEGER*4       il, info, iu, lda, ldz, lwork, m, n
REAL*8          abstol, vl, vu
INTEGER*4       ifail(n), iwork(5*n)
REAL*8          rwork(6*n), w(n)
COMPLEX*16      a(lda, n), work(lwork), z(ldz, n)
CALL ZHEEVX(jobz, range, uplo, n, a, lda, vl, vu, il, iu, abstol, m, w, z, ldz,
  work, lwork, rwork, iwork, ifail, info)
```

LAPACK8:

```
CHARACTER*1     jobz, range, uplo
INTEGER*8       il, info, iu, lda, ldz, lwork, m, n
REAL*8          abstol, vl, vu
INTEGER*8       ifail(n), iwork(5*n)
REAL*8          a(lda, n), w(n), work(lwork), z(ldz, n)
CALL SSYEVX(jobz, range, uplo, n, a, lda, vl, vu, il, iu, abstol, m, w, z, ldz,
  work, lwork, iwork, ifail, info)
```

```
CHARACTER*1     jobz, range, uplo
INTEGER*8       il, info, iu, lda, ldz, lwork, m, n
REAL*8          abstol, vl, vu
INTEGER*8       ifail(n), iwork(5*n)
REAL*8          rwork(6*n), w(n)
COMPLEX*16      a(lda, n), work(lwork), z(ldz, n)
CALL CHEEVX(jobz, range, uplo, n, a, lda, vl, vu, il, iu, abstol, m, w, z, ldz,
  work, lwork, rwork, iwork, ifail, info)
```

Input

jobz Specifies whether eigenvectors are to be computed, as follows:

jobz = 'N' or 'n':	Compute eigenvalues only.
jobz = 'V' or 'v':	Compute eigenvectors as well.

range Specifies which eigenvalues are to be computed, as follows:

range = 'A' or 'a':	All eigenvalues are to be computed.
range = 'V' or 'v':	Eigenvalues λ with **vl** $< \lambda \leq$ **vu** are to be computed.

range = 'I' or 'i': Eigenvalues λ_{il} through λ_{iu} are to be computed.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

uplo = 'U' or 'u': The upper triangular part of A is stored.

uplo = 'L' or 'l': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

a The symmetric or Hermitian matrix A.

If **uplo** = 'U' or 'u', only the upper triangular part of **a** is used to define the elements of the matrix and the strict lower triangular part of **a** is not used for input.

If **uplo** = 'L' or 'l', only the lower triangular part of **a** is used to define the elements of the matrix and the strict upper triangular part of **a** is not used for input.

lda The leading dimension of array **a** in the calling program unit. $\mathbf{lda} \geq \max(1,\mathbf{n})$.

vl If **range** = 'V' or 'v', the left endpoint of the interval of selected eigenvalues. Only eigenvalues $\lambda >$ **vl** are returned. **vl** < **vu**.

Not referenced if **range** = 'A' or 'a' or 'I' or 'i'.

vu If **range** = 'V' or 'v', the right endpoint of the interval of selected eigenvalues. Only eigenvalues $\lambda \leq$ **vu** are returned. **vu** > **vl**.

Not referenced if **range** = 'A' or 'a' or 'I' or 'i'.

il If **range** = 'I' or 'i', the index of the smallest eigenvalue to be computed. If the eigenvalues are ordered so that $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n$, only eigenvalues λ_i with $i \geq$ **il** are returned. $\mathbf{il} \geq 1$.

Not referenced if **range** = 'A' or 'a' or 'V' or 'v'.

iu If **range** = 'I' or 'i', the index of the largest eigenvalue to be computed. If the eigenvalues are ordered so that $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n$, only eigenvalues λ_i with $i \leq$ **iu** are returned. $\min(\mathbf{il},\mathbf{n}) \leq \mathbf{iu} \leq \mathbf{n}$.

Not referenced if **range** = 'A' or 'a' or 'V' or 'v'.

abstol The absolute error tolerance for the eigenvalues. An approximate eigenvalue is accepted as converged when it is determined to lie in an interval $[a,b]$ of width

$$b-a \leq \textbf{abstol} + \epsilon \, max(|a|,|b|),$$

where ϵ is the machine precision. If **abstol** ≤ 0, then $\epsilon\|T\|_1$ is used in its place, where T is the 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**('Safe minimum'), not zero. If this subprogram returns with **info** > 0, indicating that some eigenvectors did not converge, try setting **abstol** to 2**slamch**('Safe minimum').

ldz The leading dimension of array **z** in the calling program unit. **ldz** ≥ max(1,**n**).

lwork The length of array **work**. For subprograms SSYEVX and DSYEVX, **lwork** ≥ max(1,7**n**). For subprograms CHEEVX and ZHEEVX, **lwork** ≥ max(1,2**n**–1). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work, iwork, rwork Arrays used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a The triangle of **a** specified by **uplo**, including the diagonal, has been destroyed.

m The total number of selected eigenvalues found. 0 ≤ **m** ≤ **n**.

w On successful exit, the first **m** elements contain the selected eigenvalues in ascending order.

z On successful exit, if **jobz** = 'V' or 'v', the first **m** columns of **z** contain the orthonormal eigenvectors of the matrix, corresponding to the selected eigenvalues. 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**.

Not referenced if **jobz** = 'N' or 'n'.

ifail Eigenvector convergence status response. On successful exit, if **jobz** = 'V' or 'v', the first **m** elements are zero. If **info** = k > 0, then the first k elements of **ifail** contain the indices of the eigenvectors that failed to converge.

Not referenced if **jobz** = 'N' or 'n'.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	If **info** = k, then k eigenvectors failed to converge. Their indices are stored in the first k elements of **ifail**.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
range ≠ 'A' or 'a' or 'V' or 'v' or 'I' or 'i',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
lda < max(1,**n**),
range = 'V' or 'v' and **vu** ≤ **vl**,
range = 'I' or 'i' and **il** < 1,
range = 'I' or 'i' and **iu** < min(**il**,**n**) or **iu** > **n**,
ldz < max(1,**n**), and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

9 Drivers for Generalized Eigenvalue Problems

Overview

This chapter explains how to use LAPACK subprograms to compute the eigenvalues or eigenvalues and eigenvectors of

- Generalized symmetric or Hermitian definite eigenproblems of the forms

  $$Ax = \lambda Bx \quad \text{or} \quad ABx = \lambda x \quad \text{or} \quad BAx = \lambda x$$

  for real symmetric or complex Hermitian matrices A and B, with B positive definite
- Generalized symmetric or Hermitian definite banded eigenproblems of the form

  $$Ax = \lambda Bx$$

  for real symmetric or complex Hermitian band matrices A and B, with B positive definite
- Generalized general eigenproblems of the form

  $$Ax = \lambda Bx$$

  for real or complex general matrices A and B

Refer to Chapters 7 and 8 for software to compute the eigenvalues or eigenvectors and eigenvectors of a real symmetric or complex Hermitian ordinary eigenproblem.

Refer to Chapter 7 of the *HP MLIB VECLIB User's Guide* for software to compute the eigenvalues or eigenvalues and eigenvectors of a real symmetric, sparse, ordinary or generalized eigenproblem.

The following documents provide supplemental material for this chapter:

- Golub, G.H. and C.F. Van Loan. *Matrix Computations*, 2nd Edition. Baltimore, MD: The Johns Hopkins University Press. 1989.
- Parlett, B.N. *The Symmetric Eigenproblem*. Englewood Cliffs, NJ: Prentice-Hall, Inc. 1980.
- Wilkinson, J.H. *The Algebraic Eigenproblem*. New York, NY: Oxford University Press. 1965.

Chapter Objectives

After reading this chapter you will:

- Understand the forms of the generalized eigenproblems solved by LAPACK
- Know how to use the described subprograms

What You Need to Know to Use These Subprograms

To use these subprograms, it is helpful to know some basic theory of generalized eigensystems. A few facts discussed in basic textbooks are given here.

If A and B are n-by-n matrices, the set of all matrices of the form $A - \lambda B$ with $\lambda \in \mathbf{C}$ is called a *matrix pencil*. If λ is such that $det(A - \lambda B) = 0$ then λ is called an *eigenvalue* of the pencil.If λ is an eigenvalue and $Ax = \lambda Bx$ with $x \neq 0$, then x is called an *eigenvector* belonging to λ.

Alternatively, the definitions can be made without resorting to the determinant of the matrix pencil, as follows: if λ is a scalar for which there exists a nonzero vector x such that $Ax = \lambda Bx$, then λ is called an *eigenvalue* and x is called an *eigenvector* belonging to λ.

There are exactly n eigenvalues, counting multiplicity, if and only if rank(B) = n. If B is rank deficient, there may be zero, fewer than n, or an infinite number of eigenvalues. If A and B are real symmetric or complex Hermitian matrices and B is positive definite, then n eigenvalues exist, they are real, and the problem can be reduced to an ordinary symmetric or Hermitian eigenvalue problem as follows:

1. Compute the Cholesky factorization, $B = LL^*$.
2. Set $C = L^{-1}AL^{-*}$, where L^{-*} is the conjugate transpose of L^{-1}.
3. Solve the ordinary eigenvalue problem $Cy_i = \lambda_i y_i$ for λ_i and y_i.
4. Set $x_i = L^{-*}y_i$ for $i = 1, 2, ..., n$.

Then λ_i is an eigenvalue and x_i is an eigenvector of the generalized eigenproblem $Ax = \lambda Bx$. The eigenvectors are B-orthogonal: $x_i{}^*Bx_i = 1$ and $x_i{}^*Bx_j = 0$ if $i \neq j$.

Similar transformations reduce the other forms of generalized eigenvalue problems, $ABx = \lambda x$ and $BAx = \lambda x$, to ordinary symmetric or Hermitian eigenproblems when A and B are real symmetric or complex Hermitian matrices and B is positive definite. will be i am a nut

If B is invertible, the general generalized eigenproblem can be reduced to a general ordinary eigenproblem by noting that $B^{-1}Ax = \lambda x$ has the same eigenvalues and eigenvectors as the original problem. This approach will not produce generalized eigenvalues accurately if B is ill-conditioned, so LAPACK uses a robust alternative approach that avoids dealing with B^{-1}.

NAME

SGEGS/DGEGS/CGEGS/ZGEGS – Generalized Schur Form

Purpose

These subprograms compute the eigenvalues and the Schur Form of a generalized eigenproblem of the form $Az = \lambda Bz$, where A and B are n-by-n real or complex general matrices. Optionally, the left and right generalized Schur vectors of A and B also are computed. If you need only the generalized eigenvalues, use SGEGV, DGEGV, CGEGV, or ZGEGV, documented elsewhere in this chapter, instead of one of these subprograms.

Given such matrices A and B, the generalized eigenvalues are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i Bz_i.$$

λ_i is usually represented as a pair, (α_i,β_i), such that $\lambda_i = \alpha_i/\beta_i$ if the ratio is defined. There is a reasonable interpretation for $\beta_i = 0$and even for $\alpha_i = \beta_i = 0$. See (Golub and Van Loan) for details.

A pair of real matrices T and S is in generalized real Schur Form if T is block upper triangular with 1-by-1 and 2-by-2 diagonal blocks and S is upper triangular with non-negative diagonal elements. 2-by-2 blocks diagonal blocks of T are standardized so that the corresponding diagonal blocks of S have the form

$$\begin{bmatrix} a & 0 \\ 0 & c \end{bmatrix}.$$

1-by-1 blocks correspond to real generalized eigenvalues, while 2-by-2 blocks correspond to complex conjugate generalized eigenpairs.

A pair of complex matrices T and S is in complex Schur Form if T is upper triangular and S is upper triangular with non-negative real diagonal elements.

If T and S are the generalized Schur Form of A and B, then the columns of the orthogonal or unitary matrices Q and Z such that

$$T = Q^*AZ \quad \text{and} \quad S = Q^*BZ$$

are known as the left and right generalized Schur vectors of A and B, respectively.

Usage

LAPACK:

```
CHARACTER*1     jobvsl, jobvsr
INTEGER*4       info, lda, ldb, ldvsl, ldvsr, lwork, n
REAL*4          a(lda, n), alphai(n), alphar(n), b(ldb, n), beta(n),
                vsl(ldvsl, n), vsr(ldvsr, n), work(lwork)
CALL SGEGS(jobvsl, jobvsr, n, a, lda, b, ldb, alphar, alphai, beta, vsl,
  ldvsl, vsr, ldvsr, work, lwork, info)

CHARACTER*1     jobvsl, jobvsr
INTEGER*4       info, lda, ldb, ldvsl, ldvsr, lwork, n
REAL*8          a(lda, n), alphai(n), alphar(n), b(ldb, n), beta(n),
                vsl(ldvsl, n), vsr(ldvsr, n), work(lwork)
CALL DGEGS(jobvsl, jobvsr, n, a, lda, b, ldb, alphar, alphai, beta, vsl,
  ldvsl, vsr, ldvsr, work, lwork, info)

CHARACTER*1     jobvsl, jobvsr
INTEGER*4       info, lda, ldb, ldvsl, ldvsr, lwork, n
REAL*4          rwork(3*n)
COMPLEX*8       a(lda, n), alpha(n), b(ldb, n), beta(n), vsl(ldvsl, n),
                vsr(ldvsr, n), work(lwork)
CALL CGEGS(jobvsl, jobvsr, n, a, lda, b, ldb, alpha, beta, vsl, ldvsl, vsr,
  ldvsr, work, lwork, rwork, info)

CHARACTER*1     jobvsl, jobvsr
INTEGER*4       info, lda, ldb, ldvsl, ldvsr, lwork, n
REAL*8          rwork(3*n)
COMPLEX*16      a(lda, n), alpha(n), b(ldb, n), beta(n), vsl(ldvsl, n),
                vsr(ldvsr, n), work(lwork)
CALL ZGEGS(jobvsl, jobvsr, n, a, lda, b, ldb, alpha, beta, vsl, ldvsl, vsr,
  ldvsr, work, lwork, rwork, info)
```

LAPACK8:

```
CHARACTER*1     jobvsl, jobvsr
INTEGER*8       info, lda, ldb, ldvsl, ldvsr, lwork, n
REAL*8          a(lda, n), alphai(n), alphar(n), b(ldb, n), beta(n),
                vsl(ldvsl, n), vsr(ldvsr, n), work(lwork)
CALL SGEGS(jobvsl, jobvsr, n, a, lda, b, ldb, alphar, alphai, beta, vsl,
  ldvsl, vsr, ldvsr, work, lwork, info)

CHARACTER*1     jobvsl, jobvsr
INTEGER*8       info, lda, ldb, ldvsl, ldvsr, lwork, n
REAL*8          rwork(3*n)
COMPLEX*16      a(lda, n), alpha(n), b(ldb, n), beta(n), vsl(ldvsl, n),
                vsr(ldvsr, n), work(lwork)
CALL CGEGS(jobvsl, jobvsr, n, a, lda, b, ldb, alpha, beta, vsl, ldvsl, vsr,
  ldvsr, work, lwork, rwork, info)
```

Input

jobvsl Specifies whether the left generalized Schur vectors are to be computed, as follows:

- **jobvsl** = 'N' or 'n': Do not compute the left generalized Schur vectors.
- **jobvsl** = 'V' or 'v': Compute the left generalized Schur vectors.

jobvsr Specifies whether the right generalized Schur vectors are to be computed, as follows:

- **jobvsr** = 'N' or 'n': Do not compute the right generalized Schur vectors.
- **jobvsr** = 'V' or 'v': Compute the right generalized Schur vectors.

n The order of the matrices A and B. **n** ≥ 0.

a The **n**-by-**n** matrix A.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

b The **n**-by-**n** matrix B.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

ldvsl The leading dimension of array **vsl** in the calling program unit. **ldvsl** ≥ 1, and if **jobvsl** = 'V' or 'v', then **ldvsl** ≥ **n**.

ldvsr The leading dimension of array **vsr** in the calling program unit. **ldvsr** ≥ 1, and if **jobvsr** = 'V' or 'v', then **ldvsr** ≥ **n**.

lwork The length of array **work**. For SGEGS and DGEGS, **lwork** ≥ max(1,4**n**), while for CGEGS and ZGEGS, **lwork** ≥ max(1,2**n**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work, rwork Arrays used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, the generalized Schur Form of A overwrites the input.

b On successful exit, the generalized Schur Form of B overwrites the input.

alphar, alphai, beta On successful exit from SGEGS and DGEGS, **alphar**(j)/**beta**(j) and **alphai**(j)/**beta**(j) are the real and imaginary parts, respectively, of the generalized eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are not in any particular order, except that if **alphai**(j) > 0, then the jth and j+1st eigenvalues are a complex conjugate pair, with **alphai**(j+1) < 0.

NOTE The quotients **alphar**(j)/**beta**(j) and **alphai**(j)/**beta**(j) may easily overflow or underflow, and **beta**(j) may even be zero. Thus, you should avoid computing the ratios directly. However, **alphar**(j) and **alphai**(j) will be always less than and usually comparable in magnitude to $||A||$, and **beta**(j) will be always less than and usually comparable to $||B||$.

alpha, beta On successful exit from CGEGS and ZGEGS, **alpha**(j)/**beta**(j) is the generalized eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are not in any particular order.

Note: the quotients **alpha**(j)/**beta**(j) may easily overflow or underflow, and **beta**(j) may even be zero. Thus, you should avoid naively computing the ratio directly. However, **alpha**(j) will be always less than and usually comparable in magnitude to $||A||$, and **beta**(j) will be always less than and usually comparable to $||B||$.

vsl On successful exit, if **jobvsl** = 'V' or 'v', the left generalized Schur vectors of A and B. Not referenced if **jobvsl** = 'N' or 'n'.

vsr On successful exit, if **jobvsr** = 'V' or 'v', the right generalized Schur vectors of A and B. Not referenced if **jobvsr** = 'N' or 'n'.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	The algorithm terminated before completing the requested computation.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobvsl ≠ 'N' or 'n' or 'V' or 'v',
jobvsr ≠ 'N' or 'n' or 'V' or 'v',
n < 0,
lda < max(1,**n**),
ldb < max(1,**n**),
ldvsl too small, and
ldvsr too small, and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobvsl** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SGEGV/DGEGV/CGEGV/ZGEGV – General Matrix Eigenproblem

Purpose

These subprograms compute the eigenvalues and, optionally, the eigenvectors of a generalized eigenproblem of the form $Az = \lambda Bz$, where A and B are n-by-n real or complex general matrices.

Given such matrices A and B, the generalized eigenvalues are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Az_i = \lambda_i Bz_i.$$

λ_i is usually represented as a pair, (α_i,β_i), such that $\lambda_i = \alpha_i/\beta_i$ if the ratio is defined. There is a reasonable interpretation for $\beta_i = 0$ and even for $\alpha_i = \beta_i = 0$. See (Golub and Van Loan) for details.

Optionally, the z_i, which are called right generalized eigenvectors, also may be computed. In addition, these subprograms also can compute the left generalized eigenvectors, which satisfy

$$y_i{}^*A = \lambda_i y_i{}^*B.$$

Usage

LAPACK:

CHARACTER*1 **jobvl, jobvr**
INTEGER*4 **info, lda, ldb, ldvl, ldvr, lwork, n**
REAL*4 **a(lda, n), alphai(n), alphar(n), b(ldb, n), beta(n), vl(ldvl, n), vr(ldvr, n), work(lwork)**

CALL SGEGV(jobvl, jobvr, n, a, lda, b, ldb, alphar, alphai, beta, vl, ldvl, vr, ldvr, work, lwork, info)

CHARACTER*1 **jobvl, jobvr**
INTEGER*4 **info, lda, ldb, ldvl, ldvr, lwork, n**
REAL*8 **a(lda, n), alphai(n), alphar(n), b(ldb, n), beta(n), vl(ldvl, n), vr(ldvr, n), work(lwork)**

CALL DGEGV(jobvl, jobvr, n, a, lda, b, ldb, alphar, alphai, beta, vl, ldvl, vr, ldvr, work, lwork, info)

CHARACTER*1 **jobvl, jobvr**
INTEGER*4 **info, lda, ldb, ldvl, ldvr, lwork, n**
REAL*4 **rwork(8*n)**
COMPLEX*8 **a(lda, n), alpha(n), b(ldb, n), beta(n), vl(ldvl, n), vr(ldvr, n), work(lwork)**

CALL CGEGV(jobvl, jobvr, n, a, lda, b, ldb, alpha, beta, vl, ldvl, vr, ldvr, work, lwork, rwork, info)

```
CHARACTER*1     jobvl, jobvr
INTEGER*4       info, lda, ldb, ldvl, ldvr, lwork, n
REAL*8          rwork(8*n)
COMPLEX*16      a(lda, n), alpha(n), b(ldb, n), beta(n), vl(ldvl, n),
                vr(ldvr, n), work(lwork)
CALL ZGEGV(jobvl, jobvr, n, a, lda, b, ldb, alpha, beta, vl, ldvl, vr, ldvr,
  work, lwork, rwork, info)
```

LAPACK8:

```
CHARACTER*1     jobvl, jobvr
INTEGER*8       info, lda, ldb, ldvl, ldvr, lwork, n
REAL*8          a(lda, n), alphai(n), alphar(n), b(ldb, n), beta(n),
                vl(ldvl, n), vr(ldvr, n), work(lwork)
CALL SGEGV(jobvl, jobvr, n, a, lda, b, ldb, alphar, alphai, beta, vl, ldvl,
  vr, ldvr, work, lwork, info)
CHARACTER*1     jobvl, jobvr
INTEGER*8       info, lda, ldb, ldvl, ldvr, lwork, n
REAL*8          rwork(8*n)
COMPLEX*16      a(lda, n), alpha(n), b(ldb, n), beta(n), vl(ldvl, n),
                vr(ldvr, n), work(lwork)
CALL CGEGV(jobvl, jobvr, n, a, lda, b, ldb, alpha, beta, vl, ldvl, vr, ldvr,
  work, lwork, rwork, info)
```

Input

jobvl Specifies whether the left generalized eigenvectors of A and B are to be computed, as follows:

- **jobvl** = 'N' or 'n': Do not compute the left generalized eigenvectors.
- **jobvl** = 'V' or 'v': Compute the left generalized eigenvectors.

jobvr Specifies whether the right generalized eigenvectors of A and B are to be computed, as follows:

- **jobvr** = 'N' or 'n': Do not compute the right generalized eigenvectors.
- **jobvr** = 'V' or 'v': Compute the right generalized eigenvectors.

n The order of the matrices A and B. **n** ≥ 0.

a The **n**-by-**n** matrix A.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

b The **n**-by-**n** matrix B.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

ldvl The leading dimension of array **vl** in the calling program unit. **ldvl** ≥ 1, and if **jobvl** = 'V' or 'v', then **ldvl** ≥ **n**.

ldvr The leading dimension of array **vr** in the calling program unit. **ldvr** ≥ 1, and if **jobvr** = 'V' or 'v', then **ldvr** ≥ **n**.

lwork The length of array **work**. For SGEGV and DGEGV, **lwork** ≥ max(1,8**n**), while for CGEGV and ZGEGV, **lwork** ≥ max(1,2**n**). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work, rwork Arrays used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a, b Destroyed.

alphar, alphai, beta On successful exit from SGEGV and DGEGV, **alphar**(*j*)/**beta**(*j*) and **alphai**(*j*)/**beta**(*j*) are the real and imaginary parts, respectively, of the generalized eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are not in any particular order, except that if **alphai**(*j*) > 0, then the *j*th and *j*+1st eigenvalues are a complex conjugate pair, with **alphai**(*j*+1) < 0.

NOTE The quotients **alphar**(*j*)/**beta**(*j*) and **alphai**(*j*)/**beta**(*j*) may easily overflow or underflow, and **beta**(*j*) may even be zero. Thus, you should avoid computing the ratios directly. However, **alphar**(*j*) and **alphai**(*j*) will be always less than and usually comparable in magnitude to $||A||$, and **beta**(*j*) will be always less than and usually comparable to $||B||$.

alpha, beta On successful exit from CGEGV and ZGEGV, **alpha**(*j*)/**beta**(*j*) is the generalized eigenvalue $\lambda_j, j = 1, 2, ..., \mathbf{n}$. The eigenvalues are not in any particular order.

NOTE

The quotients **alpha**(*j*)/**beta**(*j*) may easily overflow or underflow, and **beta**(*j*) may even be zero. Thus, you should avoid computing the ratio directly. However, **alpha**(*j*) will be always less than and usually comparable in magnitude to ||*A*||, and **beta**(*j*) will be always less than and usually comparable to ||*B*||.

vl

On successful exit, if **jobvl** = 'V' or 'v', the left generalized eigenvectors, $y_j, j = 1, 2, ..., \mathbf{n}$, stored one after another in the columns of **vl**, in the same order as the generalized eigenvalues. The eigenvectors are normalized so the largest component will have |real part| + |imaginary part| = 1, except that for eigenvalues with **alpha**(*j*) = **beta**(*j*) = 0 or **alphar**(*j*) = **alphai**(*j*) = **beta**(*j*) = 0, a zero vector will be returned as the corresponding eigenvector.

In SGEGV and DGEGV, a left generalized eigenvector corresponding to a real generalized eigenvalue is real and takes up one column. An eigenvector pair corresponding to a complex conjugate pair of eigenvalues is complex and takes up two columns: the first column holds the real part and the second column holds the imaginary part of the eigenvector corresponding to the eigenvalue with positive imaginary part.

In CGEGV and ZGEGV, each left generalized eigenvector takes up one column.

Not referenced if **jobvl** = 'N' or 'n'.

vr

On successful exit, if **jobvr** = 'V' or 'v', the right generalized eigenvectors, $z_j, j = 1, 2, ..., \mathbf{n}$, stored one after another in the columns of **vr**, in the same order as their generalized eigenvalues. The eigenvectors are normalized so the largest component will have |real part| + |imaginary part| = 1, except that for eigenvalues with **alpha**(*j*) = **beta**(*j*) = 0 or **alphar**(*j*) = **alphai**(*j*) = **beta**(*j*) = 0, a zero vector will be returned as the corresponding eigenvector.

In SGEGV and DGEGV, a right generalized eigenvector corresponding to a real generalized eigenvalue is real and takes up one column. An eigenvector pair corresponding to a complex conjugate pair of eigenvalues is complex and takes up two columns: the first column holds the real part and the second column holds the imaginary part of the eigenvector corresponding to the eigenvalue with positive imaginary part.

In CGEGV and ZGEGV, each right generalized eigenvector takes up one column.

Not referenced if **jobvr** = 'N' or 'n'.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	The algorithm terminated before completing the requested computation.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobvl ≠ 'N' or 'n' or 'V' or 'v',
jobvr ≠ 'N' or 'n' or 'V' or 'v',
n < 0,
lda < max(1,**n**),
ldb < max(1,**n**),
ldvl too small,
ldvr too small, and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **jobvl** and **jobvr** arguments as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSBGV/DSBGV/CHBGV/ZHBGV – Symmetric or Hermitian Band Matrices

Purpose

These subprograms compute all eigenvalues and, optionally, all eigenvectors of a generalized eigenproblem of the form $Az = \lambda Bz$, where A and B are n-by-n real symmetric or complex Hermitian band matrices and B is positive definite.

A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A matrix is banded if its nonzero elements all lie fairly near the principal diagonal. Specifically, $a_{ij} = 0$ if $|i-j| > ka$ for some integer ka. The smallest such ka for a given matrix is called the half bandwidth, and $2ka+1$ is called the total bandwidth.

A real symmetric matrix B is positive definite if the quadratic form x^TBx is positive for all nonzero real vectors x; a complex Hermitian matrix B is positive definite if the quadratic form x^*Bx is positive for all nonzero complex vectors x.

Given such matrices A and B, the generalized eigenvalues are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Ax = \lambda Bx$$

Optionally, the generalized eigenvectors z_i also may be computed.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A or B, and since either triangle of A or B may be obtained from the other, you need only provide the band within one triangle of A and B. Compared to storing the entire matrix, this can save memory in two ways: only the elements within the bands are stored, and of them, only the upper or the lower triangles.

The following examples illustrate the storage of real symmetric band matrices. Consider the following matrix A of order $n = 7$ and half bandwidth $ka = 2$:

$$\begin{array}{ccccccc} 11 & 12 & 13 & 0 & 0 & 0 & 0 \\ 12 & 22 & 23 & 24 & 0 & 0 & 0 \\ 13 & 23 & 33 & 34 & 35 & 0 & 0 \\ 0 & 24 & 34 & 44 & 45 & 46 & 0 \\ 0 & 0 & 35 & 45 & 55 & 56 & 57 \\ 0 & 0 & 0 & 46 & 56 & 66 & 67 \\ 0 & 0 & 0 & 0 & 57 & 67 & 77 \end{array}$$

Upper triangular storage. The upper triangle of the matrix A is stored in an array **ab** with at least $ka+1 = 3$ rows and 7 columns as follows:

$$\begin{array}{ccccccc} * & * & 13 & 24 & 35 & 46 & 57 \\ * & 12 & 23 & 34 & 45 & 56 & 67 \\ 11 & 22 & 33 & 44 & 55 & 66 & 77 \end{array}$$

The asterisks represent elements in the ka-by-ka triangle at the upper left corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the upper triangle of A, it is stored in **ab**$(ka+1+i-j,j)$. Therefore, the columns of the upper triangle of A are stored in the columns of **ab**, and the diagonals of the upper triangle of A are stored in the rows of **ab**.

Lower triangular storage. The lower triangle of A is stored in the array **ab** as follows:

$$\begin{array}{ccccccc} 11 & 22 & 33 & 44 & 55 & 66 & 77 \\ 12 & 23 & 34 & 45 & 56 & 67 & * \\ 13 & 24 & 35 & 46 & 57 & * & * \end{array}$$

The asterisks represent elements in the ka-by-ka triangle at the lower right corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the lower triangle of A, it is stored in **ab**$(1+i-j,j)$. Therefore, the columns of the lower triangle of A are stored in the columns of **ab**, and the diagonals of the lower triangle of A are stored in the rows of **ab**.

Usage

LAPACK:

```
CHARACTER*1     jobz, uplo
INTEGER*4       info, ka, kb, ldab, ldbb, ldz, n
REAL*4          ab(ldab, n), bb(ldbb, n), w(n), work(3*n), z(ldz, n)
CALL SSBGV(jobz, uplo, n, ka, kb, ab, ldab, bb, ldbb, w, z, ldz, work, info)

CHARACTER*1     jobz, uplo
INTEGER*4       info, ka, kb, ldab, ldbb, ldz, n
REAL*8          ab(ldab, n), bb(ldbb, n), w(n), work(3*n), z(ldz, n)
CALL DSBGV(jobz, uplo, n, ka, kb, ab, ldab, bb, ldbb, w, z, ldz, work, info)

CHARACTER*1     jobz, uplo
INTEGER*4       info, ka, kb, ldab, ldbb, ldz, n
REAL*4          rwork(3*n), w(n)
COMPLEX*8       ab(ldab, n), bb(ldbb, n), work(n), z(ldz, n)
CALL CHBGV(jobz, uplo, n, ka, kb, ab, ldab, bb, ldbb, w, z, ldz, work,
  rwork, info)

CHARACTER*1     jobz, uplo
INTEGER*4       info, ka, kb, ldab, ldbb, ldz, n
REAL*8          rwork(3*n), w(n)
COMPLEX*16      ab(ldab, n), bb(ldbb, n), work(n), z(ldz, n)
CALL ZHBGV(jobz, uplo, n, ka, kb, ab, ldab, bb, ldbb, w, z, ldz, work,
  rwork, info)
```

LAPACK8:

```
CHARACTER*1     jobz, uplo
INTEGER*8       info, ka, kb, ldab, ldbb, ldz, n
REAL*8          ab(ldab, n), bb(ldbb, n), w(n), work(3*n), z(ldz, n)
CALL SSBGV(jobz, uplo, n, ka, kb, ab, ldab, bb, ldbb, w, z, ldz, work, info)

CHARACTER*1     jobz, uplo
INTEGER*8       info, ka, kb, ldab, ldbb, ldz, n
REAL*8          rwork(3*n), w(n)
COMPLEX*16      ab(ldab, n), bb(ldbb, n), work(n), z(ldz, n)
CALL CHBGV(jobz, uplo, n, ka, kb, ab, ldab, bb, ldbb, w, z, ldz, work,
  rwork, info)
```

Input

jobz Specifies whether eigenvectors are to be computed, as follows:

jobz = 'N' or 'n': Compute eigenvalues only.

jobz = 'V' or 'v': Compute eigenvectors as well.

uplo Specifies whether the upper or lower triangular parts of the symmetric or Hermitian matrices A and B are stored in arrays **ab** and **bb**, respectively, as follows:

uplo = 'U' or 'u': The upper triangular parts are stored.

uplo = 'L' or 'l': The lower triangular parts are stored.

n The order of the matrices A and B. $\mathbf{n} \geq 0$.

ka The number of super-diagonals of the matrix A if **uplo** = 'U' or 'u', or the number of subdiagonals if **uplo** = 'L' or 'l'. $\mathbf{ka} \geq 0$.

kb The number of super-diagonals of the matrix B if **uplo** = 'U' or 'u', or the number of subdiagonals if **uplo** = 'L' or 'l'. $0 \leq \mathbf{kb} \leq \mathbf{ka}$.

ab The upper or lower triangle of the symmetric or Hermitian band matrix A, stored in the first **ka**+1 rows of array **ab**. The j-th column of A is stored in the j-th column of array **ab** as follows:

If **uplo** = 'U' or 'u', $\mathbf{ab}(\mathbf{ka}+1+i-j,j) = A(i,j)$ for $\max(1,j-\mathbf{ka}) \leq i \leq j$;

If **uplo** = 'L' or 'l', $\mathbf{ab}(1+i-j,j) = A(i,j)$ for $j \leq i \leq \min(\mathbf{n},j+\mathbf{ka})$.

ldab The leading dimension of array **ab** in the calling program unit. $\mathbf{ldab} \geq \mathbf{ka}+1$.

bb The upper or lower triangle of the symmetric or Hermitian band matrix B, stored in the first **kb**+1 rows of array **bb**. The j-th column of B is stored in the j-th column of array **bb** as follows:

If **uplo** = 'U' or 'u', $\mathbf{bb}(\mathbf{kb}+1+i-j,j) = B(i,j)$ for $\max(1,j-\mathbf{kb}) \leq i \leq j$;

If **uplo** = 'L' or 'l', $\mathbf{bb}(1+i-j,j) = B(i,j)$ for $j \leq i \leq \min(\mathbf{n},j+\mathbf{kb})$.

ldbb The leading dimension of array **bb** in the calling program unit. $\mathbf{ldbb} \geq \mathbf{kb}+1$.

ldz The leading dimension of array **z** in the calling program unit. $\mathbf{ldz} \geq 1$, and if **jobz** = 'V' or 'v', then $\mathbf{ldz} \geq \mathbf{n}$.

Working Storage

work, rwork Arrays used for work space.

Output

ab, bb	Destroyed.	
w	On successful exit, the generalized eigenvalues in ascending order.	
z	On successful exit, if **jobz** = 'V' or 'v', the generalized eigenvectors.	
	Not referenced if **jobz** = 'N' or 'n'.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = $k \le$ **n**, the algorithm failed to converge; k off-diagonal elements of an intermediate tridiagonal form did not converge to zero. If **info** = $k >$ **n**, then the leading minor of order k–**n** of B is not positive definite and no eigenvalues or eigenvectors could be computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobz ≠ 'N' or 'n' or 'V' or 'v',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
ka < 0,
kb < 0,
kb > **ka**,
ldab < **ka**+1,
ldbb < **kb**+1, and
ldz too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSPGV/DSPGV/.../ZHPGV – Symmetric or Hermitian Packed Matrices

Purpose

These subprograms compute all eigenvalues and, optionally, all eigenvectors of generalized eigenproblems of the form $Az = \lambda Bz$, $ABz = \lambda z$, or $BAz = \lambda z$, where A and B are n-by-n real symmetric or complex Hermitian matrices stored in packed form and B is positive definite.

A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A real symmetric matrix B is positive definite if the quadratic form x^TBx is positive for all nonzero real vectors x; a complex Hermitian matrix B is positive definite if the quadratic form x^*Bx is positive for all nonzero complex vectors x.

Given such matrices A and B, the generalized eigenvalues are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Ax = \lambda Bx \quad \text{or} \quad ABx = \lambda x \quad \text{or} \quad BAx = \lambda x.$$

Optionally, the generalized eigenvectors z_i also may be computed.

Matrix Storage

Because either triangle of A or B may be obtained from its other triangle, you need only provide either the upper or the lower triangle of A, and the same triangle of B. Compared to storing the entire matrices, you save memory by supplying only one triangle of each matrix, stored column-by-column in packed form in two 1-dimensional arrays.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**($i+j\times(j-1)/2$).

Lower triangular storage. If the lower triangle of A is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**($i+(j-1)\times(2n-j)/2$).

Usage

LAPACK:

```
CHARACTER*1     jobz, uplo
INTEGER*4       info, itype, ldz, n
REAL*4          ap((n*(n+1))/2), bp((n*(n+1))/2), w(n), work(3*n),
                z(ldz, n)
CALL SSPGV(itype, jobz, uplo, n, ap, bp, w, z, ldz, work, info)

CHARACTER*1     jobz, uplo
INTEGER*4       info, itype, ldz, n
REAL*8          ap((n*(n+1))/2), bp((n*(n+1))/2), w(n), work(3*n),
                z(ldz, n)
CALL DSPGV(itype, jobz, uplo, n, ap, bp, w, z, ldz, work, info)
```

```
CHARACTER*1     jobz, uplo
INTEGER*4       info, itype, ldz, n
REAL*4          rwork(max(1,3*n–2)), w(n)
COMPLEX*8       ap((n*(n+1))/2), bp((n*(n+1))/2),
                work(max(1,2*n–1)), z(ldz, n)
CALL CHPGV(itype, jobz, uplo, n, ap, bp, w, z, ldz, work, rwork, info)
```

```
CHARACTER*1     jobz, uplo
INTEGER*4       info, itype, ldz, n
REAL*8          rwork(max(1,3*n–2)), w(n)
COMPLEX*16      ap((n*(n+1))/2), bp((n*(n+1))/2),
                work(max(1,2*n–1)), z(ldz, n)
CALL ZHPGV(itype, jobz, uplo, n, ap, bp, w, z, ldz, work, rwork, info)
```

LAPACK8:

```
CHARACTER*1     jobz, uplo
INTEGER*8       info, itype, ldz, n
REAL*8          ap((n*(n+1))/2), bp((n*(n+1))/2), w(n), work(3*n),
                z(ldz, n)
CALL SSPGV(itype, jobz, uplo, n, ap, bp, w, z, ldz, work, info)
```

```
CHARACTER*1     jobz, uplo
INTEGER*8       info, itype, ldz, n
REAL*8          rwork(max(1,3*n–2)), w(n)
COMPLEX*16      ap((n*(n+1))/2), bp((n*(n+1))/2),
                work(max(1,2*n–1)), z(ldz, n)
CALL CHPGV(itype, jobz, uplo, n, ap, bp, w, z, ldz, work, rwork, info)
```

Input

itype Specifies the problem type to be solved, as follows:

itype = 1:	Solve $Az = \lambda Bz$.
itype = 2:	Solve $ABz = \lambda z$.
itype = 3:	Solve $BAz = \lambda z$.

jobz Specifies whether eigenvectors are to be computed, as follows:

jobz = 'N' or 'n':	Compute eigenvalues only.
jobz = 'V' or 'v':	Compute eigenvectors as well.

uplo Specifies whether the upper or lower triangular parts of the symmetric or Hermitian matrices A and B are stored in arrays **ap** and **bp**, respectively, as follows:

uplo = 'U' or 'u':	The upper triangular parts are stored.
uplo = 'L' or '1':	The lower triangular parts are stored.

n The order of the matrices A and B. $\mathbf{n} \geq 0$.

ap The upper or lower triangular part of the symmetric or Hermitian matrix A, packed columnwise in a linear array as follows:

If **uplo** = 'U' or 'u', **ap**$(i + (j-1) \times j/2) = A(i,j)$ for $1 \le i \le j$;

If **uplo** = 'L' or 'l', **ap**$(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \le i \le \mathbf{n}$.

bp The upper or lower triangular part of the symmetric or Hermitian matrix B, packed columnwise in a linear array as follows:

If **uplo** = 'U' or 'u', **bp**$(i + (j-1) \times j/2) = B(i,j)$ for $1 \le i \le j$;

If **uplo** = 'L' or 'l', **bp**$(i + (j-1) \times (2\mathbf{n}-j)/2) = B(i,j)$ for $j \le i \le \mathbf{n}$.

ldz The leading dimension of array **z** in the calling program unit. **ldz** ≥ 1, and if **jobz** = 'V' or 'v', then **ldz** ≥ **n**.

Working Storage

work, rwork Arrays used for work space.

Output

ap Destroyed.

bp On exit with **info** ≤ **n**, the triangular factor U or L from the Cholesky factorization $B = U^*U$ or $B = LL^*$, in the same storage format as B.

w On successful exit, the eigenvalues in ascending order. On exit with **info** ≤ **n**, the eigenvalues are correct for indices 1, 2, ..., **info**–1, but they are unordered and may not be the smallest eigenvalues of the problem.

z On successful exit, if **jobz** = 'V' or 'v', the eigenvectors. If an error exit is made, **z** contains the eigenvectors associated with the stored eigenvalues. The eigenvectors are normalized as follows: if **itype** = 1 or 2, then $z_j^*Bz_j = 1$; if **itype** = 3, then $z_j^*B^{-1}z_j = 1$.

Not referenced if **jobz** = 'N' or 'n'.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.

info > 0:	If **info** = $k \leq$ **n**, the algorithm terminated before finding the k-th eigenvalue. If **info** = $k >$ **n**, then the leading minor of order k–**n** of B is not positive definite and no eigenvalues or eigenvectors could be computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

itype ≠ 1, 2, or 3,
jobz ≠ 'N' or 'n' or 'V' or 'v',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0, and
ldz too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

NAME

SSYGV/DSYGV/CHEGV/ZHEGV – Symmetric or Hermitian Matrices

Purpose

These subprograms compute all eigenvalues and, optionally, all eigenvectors of generalized eigenproblems of the form $Az = \lambda Bz$, $ABz = \lambda z$, or $BAz = \lambda z$, where A and B are n-by-n real symmetric or complex Hermitian matrices and B is positive definite.

A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A real symmetric matrix B is positive definite if the quadratic form x^TBx is positive for all nonzero real vectors x; a complex Hermitian matrix B is positive definite if the quadratic form x^*Bx is positive for all nonzero complex vectors x.

Given such matrices A and B, the generalized eigenvalues are scalars λ_i, $i = 1, 2, ..., n$, for which there exist corresponding nonzero vectors, z_i, $i = 1, 2, ..., n$, such that

$$Ax = \lambda Bx \quad \text{or} \quad ABx = \lambda x \quad \text{or} \quad BAx = \lambda x$$

Optionally, the generalized eigenvectors z_i also may be computed.

Matrix Storage

Because either triangle of A or B may be obtained from its other triangle, you need only provide one triangle of A and one triangle of B. You may supply either the upper or the lower triangle of A, and the same triangle of B, in 2 two-dimensional arrays large enough to hold the entire matrices. The other triangle of the arrays are not referenced.

Usage

LAPACK:

```
CHARACTER*1     jobz, uplo
INTEGER*4       info, itype, lda, ldb, lwork, n
REAL*4          a(lda, n), b(ldb, n), w(n), work(lwork)
CALL SSYGV(itype, jobz, uplo, n, a, lda, b, ldb, w, work, lwork, info)

CHARACTER*1     jobz, uplo
INTEGER*4       info, itype, lda, ldb, lwork, n
REAL*8          a(lda, n), b(ldb, n), w(n), work(lwork)
CALL DSYGV(itype, jobz, uplo, n, a, lda, b, ldb, w, work, lwork, info)
```

```
CHARACTER*1      jobz, uplo
INTEGER*4        info, itype, lda, ldb, lwork, n
REAL*4           rwork(max(1,3*n–2)), w(n)
COMPLEX*8        a(lda, n), b(ldb, n), work(lwork)
CALL CHEGV(itype, jobz, uplo, n, a, lda, b, ldb, w, work, lwork, rwork,
  info)

CHARACTER*1      jobz, uplo
INTEGER*4        info, itype, lda, ldb, lwork, n
REAL*8           rwork(max(1,3*n–2)), w(n)
COMPLEX*16       a(lda, n), b(ldb, n), work(lwork)
CALL ZHEGV(itype, jobz, uplo, n, a, lda, b, ldb, w, work, lwork, rwork,
  info)
```

LAPACK8:

```
CHARACTER*1      jobz, uplo
INTEGER*8        info, itype, lda, ldb, lwork, n
REAL*8           a(lda, n), b(ldb, n), w(n), work(lwork)
CALL SSYGV(itype, jobz, uplo, n, a, lda, b, ldb, w, work, lwork, info)

CHARACTER*1      jobz, uplo
INTEGER*8        info, itype, lda, ldb, lwork, n
REAL*8           rwork(max(1,3*n–2)), w(n)
COMPLEX*16       a(lda, n), b(ldb, n), work(lwork)
CALL CHEGV(itype, jobz, uplo, n, a, lda, b, ldb, w, work, lwork, rwork,
  info)
```

Input

itype Specifies the problem type to be solved, as follows:

itype = 1:	Solve $Az = \lambda Bz$.
itype = 2:	Solve $ABz = \lambda z$.
itype = 3:	Solve $BAz = \lambda z$.

jobz Specifies whether eigenvectors are to be computed, as follows:

jobz = 'N' or 'n':	Compute eigenvalues only.
jobz = 'V' or 'v':	Compute eigenvectors as well.

uplo Specifies whether the upper or lower triangular parts of the symmetric or Hermitian matrices A and B are stored in arrays **a** and **b**, respectively, as follows:

uplo = 'U' or 'u':	The upper triangular parts are stored.
uplo = 'L' or 'l':	The lower triangular parts are stored.

n The order of the matrices A and B. $\mathbf{n} \geq 0$.

a The symmetric or Hermitian matrix A.

If **uplo** = 'U' or 'u', only the upper triangular part of **a** is used to define the elements of the matrix and the strict lower triangular part of **a** is not used for input.

If **uplo** = 'L' or '1', only the lower triangular part of **a** is used to define the elements of the matrix and the strict upper triangular part of **a** is not used for input.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).

b The symmetric positive definite matrix B.

If **uplo** = 'U' or 'u', only the upper triangular part of **b** is used to define the elements of the matrix and the strict lower triangular part of **b** is not used for input.

If **uplo** = 'L' or '1', only the lower triangular part of **b** is used to define the elements of the matrix and the strict upper triangular part of **b** is not used for input.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**n**).

lwork The length of array **work**. **lwork** ≥ max(1,3**n**–1). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work, rwork Arrays used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, if **jobz** = 'V' or 'v', the orthonormal eigenvectors of the matrix. If an error exit is made, **a** contains the eigenvectors associated with the stored eigenvalues. The eigenvectors are normalized as follows: if **itype** = 1 or 2, then $z_j^* B z_j = 1$; if **itype** = 3, then

$z_j^* B^{-1} z_j = 1.$

If **jobz** = 'N' or 'n', then the triangle of **a** specified by **uplo**, including the diagonal, has been destroyed.

b	On exit with **info** ≤ **n**, the triangular factor U or L from the Cholesky factorization $B = U^*U$ or $B = LL^*$, in the same storage format as B.	
w	On successful exit, the eigenvalues in ascending order. On exit with **info** ≤ **n**, the eigenvalues are correct for indices 1, 2, ..., **info**–1, but they are unordered and may not be the smallest eigenvalues of the problem.	
info	Status response:	
	info = 0:	Successful exit.
	info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
	info > 0:	If **info** = k ≤ **n**, the algorithm terminated before finding the k-th eigenvalue. If **info** = k > **n**, then the leading minor of order k–**n** of B is not positive definite and no eigenvalues or eigenvectors could be computed.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

itype ≠ 1, 2, or 3,
jobz ≠ 'N' or 'n' or 'V' or 'v',
uplo ≠ 'L' or 'l' or 'U' or 'u',
n < 0,
lda < max(1,**n**),
ldb < max(1,**n**), and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobz** argument as 'NoVectors' for 'N' or 'Vectors' for 'V'.

10 Drivers for the Singular Value Decomposition

Overview

This chapter explains how to use LAPACK subprograms to compute the singular value decomposition of a matrix or the generalized singular value decomposition of a pair of matrices.

The following document provides supplemental material for this chapter:

- Golub, G.H. and C.F. Van Loan. *Matrix Computations*, 2nd Edition. Baltimore, MD: The Johns Hopkins University Press. 1989.

Chapter Objectives

After reading this chapter you will know how to use the described subprograms.

What You Need to Know to Use These Subprograms

To use these subprograms you should know what the singular value decomposition of a matrix is and that such a decomposition exists for any matrix. It would be helpful to be familiar with some of the interpretations and applications of singular values, and especially to understand how small singular values may indicate ill-conditioning or numerical singularity, and how the SVD can be used to deal with matrices that, for computational purposes, are rank deficient. These concepts are beyond the scope of this chapter introduction; refer to (Golub and Van Loan).

NAME

SGESVD/DGESVD/CGESVD/ZGESVD – SVD of a General Matrix

Purpose

These subprograms compute the singular value decomposition (SVD) of an m-by-n matrix A, optionally computing some or all of the left and right singular vectors. The SVD of A is written

$$A = U\Sigma V^*$$

where Σ is a diagonal matrix with the singular values on the diagonal, and U and V are orthogonal or unitary. The columns of U are the left singular vectors and the columns of V are the right singular vectors. If the right singular vectors are requested, V^T is returned.

Usage

LAPACK:

```
CHARACTER*1     jobu, jobvt
INTEGER*4       info, lda, ldu, ldvt, lwork, m, n
REAL*4          a(lda, n), s(min(m,n)), u(ldu, ucol), vt(ldvt, n),
                work(lwork)
CALL SGESVD(jobu, jobvt, m, n, a, lda, s, u, ldu, vt, ldvt, work, lwork,
  info)

CHARACTER*1     jobu, jobvt
INTEGER*4       info, lda, ldu, ldvt, lwork, m, n
REAL*8          a(lda, n), s(min(m,n)), u(ldu, ucol), vt(ldvt, n),
                work(lwork)
CALL DGESVD(jobu, jobvt, m, n, a, lda, s, u, ldu, vt, ldvt, work, lwork,
  info)

CHARACTER*1     jobu, jobvt
INTEGER*4       info, lda, ldu, ldvt, lwork, m, n
REAL*4          rwork(5*min(m,n)), s(min(m,n))
COMPLEX*8       a(lda, n), u(ldu, ucol), vt(ldvt, n), work(lwork)
CALL CGESVD(jobu, jobvt, m, n, a, lda, s, u, ldu, vt, ldvt, work, lwork,
  rwork, info)

CHARACTER*1     jobu, jobvt
INTEGER*4       info, lda, ldu, ldvt, lwork, m, n
REAL*8          rwork(5*min(m,n)), s(min(m,n))
COMPLEX*16      a(lda, n), u(ldu, ucol), vt(ldvt, n), work(lwork)
CALL ZGESVD(jobu, jobvt, m, n, a, lda, s, u, ldu, vt, ldvt, work, lwork,
  rwork, info)
```

LAPACK8:

```
CHARACTER*1     jobu, jobvt
INTEGER*8       info, lda, ldu, ldvt, lwork, m, n
REAL*8          a(lda, n), s(min(m,n)), u(ldu, ucol), vt(ldvt, n),
                work(lwork)
CALL SGESVD(jobu, jobvt, m, n, a, lda, s, u, ldu, vt, ldvt, work, lwork,
  info)

CHARACTER*1     jobu, jobvt
INTEGER*8       info, lda, ldu, ldvt, lwork, m, n
REAL*8          rwork(5*min(m,n)), s(min(m,n))
COMPLEX*16      a(lda, n), u(ldu, ucol), vt(ldvt, n), work(lwork)
CALL CGESVD(jobu, jobvt, m, n, a, lda, s, u, ldu, vt, ldvt, work, lwork,
  rwork, info)
```

Input

jobu Specifies which left singular vectors to compute, as follows:

- **jobu** = 'A' or 'a': All **m** m-dimensional left singular vectors are returned in **u**.
- **jobu** = 'S' or 's': Only min(**m**,**n**) **m**-dimensional left singular vectors are returned in **u**.
- **jobu** = 'O' or 'o': Only min(**m**,**n**) **m**-dimensional left singular vectors overwrite **a**.
- **jobu** = 'N' or 'n': No left singular vectors are computed.

jobvt Specifies which right singular vectors to compute, as follows:

- **jobvt** = 'A' or 'a': All **n** n-dimensional right singular vectors are returned in **vt**.
- **jobvt** = 'S' or 's': Only min(**m**,**n**) **n**-dimensional right singular vectors are returned in **vt**.
- **jobvt** = 'O' or 'o': Only min(**m**,**n**) **n**-dimensional right singular vectors overwrite **a**.
- **jobvt** = 'N' or 'n': No right singular vectors are computed.

jobvt and **jobu** cannot simultaneously be 'O' or 'o'.

m The number of rows of the matrix A. $\mathbf{m} \geq 0$.

n The number of columns of the matrix A. $\mathbf{n} \geq 0$.

a The **m**-by-**n** matrix A.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**m**).

ldu The leading dimension of array **u** in the calling program unit. **ldu** ≥ 1. If **jobu** = 'S' or 's' or 'A' or 'a', then **ldu** ≥ **m**.

ldvt The leading dimension of array **vt** in the calling program unit. **ldvt** ≥ 1, and if **jobvt** = 'S' or 's', then **ldvt** ≥ min(**m**,**n**), or if **jobvt** = 'A' or 'a', then **ldvt** ≥ **n**.

lwork The length of array **work**. **lwork** ≥ max(1,3min(**m**,**n**)+max(**m**,**n**), 5min(**m**,**n**)–4). For good performance, **lwork** must generally be larger. The optimum value of **lwork** for high performance is returned in **work**(1).

Working Storage

work, rwork Arrays used for work space. On successful exit, **work**(1) contains the optimal work space length **lwork** for high performance.

Output

a On successful exit, if **jobu** = 'O' or 'o', **a** contains min(**m**,**n**) left singular vectors.

On successful exit, if **jobvt** = 'O' or 'o', **a** contains min(**m**,**n**) right singular vectors.

Otherwise, destroyed.

s On successful exit, the singular values of A, sorted into nonincreasing order.

u On successful exit, none, some, or all of the left singular vectors of A, that is, columns of the matrix U. The left singular vectors are of dimension **m**. The number of left singular vectors returned, and hence the second dimension, **ucol**, of the array **u**, depends on **jobu** as follows:

If **jobu** = 'A' or 'a', then **m** left singular vectors are returned and **ucol** ≥ **m**.

If **jobu** = 'S' or 's', then min(**m**,**n**) left singular vectors are returned and **ucol** ≥ min(**m**,**n**).

If **jobu** = 'N' or 'n' or 'O' or 'o' then no left singular vectors are returned and **u** is not referenced.

vt On successful exit, the rows of **vt** hold none, some, or all of the right singular vectors of A, that is, columns of the matrix V. The right singular vectors are of dimension **n**.

If **jobvt** = 'A' or 'a', then **n** right singular vectors are returned.

If **jobvt** = 'S' or 's', then min(**m**,**n**) right singular vectors are returned

If **jobvt** = 'N' or 'n' or 'O' or 'o' then no right singular vectors are returned and **vt** is not referenced

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	The algorithm did not converge.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobu ≠ 'A' or 'a' or 'S' or 's' or 'O' or 'o' or 'N' or 'n',
jobvt ≠ 'A' or 'a' or 'S' or 's' or 'O' or 'o' or 'N' or 'n',
m < 0,
n < 0,
lda < max(1,**m**),
ldu too small,
ldvt too small, and
lwork too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobu** argument as 'AllVectors' for 'A', 'SomeVectors' for 'S', 'OverwriteA' for 'O', or 'NoVectors' for 'N'.

NAME

SGGSVD/DGGSVD/CGGSVD/ZGGSVD – Generalized SVD

Purpose

These subprograms compute the generalized singular value decomposition (GSVD) of the m-by-n matrix A and the p-by-n matrix B.

Let l be the effective numerical rank of the matrix B and let $k+l$ be the effective numerical rank of the matrix $[A^* \quad B^*]^*$, where * indicates conjugate transpose (ordinary transpose if the matrices are real). Then the GSVD of A and B is written

$$U^*AQ = D_1 [0 \quad R], \qquad V^*BQ = D_2 [0 \quad R] \qquad (1)$$

where U is an m-by-m orthogonal or unitary matrix, V is a p-by-p orthogonal or unitary matrix, Q is an n-by-n orthogonal or unitary matrix, D_1 is a real m-by-$(k+l)$ diagonal matrix, D_2 is a real p-by-$(k+l)$ diagonal matrix, 0 is a $(k+l)$-by-$(n-k-l)$ zero matrix, and R is a $(k+l)$-by-$(k+l)$ nonsingular upper triangular matrix.

Alternatively, the GSVD of A and B is sometimes presented in the form

$$U^*AX = [0 \quad D_1], \qquad V^*BX = [0 \quad D_2]. \qquad (2)$$

where U, V, D_1, and D_2 are as above and X is an n-by-n nonsingular matrix. Forms (1) and (2) are equivalent if

$$X = Q \begin{bmatrix} I & 0 \\ 0 & R^{-1} \end{bmatrix}.$$

D_1, D_2, and R have the following structures, where subscripts on zero and identity matrices indicate their dimensions:

If $k+l \leq m$:

$$D_1 = \begin{bmatrix} I_{kk} & 0_{kl} \\ 0_{lk} & C \\ 0_{m-k-l,k} & 0_{m-k-l,l} \end{bmatrix}$$

$$D_2 = \begin{bmatrix} 0_{l,k} & S \\ 0_{p-l,k} & 0_{p-l,l} \end{bmatrix}$$

$$R = \begin{bmatrix} R_{11} & R_{12} \\ 0_{lk} & R_{22} \end{bmatrix}$$

where

$$C = \text{diag}(\alpha_{k+1}, \alpha_{k+2}, ..., \alpha_{k+l}),$$

$$S = \text{diag}(\beta_{k+1}, \beta_{k+2}, ..., \beta_{k+l}),$$

with

$$0 \leq \alpha_i \leq 1, \quad i = k+1, k+2, ..., k+l,$$

$$0 \leq \beta_i \leq 1, \quad i = k+1, k+2, ..., k+l,$$

and

$$\alpha_i^2+\beta_i^2 = 1, \quad i = k+1, k+2, ..., k+l.$$

If $k+l > m$:

$$D_1 = \begin{bmatrix} I_{kk} & 0_{k,m-k} & 0_{k,k+l-m} \\ 0_{m-k,k} & C & 0_{m-k,k+l-m} \end{bmatrix}$$

$$D_2 = \begin{bmatrix} 0_{m-k,k} & S & 0_{m-k,k+l-m} \\ 0_{k+l-m,k} & 0_{k+l-m,m-k} & I_{k+l-m,k+l-m} \\ 0_{p-l,k} & 0_{p-l,m-k} & 0_{p-l,k+l-m} \end{bmatrix}$$

$$\mathcal{R} = \begin{bmatrix} R_{11} & R_{12} & R_{13} \\ 0_{m-k,k} & R_{22} & R_{23} \\ 0_{k+l-m,k} & 0_{k+l-m,m-k} & R_{33} \end{bmatrix}$$

where

$$C = \text{diag}(\alpha_{k+1}, \alpha_{k+2}, \ldots, \alpha_m),$$

$$S = \text{diag}(\beta_{k+1}, \beta_{k+2}, \ldots, \beta_m),$$

with

$$0 \le \alpha_i \le 1, \quad i = k+1, k+2, \ldots, m,$$

$$0 \le \beta_i \le 1, \quad i = k+1, k+2, \ldots, m,$$

and

$$\alpha_i^2 + \beta_i^2 = 1, \quad i = k+1, k+2, \ldots, m.$$

The ratios α_i/β_i, $i = k+1, k+2, \ldots, min(k+l,m)$, are called the generalized singular values of A and B. Avoid computing these ratios directly, or compute them with caution, to prevent overflow or division by zero.

The subprograms compute C, S, R, and optionally the orthogonal or unitary transformation matrices U, V, and Q.

If B is square and nonsingular, the GSVD of A and B implicitly gives the singular value decomposition of the matrix AB^{-1}:

$$AB^{-1} = U(D_1 D_2^{-1})V^*.$$

Usage

LAPACK:

CHARACTER*1 **jobq, jobu, jobv**
INTEGER*4 **info, k, l, lda, ldb, ldq, ldu, ldv, m, n, p**
INTEGER*4 **iwork(n)**
REAL*4 **a(lda, n), alpha(n), b(ldb, n), beta(n), q(ldq, n), u(ldu, m), v(ldv, n), work(max(3*n,m,p)+n)**

CALL SGGSVD(jobu, jobv, jobq, m, n, p, k, l, a, lda, b, ldb, alpha, beta, u, ldu, v, ldv, q, ldq, work, iwork, info)

CHARACTER*1 **jobq, jobu, jobv**
INTEGER*4 **info, k, l, lda, ldb, ldq, ldu, ldv, m, n, p**
INTEGER*4 **iwork(n)**

```
REAL*8          a(lda, n), alpha(n), b(ldb, n), beta(n), q(ldq, n),
                u(ldu, m), v(ldv, n), work(max(3*n,m,p)+n)
CALL DGGSVD(jobu, jobv, jobq, m, n, p, k, l, a, lda, b, ldb, alpha, beta, u,
  ldu, v, ldv, q, ldq, work, iwork, info)

CHARACTER*1     jobq, jobu, jobv
INTEGER*4       info, k, l, lda, ldb, ldq, ldu, ldv, m, n, p
INTEGER*4       iwork(n)
REAL*4          alpha(n), beta(n), rwork(2*n)
COMPLEX*8       a(lda, n), b(ldb, n), q(ldq, n), u(ldu, m), v(ldv, n),
                work(max(3*n,m,p)+n)
CALL CGGSVD(jobu, jobv, jobq, m, n, p, k, l, a, lda, b, ldb, alpha, beta, u,
  ldu, v, ldv, q, ldq, work, rwork, iwork, info)

CHARACTER*1     jobq, jobu, jobv
INTEGER*4       info, k, l, lda, ldb, ldq, ldu, ldv, m, n, p
INTEGER*4       iwork(n)
REAL*8          alpha(n), beta(n), rwork(2*n)
COMPLEX*16      a(lda, n), b(ldb, n), q(ldq, n), u(ldu, m), v(ldv, n),
                work(max(3*n,m,p)+n)
CALL ZGGSVD(jobu, jobv, jobq, m, n, p, k, l, a, lda, b, ldb, alpha, beta, u,
  ldu, v, ldv, q, ldq, work, rwork, iwork, info)
```

LAPACK8:

```
CHARACTER*1     jobq, jobu, jobv
INTEGER*8       info, k, l, lda, ldb, ldq, ldu, ldv, m, n, p
INTEGER*8       iwork(n)
REAL*8          a(lda, n), alpha(n), b(ldb, n), beta(n), q(ldq, n),
                u(ldu, m), v(ldv, n), work(max(3*n,m,p)+n)
CALL SGGSVD(jobu, jobv, jobq, m, n, p, k, l, a, lda, b, ldb, alpha, beta, u,
  ldu, v, ldv, q, ldq, work, iwork, info)

CHARACTER*1     jobq, jobu, jobv
INTEGER*8       info, k, l, lda, ldb, ldq, ldu, ldv, m, n, p
INTEGER*8       iwork(n)
REAL*8          alpha(n), beta(n), rwork(2*n)
COMPLEX*16      a(lda, n), b(ldb, n), q(ldq, n), u(ldu, m), v(ldv, n),
                work(max(3*n,m,p)+n)
CALL CGGSVD(jobu, jobv, jobq, m, n, p, k, l, a, lda, b, ldb, alpha, beta, u,
  ldu, v, ldv, q, ldq, work, rwork, iwork, info)
```

Input

jobu Specifies whether to compute the *U* matrix or not, as follows:

jobu = 'N' or 'n': Do not compute the *U* matrix.

jobu = 'U' or 'u': Compute the *U* matrix.

jobv Specifies whether to compute the V matrix or not, as follows:

jobv = 'N' or 'n': Do not compute the V matrix.

jobv = 'V' or 'v': Compute the V matrix.

jobq Specifies whether to compute the Q matrix or not, as follows:

jobv = 'N' or 'n': Do not compute the Q matrix.

jobv = 'Q' or 'q': Compute the Q matrix.

m The number of rows of the matrix A. **m** ≥ 0.

n The number of columns of the matrices A and B. **n** ≥ 0.

p The number of rows of the matrix B. **p** ≥ 0.

a The **m**-by-**n** matrix A.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**m**).

b The **p**-by-**n** matrix B.

ldb The leading dimension of array **b** in the calling program unit. **ldb** ≥ max(1,**p**).

ldu The leading dimension of array **u** in the calling program unit. **ldu** ≥ 1, and if **jobu** = 'U' or 'u', then **ldu** ≥ **m**.

ldv The leading dimension of array **v** in the calling program unit. **ldv** ≥ 1, and if **jobv** = 'V' or 'v', then **ldq** ≥ **p**.

ldq The leading dimension of array **q** in the calling program unit. **ldq** ≥ 1, and if **jobq** = 'Q' or 'q', then **ldq** ≥ **n**.

Working Storage

work, rwork, iwork Arrays used for work space.

Output

k, l On successful exit, **k** and **l** specify the dimensions of the subblocks of D_1, D_2, and R as described in "Purpose."

a On successful exit with **k+l** ≤ **m**, the (**k+l**)-by-(**k+l**) nonsingular triangular matrix R is stored in rows 1 to **k+l** of columns **n–k–l+1** to **n** of **a**.

On successful exit with **k+l** > **m**, rows 1 to **m** of the (**k+l**)-by-(**k+l**) nonsingular triangular matrix $R$are stored in rows 1 to **m** of columns **n–k–l+1** to **n** of **a**.

b On successful exit with **k+l** > **m**, the R_{33} block of R is stored in rows **m–k+1** to **l** of columns **m+n–k–l+1** to **n** of **b**.

Destroyed if **k+l** ≤ **m**.

alpha, beta On successful exit, **alpha** and **beta** contain the generalized singular value pairs of A and B, as described in "Purpose." The α_i and β_i are not sorted into any particular order.

If **k+l** ≤ **m**:

$$\text{alpha}(i) = \begin{cases} 1 & \text{if } i = 1, 2, \ldots, \mathbf{k}, \\ \alpha_i & \text{if } i = \mathbf{k}+1, \ldots, \mathbf{k}+\mathbf{l}, \\ 0 & \text{if } i = \mathbf{k}+\mathbf{l}+1, \ldots, \mathbf{n}. \end{cases}$$

$$\text{beta}(i) = \begin{cases} 0 & \text{if } i = 1, 2, \ldots, \mathbf{k}, \\ \beta_i & \text{if } i = \mathbf{k}+1, \ldots, \mathbf{k}+\mathbf{l}, \\ 0 & \text{if } i = \mathbf{k}+\mathbf{l}+1, \ldots, \mathbf{n}. \end{cases}$$

If **k+l** > **m**:

$$\text{alpha}(i) = \begin{cases} 1 & \text{if } i = 1, 2, \ldots, \mathbf{k}, \\ \alpha_i & \text{if } i = \mathbf{k}+1, \ldots, \mathbf{m}, \\ 0 & \text{if } i = \mathbf{m}+1, \ldots, \mathbf{n}. \end{cases}$$

$$\text{beta}(i) = \begin{cases} 0 & \text{if } i = 1, 2, \ldots, \mathbf{k}, \\ \beta_i & \text{if } i = \mathbf{k}+1, \ldots, \mathbf{m}, \\ 1 & \text{if } i = \mathbf{m}+1, \ldots, \mathbf{k}+\mathbf{l}, \\ 0 & \text{if } i = \mathbf{k}+\mathbf{l}+1, \ldots, \mathbf{n}. \end{cases}$$

u On successful exit, if **jobu** = 'U' or 'u', the matrix U. Not referenced if **jobu** = 'N' or 'n'.

v On successful exit, if **jobv** = 'V' or 'v', the matrix V. Not referenced if **jobv** = 'N' or 'n'.

q On successful exit, if **jobq** = 'Q' or 'q', the matrix Q. Not referenced if **jobq** = 'N' or 'n'.

info Status response:

info = 0:	Successful exit.
info < 0:	If **info** = $-k$, the k-th argument had an invalid value.
info > 0:	The algorithm did not converge.

Notes

If an error in the arguments is detected, the subprograms call error handler XERBLA, which writes an error message onto the standard error file and terminates execution. The standard version of XERBLA (see Chapter 11), may be replaced with a user-supplied version to change the error procedure. Error conditions are

jobu ≠ 'U' or 'u',
jobv ≠ 'V' or 'v',
jobq ≠ 'Q' or 'q',
m < 0,
n < 0,
p < 0,
lda < max(1,**m**),
ldb < max(1,**p**),
ldu too small,
ldv too small, and
ldq too small.

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding, for example, the **jobu** argument as 'U wanted' for 'U' or 'NoU' for 'N'.

11 LAPACK Auxiliary Subprograms

Overview

This chapter describes selected LAPACK auxiliary subprograms. Although the auxiliary subprograms are a part of the public domain release of LAPACK, the Hewlett-Packard implementation of LAPACK does not support all of them. They are viewed as internal to the package and subject to change. The auxiliary subprograms described in this chapter, however, are supported as part of LAPACK and will exist in subsequent releases of the product. The operations covered are:

- Choosing machine- or problem-dependent parameters
- Computing a norm of a matrix, for matrices stored in several different formats
- Reporting errors in a consistent manner

The following document provides supplemental material for this chapter:

- Golub, G.H. and C.F. Van Loan. *Matrix Computations*, 2nd Edition. Baltimore, MD: The Johns Hopkins University Press. 1989.

Chapter Objectives

After reading this chapter you will:

- Know what a vector norm and a matrix norm is and which matrix norms can be computed by LAPACK auxiliary subprograms.
- Know how blocking parameters are set and used
- Understand how to use the described subprograms

What You Need to Know to Use These Subprograms

Norms of Vectors and Matrices

To use the norm-computing subprograms, you need to understand the basics of vector and matrix norms. For completeness, the following is a brief discussion of vector and matrix norms. Most standard texts on linear algebra cover the prerequisite material in greater detail.

Definition: A *vector norm* on $\mathbf{R}^n$, the vector space of n-dimensional real vectors, is a function $f:\mathbf{R}^n \rightarrow \mathbf{R}$ that has the following properties:

$f(x) \geq 0$	$x \in \mathbf{R}^v$
$f(x) = 0$	if and only if $x = 0$
$f(x+y) \leq f(\xi)+\phi(\psi)$	$x, y \in \mathbf{R}^v$
$f(\alpha x) = \lvert\alpha\rvert f(\xi)$	$\alpha \in \mathbf{R}, \xi \in \mathbf{R}^v$

Such a function is denoted with a double-bar notation: $f(x) = \|x\|$. Subscripts on the double bar are used to distinguish between various norms. The most important vector norms are the 1-, 2-, and ∞-norms, defined in Table 11-1.

The vector space of m-by-n matrices is isomorphic to the vector space of mn-dimensional vectors. Therefore, the definition of a matrix norm follows from the definition of a vector norm.

Definition: A *matrix norm* on $\mathbf{R}^{m\times n}$, the vector space of m-by-n real matrices, is a function $f:\mathbf{R}^{m\times n} \rightarrow \mathbf{R}$ that has the following properties:

$f(A) \geq 0$	$A \in \mathbf{R}^{\mu\times n}$
$f(A) = 0$	if and only if $A = 0$
$f(A+B) \leq f(A)+\phi(B)$	$A, B \in \mathbf{R}^{\mu\times n}$
$f(\alpha A) = \lvert\alpha\rvert f(A)$	$\alpha \in \mathbf{R}, A \in \mathbf{R}^{\mu\times n}$

As with vector norms, f is denoted with the double-bar notation: $f(A) = \|A\|$, again using subscripts to designate different matrix norms.

The formal definition of a matrix norm, given above, ignores the uses of matrices as operators in matrix-vector and matrix-matrix multiplication. Therefore, a matrix norm usually is required to satisfy several additional conditions related to such products.

Let $\|\ \|_\alpha$ be a vector norm on $\mathbf{R}^m$, $\|\ \|_\beta$ be a vector norm on $\mathbf{R}^n$, and $\|\ \|_{\alpha,\beta}$ be a matrix norm on $\mathbf{R}^{m\times n}$. The matrix norm is said to be *consistent with* the vector norm if

$$\|Ax\|_\beta \le \|A\|_{\alpha,\beta}\|x\|_\alpha.$$

Let $\|\ \|_\alpha$ be a vector norm on $\mathbf{R}^m$, $\|\ \|_\beta$ be a vector norm on $\mathbf{R}^n$, and $\|\ \|_{\alpha,\beta}$ be a matrix norm on $\mathbf{R}^{m\times n}$. The matrix norm is said to be *induced by* or *subordinate to* the vector norm if

$$\|A\|_{\alpha,\beta} = \max_{x\neq 0} \frac{\|Ax\|_\beta}{\|x\|_\alpha}.$$

Finally, let $\|\ \|_\alpha$, $\|\ \|_\beta$, and $\|\ \|_\gamma$ be matrix norms on $\mathbf{R}^{m\times q}$, $\mathbf{R}^{m\times n}$, and $\mathbf{R}^{n\times q}$, respectively. Then the norms are *consistent* if the submultiplicative property

$$\|AB\|_\alpha \le \|A\|_\beta\ \|B\|_\gamma$$

is satisfied for all $A \in \mathbf{R}^{m\times n}$ and $B \in \mathbf{R}^{n\times q}$.

The norm-computing auxiliary subprograms in LAPACK will evaluate the 1-, ∞-, Frobenius-, or Δ-norms of a matrix stored in a variety of forms.

Table 11-1 Norms of Vectors and Matrices

Name	Vector Norm	Matrix Norm
1-norm	$\|x\|_1 = \sum_i \|x_i\|$	$\|A\|_1 = \max_j \sum_i \|a_{ij}\|$
2-norm	$\|x\|_2 = (\sum_i \|x_i\|^2)^{1/2}$	$\|A\|_2 = \max_{x\neq 0} \|Ax\|/\|x\|$
∞-norm	$\|x\|_\infty = \max_i \|x_i\|$	$\|A\|_\infty = \max_i \sum_j \|a_{ij}\|$
Frobenius norm	$\|x\|_F = \|x\|_2$	$\|A\|_F = (\sum_{ij} \|a_{ij}\|^2)^{1/2}$
Δ-norm	—	$\|A\|_\Delta = \max_{ij} \|a_{ij}\|$

The Frobenius matrix norm is not subordinate to the Frobenius vector norm. The Δ matrix norm is not subordinate to any vector norm, nor is it consistent with itself as a matrix norm.

NAME

ILAENV – Choose Problem-Dependent Parameters

Purpose

ILAENV is called by various LAPACK subprograms to set problem-dependent parameters.

Usage

LAPACK:

```
CHARACTER*(*)      name, opts
INTEGER*4          ispec, n1, n2, n3, n4
INTEGER*4          ivalue, ILAENV
ivalue = ILAENV(ispec, name, opts, n1, n2, n3, n4)
```

LAPACK8:

```
CHARACTER*(*)      name, opts
INTEGER*8          ispec, n1, n2, n3, n4
INTEGER*8          ivalue, ILAENV
ivalue = ILAENV(ispec, name, opts, n1, n2, n3, n4)
```

Input

ispec Specifies which parameter is to be returned as the value of ILAENV, as follows:

ispec = 1:	The optimal block size; if this value is 1, an unblocked algorithm will give the best performance.
ispec = 2:	The minimum block size for which the blocked algorithm should be used; if the usable block size is less than this value, an unblocked algorithm should be used.
ispec = 3:	The crossover point: in a blocked algorithm, for **n** less than this value, an unblocked algorithm should be used.
ispec = 4:	The number of shifts, used in the nonsymmetric eigenvalue subroutines.

	ispec = 5:	The minimum column size for blocking to be used; rectangular blocks must have size at least **k**-by-**m**, where **k** is given by ILAENV(2,...) and **m** by ILAENV(5,...).
	ispec = 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 QR factorization is used first to reduce the matrix to a triangular form.
	ispec = 7:	The number of processors (unused in the current LAPACK implementation).
	ispec = 8:	The crossover point for the multishift QR and QZ methods for nonsymmetric eigenvalue problems.
name	The name of the calling subprogram in either all uppercase or all lowercase characters.	
opts	The character options passed to subroutine **name**, concatenated into a single character string in the same order in which they appear in the argument list for subroutine **name**. For example, **uplo** = 'U', **trans** = 'T', and **diag** = 'N' for a triangular subroutine would be specified as **opts** = 'UTN'.	
n1, n2, n3, n4	The problem size arguments passed to subroutine **name**, in the same order in which they appear in the argument list for subroutine **name**; these may not all be required.	

Output

ivalue	The function value is the value of the requested problem-dependent parameter, or an error code, as follows:	
	ivalue ≥ 0:	The value of the problem parameter specified by **ispec**.
	ivalue < 0:	If **ivalue** = $-k$, the k-th argument had an invalid value.

Notes

The following conventions have been used when calling ILAENV from LAPACK subprograms:

opts is a concatenation of all of the character options to subroutine **name**, in the same order in which they appear in the argument list for **name**, even if they are not used in determining the value of the problem-dependent parameter specified by **ispec**.

The problem size arguments **n1**, **n2**, **n3**, and **n4** are specified in the order in which they appear in the argument list for **name**. **n1** is used first, **n2** second, and so on, and unused problem size arguments are passed a value of -1.

The parameter value returned by ILAENV is checked for validity in the calling subroutine. For example, ILAENV is used to retrieve the optimal block size for STRTRI as follows:

```
NB = ILAENV (1, 'STRTRI', UPLO // DIAG, N, -1, -1, -1)
IF ( NB .LE. 1 ) NB = MAX(1, N)
```

NAME

SLAMCH/DLAMCH – Return Machine-Dependent Parameters

Purpose

These subprograms are called by various LAPACK subprograms to return machine-dependent parameters, thus promoting machine independence in LAPACK.

Usage

LAPACK:

```
CHARACTER*1        name
REAL*4             SLAMCH, value
value = SLAMCH(name)

CHARACTER*1        name
REAL*8             DLAMCH, value
value = DLAMCH(name)
```

LAPACK8:

```
CHARACTER*1        name
REAL*8             SLAMCH, value
value = SLAMCH(name)
```

Input

name Specifies which machine-dependent parameter is to be returned, as follows:

name = 'E' or 'e':	*eps*	The relative machine precision: the smallest number ε such that 1 + ε may be represented as a floating-point number with 1 + ε > 1.
name = 'S' or 's':	*sfmin*	The safe minimum: the smallest number such that 1/*sfmin* does not overflow.
name = 'B' or 'b':	*base*	The base of the machine, *base* = 2.0 on all CONVEX machine types.
name = 'P' or 'p':	*prec*	*eps*×*base*.
name = 'N' or 'n':	*t*	The number of base-2 digits in the mantissa.
name = 'R' or 'r':	*rnd*	1.0 on machines where rounding occurs on addition; zero otherwise. *rnd* = 1.0 on all CONVEX machine types.
name = 'M' or 'm':	*emin*	The smallest exponent before underflow.
name = 'U' or 'u':	*rmin*	The underflow threshold: $base^{emin-1}$.
name = 'L' or 'l':	*emax*	The largest exponent before overflow.
name = 'O' or 'o':	*rmin*	The overflow threshold: $base^{emax} \times (1 - \varepsilon)$.

Output

value The function value is the value of the requested machine-dependent parameter.

Notes

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the function reference may be improved by coding, for example, the **name** argument as 'Eps' for 'E' or 'Safemin' for 'S'.

NAME

SLANGB/DLANGB/.../ZLANGB – Compute Norm of General Band Matrix

Purpose

These subprograms compute a norm of an m-by-n general band matrix A. A band matrix is a matrix whose nonzero elements all lie near the principal diagonal. Specifically, $a_{ij} = 0$ if $i-j > kl$ or $j-i > ku$ for some integers kl and ku. The smallest such kl and ku for a given matrix are called the lower and upper bandwidths, respectively, and $k = kl+ku+1$ is the total bandwidth.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, you need only provide the elements within the band of A. Compared to storing the entire matrix, this can save memory if $kl+ku+1 < n$.

The following example illustrates the storage of general band matrices. Consider the following matrix A of order $n = 9$ and lower and upper bandwidths $kl = 2$ and $ku = 3$, respectively:

11	12	13	14	0	0	0	0	0
21	22	23	24	25	0	0	0	0
31	32	33	34	35	36	0	0	0
0	42	43	44	45	46	47	0	0
0	0	53	54	55	56	57	58	0
0	0	0	64	65	66	67	68	69
0	0	0	0	75	76	77	78	79
0	0	0	0	0	86	87	88	89
0	0	0	0	0	0	97	98	99

A is given in an array **ab** with at least $kl+ku+1 = 6$ rows and $n = 9$ columns as follows:

*	*	*	14	25	36	47	58	69
*	*	13	24	35	46	57	68	79
*	12	23	34	45	56	67	78	89
11	22	33	44	55	66	77	88	99
21	32	43	54	65	76	87	98	*
31	42	53	64	75	86	97	*	*

The asterisks in the *ku*-by-*ku* triangle at the upper left corner and in the *kl*-by-*kl* triangle at the lower right corner represent elements of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of A, then it is stored in **ab**(ku+1+i–j,j). Therefore, the columns of A are stored in the columns of **ab**, and the diagonals of A are stored in the rows of **ab**, such that the principal diagonal is stored in row ku+1 of **ab**.

Note that this storage format omits the first *kl* rows reserved for fill-in in the general band storage for _GBSV and _GBTRF.

Usage

LAPACK:

```
CHARACTER*1          norm
INTEGER*4            kl, ku, ldab, n
REAL*4               ab(ldab, n), work(n)
REAL*4               anorm, SLANGB
anorm = SLANGB(norm, n, kl, ku, ab, ldab, work)

CHARACTER*1          norm
INTEGER*4            kl, ku, ldab, n
REAL*8               ab(ldab, n), work(n)
REAL*8               anorm, DLANGB
anorm = DLANGB(norm, n, kl, ku, ab, ldab, work)

CHARACTER*1          norm
INTEGER*4            kl, ku, ldab, n
REAL*4               rwork(n)
COMPLEX*8            ab(ldab, n)
REAL*4               anorm, CLANGB
anorm = CLANGB(norm, n, kl, ku, ab, ldab, rwork)

CHARACTER*1          norm
INTEGER*4            kl, ku, ldab, n
REAL*8               rwork(n)
COMPLEX*16           ab(ldab, n)
REAL*8               anorm, ZLANGB
anorm = ZLANGB(norm, n, kl, ku, ab, ldab, rwork)
```

LAPACK8:

```
CHARACTER*1          norm
INTEGER*8            kl, ku, ldab, n
REAL*8               ab(ldab, n), work(n)
REAL*8               anorm, SLANGB
anorm = SLANGB(norm, n, kl, ku, ab, ldab, work)

CHARACTER*1          norm
INTEGER*8            kl, ku, ldab, n
REAL*8               rwork(n)
```

```
COMPLEX*16          ab(ldab, n)
REAL*8              anorm, CLANGB
anorm = CLANGB(norm, n, kl, ku, ab, ldab, rwork)
```

Input

norm Specifies which norm is to be computed, as follows:

norm = 'F', 'f', 'E', or 'e':	Compute $\|\|A\|\|_F$ = the Frobenius norm.
norm = 'I' or 'i':	Compute $\|\|A\|\|_\infty$ = maximum row sum.
norm = '1', 'O', or 'o':	Compute $\|\|A\|\|_1$ = maximum column sum.
norm = 'M' or 'm':	Compute $max(\|A_{ij}\|)$.

n The order of the matrix A. **n** ≥ 0.

kl The number of subdiagonals within the band of A. **kl** ≥ 0.

ku The number of superdiagonals within the band of A. **ku** ≥ 0.

ab The matrix A in band storage, in the first **kl**+**ku**+1 rows. The j-th column of A is stored in the j-th column of array **ab** as follows: **ab**(**ku**+1+i–j,j) = $A(i,j)$ for max(1,j–**ku**) ≤ i ≤ min(**n**,j+**kl**)

ldab The leading dimension of array **ab** in the calling program unit. **ldab** ≥ **kl**+**ku**+1.

Working Storage

work, rwork Arrays used for work space. Not referenced unless **norm** = 'I' or 'i'.

Output

anorm The function value is the value of the requested norm of A.

Notes

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **norm** argument as 'Frobenius' for 'F', 'Infinity-Norm' for 'I', 'One-norm' or '1-norm' for 'O', or 'Max-Element' for 'M'.

NAME

SLANGE/DLANGE/.../ZLANGE – Compute Norm of General Matrix

Purpose

These subprograms compute a norm of a general m-by-n matrix A.

Usage

LAPACK:

```
CHARACTER*1        norm
INTEGER*4          lda, m, n
REAL*4             a(lda, n), work(n)
REAL*4             anorm, SLANGE
anorm = SLANGE(norm, m, n, a, lda, work)

CHARACTER*1        norm
INTEGER*4          lda, m, n
REAL*8             a(lda, n), work(n)
REAL*8             anorm, DLANGE
anorm = DLANGE(norm, m, n, a, lda, work)

CHARACTER*1        norm
INTEGER*4          lda, m, n
REAL*4             rwork(n)
COMPLEX*8          a(lda, n)
REAL*4             anorm, CLANGE
anorm = CLANGE(norm, m, n, a, lda, rwork)

CHARACTER*1        norm
INTEGER*4          lda, m, n
REAL*8             rwork(n)
COMPLEX*16         a(lda, n)
REAL*8             anorm, ZLANGE
anorm = ZLANGE(norm, m, n, a, lda, rwork)
```

LAPACK8:

```
CHARACTER*1        norm
INTEGER*8          lda, m, n
REAL*8             a(lda, n), work(n)
REAL*8             anorm, SLANGE
anorm = SLANGE(norm, m, n, a, lda, work)

CHARACTER*1        norm
INTEGER*8          lda, m, n
REAL*8             rwork(n)
COMPLEX*16         a(lda, n)
REAL*8             anorm, CLANGE
anorm = CLANGE(norm, m, n, a, lda, rwork)
```

Input

norm Specifies which norm is to be computed, as follows:

norm = 'F', 'f', 'E', or 'e':	Compute $\|\|A\|\|_F$ = the Frobenius norm.
norm = 'I' or 'i':	Compute $\|\|A\|\|_\infty$ = maximum row sum.
norm = '1', 'O', or 'o':	Compute $\|\|A\|\|_1$ = maximum column sum.
norm = 'M' or 'm':	Compute $max(\|A_{ij}\|)$.

m The number of rows of the matrix A. **m** ≥ 0.

n The number of columns of the matrix A. **n** ≥ 0.

a The **m**-by-**n** matrix A.

lda The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**m**).

Working Storage

work, rwork Arrays used for work space. Not referenced unless **norm** = 'I' or 'i'.

Output

anorm The function value is the value of the requested norm of A.

Notes

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **norm** argument as 'Frobenius' for 'F', 'Infinity-Norm' for 'I', 'One-norm' or '1-norm' for 'O', or 'Max-Element' for 'M'.

NAME

SLANGT/.../ZLANGT – Compute Norm of General Tridiagonal Matrix

Purpose

These subprograms compute a norm of a general tridiagonal matrix A. A matrix $A = (a_{ij})$ is tridiagonal if its nonzero elements lie only on the principal diagonal ($i = j$), the subdiagonal ($i = j+1$), and the superdiagonal ($i = j-1$) of the matrix.

Matrix Storage

The following example illustrates the storage of general tridiagonal matrices. Consider the following tridiagonal matrix of order $n = 7$:

11	12	0	0	0	0	0
21	22	23	0	0	0	0
0	32	33	34	0	0	0
0	0	43	44	45	0	0
0	0	0	54	55	56	0
0	0	0	0	65	66	67
0	0	0	0	0	76	77

The subdiagonal is stored in array **dl**, the principal diagonal is stored in array **d**, and the superdiagonal is stored in array **du**, as follows:

i	**dl**(i)	**d**(i)	**du**(i)
1	21	11	12
2	32	22	23
3	43	33	34
4	54	44	45
5	65	55	56
6	76	66	67
7		77	

Usage

LAPACK:

```
CHARACTER*1     norm
INTEGER*4       n
REAL*4          d(n), dl(n–1), du(n–1)
REAL*4          anorm, SLANGT
anorm = SLANGT(norm, n, dl, d, du)
```

```
CHARACTER*1        norm
INTEGER*4          n
REAL*8             d(n), dl(n–1), du(n–1)
REAL*8             anorm, DLANGT
anorm = DLANGT(norm, n, dl, d, du)

CHARACTER*1        norm
INTEGER*4          n
COMPLEX*8          d(n), dl(n–1), du(n–1)
REAL*4             anorm, CLANGT
anorm = CLANGT(norm, n, dl, d, du)

CHARACTER*1        norm
INTEGER*4          n
COMPLEX*16         d(n), dl(n–1), du(n–1)
REAL*8             anorm, ZLANGT
anorm = ZLANGT(norm, n, dl, d, du)
```

LAPACK8:

```
CHARACTER*1        norm
INTEGER*8          n
REAL*8             d(n), dl(n–1), du(n–1)
REAL*8             anorm, SLANGT
anorm = SLANGT(norm, n, dl, d, du)

CHARACTER*1        norm
INTEGER*8          n
COMPLEX*16         d(n), dl(n–1), du(n–1)
REAL*8             anorm, CLANGT
anorm = CLANGT(norm, n, dl, d, du)
```

Input

norm Specifies which norm is to be computed, as follows:

norm = 'F', 'f', 'E', or 'e':	Compute $\|\|A\|\|_F$ = the Frobenius norm.
norm = 'I' or 'i':	Compute $\|\|A\|\|_\infty$ = maximum row sum.
norm = '1', 'O', or 'o':	Compute $\|\|A\|\|_1$ = maximum column sum.
norm = 'M' or 'm':	Compute $max(\|A_{ij}\|)$.

n The order of the matrix A. **n** ≥ 0.

dl The **n**–1 subdiagonal elements of A.

d The diagonal elements of A.

du The **n**–1 superdiagonal elements of A.

Output

anorm The function value is the value of the requested norm of A.

Notes

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **norm** argument as 'Frobenius' for 'F', 'Infinity-Norm' for 'I', 'One-norm' or '1-norm' for 'O', or 'Max-Element' for 'M'.

NAME

SLANSB/... – Compute Norm of Symmetric or Hermitian Band Matrix

Purpose

These subprograms compute a norm of a real or complex symmetric or complex Hermitian band matrix A. A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

Tridiagonal matrices are the special case $kd = 1$. They can be handled more efficiently by the LAPACK subprograms SLANST, DLANST, CLANHT, and ZLANHT.

The structure of A is indicated by the name of the subprogram used:

SLANSB	or	DLANSB	A is a real symmetric matrix.
CLANSB	or	ZLANSB	A is a complex symmetric matrix.
CLANHB	or	ZLANHB	A is a complex Hermitian matrix.

Matrix Storage

Because it is not necessary to store or operate on the zeros outside the band of A, and since either triangle of A may be obtained from the other, you need only provide the band within one triangle of A. Compared to storing the entire matrix, this can save memory in two ways: only the elements within the band are stored, and of them, only the upper or the lower triangle.

The following examples illustrate the storage of symmetric or Hermitian band matrices. Consider the following matrix A of order $n = 7$ and half bandwidth $kd = 2$:

11	12	13	0	0	0	0
12	22	23	24	0	0	0
13	23	33	34	35	0	0
0	24	34	44	45	46	0
0	0	35	45	55	56	57
0	0	0	46	56	66	67
0	0	0	0	57	67	77

Upper triangular storage. The upper triangle of A is stored in an array **ab** with at least $kd+1 = 3$ rows and 7 columns as follows:

*	*	13	24	35	46	57
*	12	23	34	45	56	67
11	22	33	44	55	66	77

The asterisks represent elements in the *kd*-by-*kd* triangle at the upper left corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the upper triangle of *A*, it is stored in **ab**(*kd*+1+*i*–*j*,*j*). Therefore, the columns of the upper triangle of *A* are stored in the columns of **ab**, and the diagonals of the upper triangle of *A* are stored in the rows of **ab**.

Lower triangular storage. The lower triangle of A is stored in the array **ab** as follows:

11	22	33	44	55	66	77
12	23	34	45	56	67	*
13	24	35	46	57	*	*

The asterisks represent elements in the *kd*-by-*kd* triangle at the lower right corner of **ab** that are not referenced. Thus, if a_{ij} is an element within the band of the lower triangle of *A*, it is stored in **ab**(*kd*+1+*i*–*j*,*j*). Therefore, the columns of the lower triangle of *A* are stored in the columns of **ab**, and the diagonals of the lower triangle of *A* are stored in the rows of **ab**.

Usage

LAPACK:

```
CHARACTER*1          norm, uplo
INTEGER*4            kd, ldab, n
REAL*4               ab(ldab, n), work(n)
REAL*4               anorm, SLANSB
anorm = SLANSB(norm, uplo, n, kd, ab, ldab, work)

CHARACTER*1          norm, uplo
INTEGER*4            kd, ldab, n
REAL*8               ab(ldab, n), work(n)
REAL*8               anorm, DLANSB
anorm = DLANSB(norm, uplo, n, kd, ab, ldab, work)

CHARACTER*1          norm, uplo
INTEGER*4            kd, ldab, n
REAL*4               rwork(n)
COMPLEX*8            ab(ldab, n)
REAL*4               anorm, CLANHB
anorm = CLANHB(norm, uplo, n, kd, ab, ldab, rwork)

CHARACTER*1          norm, uplo
INTEGER*4            kd, ldab, n
REAL*4               rwork(n)
COMPLEX*8            ab(ldab, n)
REAL*4               anorm, CLANSB
anorm = CLANSB(norm, uplo, n, kd, ab, ldab, rwork)
```

```
CHARACTER*1        norm, uplo
INTEGER*4          kd, ldab, n
REAL*8             rwork(n)
COMPLEX*16         ab(ldab, n)
REAL*8             anorm, ZLANHB
anorm = ZLANHB(norm, uplo, n, kd, ab, ldab, rwork)

CHARACTER*1        norm, uplo
INTEGER*4          kd, ldab, n
REAL*8             rwork(n)
COMPLEX*16         ab(ldab, n)
REAL*8             anorm, ZLANSB
anorm = ZLANSB(norm, uplo, n, kd, ab, ldab, rwork)
```

LAPACK8:

```
CHARACTER*1        norm, uplo
INTEGER*8          kd, ldab, n
REAL*8             ab(ldab, n), work(n)
REAL*8             anorm, SLANSB
anorm = SLANSB(norm, uplo, n, kd, ab, ldab, work)

CHARACTER*1        norm, uplo
INTEGER*8          kd, ldab, n
REAL*8             rwork(n)
COMPLEX*16         ab(ldab, n)
REAL*8             anorm, CLANHB
anorm = CLANHB(norm, uplo, n, kd, ab, ldab, rwork)

CHARACTER*1        norm, uplo
INTEGER*8          kd, ldab, n
REAL*8             rwork(n)
COMPLEX*16         ab(ldab, n)
REAL*8             anorm, CLANSB
anorm = CLANSB(norm, uplo, n, kd, ab, ldab, rwork)
```

Input

norm Specifies which norm is to be computed, as follows:

norm = 'F', 'f', 'E', or 'e':	Compute $\|\|A\|\|_F$ = the Frobenius norm.
norm = 'I' or 'i':	Compute $\|\|A\|\|_\infty$ = maximum row sum.
norm = '1', 'O', or 'o':	Compute $\|\|A\|\|_1$ = maximum column sum.
norm = 'M' or 'm':	Compute $max(\|A_{ij}\|)$.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

- **uplo** = 'U' or 'u': The upper triangular part of A is stored.
- **uplo** = 'L' or 'l': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

kd The number of super-diagonals of the matrix A if **uplo** = 'U' or 'u', or the number of sub-diagonals if **uplo** = 'L' or 'l'. $\mathbf{kd} \geq 0$.

ab The upper or lower triangle of the symmetric or Hermitian band matrix A, stored in the first **kd**+1 rows of the array. The j-th column of A is stored in the j-th column of array **ab** as follows:

If **uplo** = 'U' or 'u', $\mathbf{ab}(\mathbf{kd}+1+i-j,j) = A(i,j)$ for $\max(1,j-\mathbf{kd}) \leq i \leq j$;

If **uplo** = 'L' or 'l', $\mathbf{ab}(1+i-j,j) = A(i,j)$ for $j \leq i \leq \min(\mathbf{n},j+\mathbf{kd})$.

ldab The leading dimension of array **ab** in the calling program unit. $\mathbf{ldab} \geq \mathbf{kd}+1$.

Working Storage

work, rwork Arrays used for work space. Not referenced unless **norm** = '1' or 'I' or 'i' or 'O' or 'o'.

Output

anorm The function value is the value of the requested norm of A.

Notes

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **norm** argument as 'Frobenius' for 'F', 'Infinity-Norm' for 'I', 'One-norm' or '1-norm' for 'O', or 'Max-Element' for 'M'.

NAME

SLANSP/... – Compute Norm of Symmetric or Hermitian Packed Matrix

Purpose

These subprograms compute a norm of a real or complex symmetric or complex Hermitian matrix A that is stored in an array in packed form.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

The structure of A is indicated by the name of the subprogram used:

SLANSP	or	DLANSP	A is a real symmetric packed matrix.
CLANSP	or	ZLANSP	A is a complex symmetric packed matrix.
CLANHP	or	ZLANHP	A is a complex Hermitian packed matrix.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A, either the upper or the lower triangle. Compared to storing the entire matrix, you save memory by supplying that triangle stored column-by-column in packed form in a 1-dimensional array.

The following examples illustrate the packed storage of symmetric or Hermitian matrices.

Upper triangular storage. If the upper triangle of A is

$$\begin{matrix} 11 & 12 & 13 & 14 \\ & 22 & 23 & 24 \\ & & 33 & 34 \\ & & & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	12	22	13	23	33	14	24	34	44

Upper triangular matrix element a_{ij} is stored in array element **ap**(i+j×(j–1)/2).

Lower triangular storage. If the lower triangle of A is

$$\begin{matrix} 11 & & & \\ 21 & 22 & & \\ 31 & 32 & 33 & \\ 41 & 42 & 43 & 44 \end{matrix}$$

then A is packed column-by-column into an array **ap** as follows:

k	1	2	3	4	5	6	7	8	9	10
ap(k)	11	21	31	41	22	32	42	33	43	44

Lower triangular matrix element a_{ij} is stored in array element **ap**($i+(j-1)\times(2n-j)/2$).

Usage

LAPACK:

```
CHARACTER*1          norm, uplo
INTEGER*4            n
REAL*4               ap((n*(n+1))/2), work(n)
REAL*4               anorm, SLANSP
anorm = SLANSP(norm, uplo, n, ap, work)

CHARACTER*1          norm, uplo
INTEGER*4            n
REAL*8               ap((n*(n+1))/2), work(n)
REAL*8               anorm, DLANSP
anorm = DLANSP(norm, uplo, n, ap, work)

CHARACTER*1          norm, uplo
INTEGER*4            n
REAL*4               rwork(n)
COMPLEX*8            ap((n*(n+1))/2)
REAL*4               anorm, CLANHP
anorm = CLANHP(norm, uplo, n, ap, rwork)

CHARACTER*1          norm, uplo
INTEGER*4            n
REAL*4               rwork(n)
COMPLEX*8            ap((n*(n+1))/2)
REAL*4               anorm, CLANSP
anorm = CLANSP(norm, uplo, n, ap, rwork)

CHARACTER*1          norm, uplo
INTEGER*4            n
REAL*8               rwork(n)
COMPLEX*16           ap((n*(n+1))/2)
REAL*8               anorm, ZLANHP
```

```
anorm = ZLANHP(norm, uplo, n, ap, rwork)
CHARACTER*1        norm, uplo
INTEGER*4          n
REAL*8             rwork(n)
COMPLEX*16         ap((n*(n+1))/2)
REAL*8             anorm, CLANSP
anorm = ZLANSP(norm, uplo, n, ap, rwork)
```

LAPACK8:

```
CHARACTER*1        norm, uplo
INTEGER*8          n
REAL*8             ap((n*(n+1))/2), work(n)
REAL*8             anorm, SLANSP
anorm = SLANSP(norm, uplo, n, ap, work)
CHARACTER*1        norm, uplo
INTEGER*8          n
REAL*8             rwork(n)
COMPLEX*16         ap((n*(n+1))/2)
REAL*8             anorm, CLANHP
anorm = CLANHP(norm, uplo, n, ap, rwork)
CHARACTER*1        norm, uplo
INTEGER*8          n
REAL*8             rwork(n)
COMPLEX*16         ap((n*(n+1))/2)
REAL*8             anorm, CLANSP
anorm = CLANSP(norm, uplo, n, ap, rwork)
```

Input

norm Specifies which norm is to be computed, as follows:

norm = 'F', 'f', 'E', or 'e':	Compute $\|\|A\|\|_F$ = the Frobenius norm.
norm = 'I' or 'i':	Compute $\|\|A\|\|_\infty$ = maximum row sum.
norm = '1', 'O', or 'o':	Compute $\|\|A\|\|_1$ = maximum column sum.
norm = 'M' or 'm':	Compute $max(\|A_{ij}\|)$.

uplo Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:

uplo = 'U' or 'u':	The upper triangular part of A is stored.

uplo = 'L' or '1': The lower triangular part of A is stored.

n The order of the matrix A. $\mathbf{n} \geq 0$.

ap The upper or lower triangular part of the symmetric or Hermitian matrix A, packed columnwise in a linear array as follows:

If **uplo** = 'U' or 'u', $\mathbf{ap}(i + (j-1) \times j/2) = A(i,j)$ for $1 \leq i \leq j$;

If **uplo** = 'L' or '1', $\mathbf{ap}(i + (j-1) \times (2\mathbf{n}-j)/2) = A(i,j)$ for $j \leq i \leq \mathbf{n}$.

Working Storage

work, rwork Arrays used for work space. Not referenced unless **norm** = '1' or 'I' or 'i' or 'O' or 'o'.

Output

anorm The function value is the value of the requested norm of A.

Notes

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **norm** argument as 'Frobenius' for 'F', 'Infinity-Norm' for 'I', 'One-norm' or '1-norm' for 'O', or 'Max-Element' for 'M'.

NAME

SLANST/... – Compute Norm of Symmetric or Hermitian Tridiagonal Matrix

Purpose

These subprograms compute a norm of a real symmetric or complex Hermitian tridiagonal matrix A. A real matrix is symmetric if $A = A^T$, its transpose; a complex matrix is Hermitian if $A = A^*$, its conjugate transpose.

A matrix $A = (a_{ij})$ is tridiagonal if its nonzero elements lie only on the principal diagonal ($i = j$), the subdiagonal ($i = j+1$), and the superdiagonal ($i = j-1$) of the matrix.

Matrix Storage

The following example illustrates the storage of symmetric or Hermitian tridiagonal matrices. Consider the following symmetric tridiagonal matrix of order $n = 7$:

11	21	0	0	0	0	0
21	22	32	0	0	0	0
0	32	33	43	0	0	0
0	0	43	44	54	0	0
0	0	0	54	55	65	0
0	0	0	0	65	66	76
0	0	0	0	0	76	77

The subdiagonal is stored in array **e** and the principal diagonal is stored in array **d**, as follows:

i	**e**(i)	**d**(i)
1	21	11
2	32	22
3	43	33
4	54	44
5	65	55
6	76	66
7		77

Usage

LAPACK:

```
CHARACTER*1        norm
INTEGER*4          n
REAL*4             d(n), e(n–1)
REAL*4             anorm, SLANST
anorm = SLANST(norm, n, d, e)

CHARACTER*1        norm
INTEGER*4          n
REAL*8             d(n), e(n–1)
REAL*8             anorm, DLANST
anorm = DLANST(norm, n, d, e)

CHARACTER*1        norm
INTEGER*4          n
REAL*4             d(n)
COMPLEX*8          e(n–1)
REAL*4             anorm, CLANHT
anorm = CLANHT(norm, n, d, e)

CHARACTER*1        norm
INTEGER*4          n
REAL*8             d(n)
COMPLEX*16         e(n–1)
REAL*8             anorm, ZLANHT
anorm = ZLANHT(norm, n, d, e)
```

LAPACK8:

```
CHARACTER*1        norm
INTEGER*8          n
REAL*8             d(n), e(n–1)
REAL*8             anorm, SLANST
anorm = SLANST(norm, n, d, e)

CHARACTER*1        norm
INTEGER*8          n
REAL*8             d(n)
COMPLEX*16         e(n–1)
REAL*8             anorm, CLANHT
anorm = CLANHT(norm, n, d, e)
```

Input

norm Specifies which norm is to be computed, as follows:

norm = 'F', 'f', 'E', or 'e':	Compute $\|A\|_F$ = the Frobenius norm.
norm = 'I' or 'i':	Compute $\|A\|_\infty$ = maximum row sum.

	norm = '1', 'O', or 'o':	Compute $\|\|A\|\|_1$ = maximum column sum.
	norm = 'M' or 'm':	Compute $max(\|A_{ij}\|)$.
n	The order of the matrix A. $\mathbf{n} \geq 0$.	
d	The **n** diagonal elements of the tridiagonal matrix A.	
e	The **n**–1 subdiagonal elements of the tridiagonal matrix A.	

Output

anorm	The function value is the value of the requested norm of A.

Notes

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **norm** argument as 'Frobenius' for 'F', 'Infinity-Norm' for 'I', 'One-norm' or '1-norm' for 'O', or 'Max-Element' for 'M'.

NAME

SLANSY/.../ZLANSY – Compute Norm of Symmetric or Hermitian Matrix

Purpose

These subprograms compute a norm of a real or complex symmetric or complex Hermitian matrix A.

A matrix is symmetric if $A = A^T$, its transpose; a matrix is Hermitian if $A = A^*$, its conjugate transpose.

The structure of A is indicated by the name of the subprogram used:

SLANSY	or	DLANSY	A is a real symmetric matrix.
CLANSY	or	ZLANSY	A is a complex symmetric matrix.
CLANHE	or	ZLANHE	A is a complex Hermitian matrix.

Matrix Storage

Because either triangle of A may be obtained from the other, you need only provide one triangle of A. You may supply either the upper or the lower triangle of A, in a two-dimensional array large enough to hold the entire matrix. The other triangle of the array is not referenced.

Usage

LAPACK:

```
CHARACTER*1          norm, uplo
INTEGER*4            lda, n
REAL*4               a(lda, n), work(n)
REAL*4               anorm, SLANSY
anorm = SLANSY(norm, uplo, n, a, lda, work)

CHARACTER*1          norm, uplo
INTEGER*4            lda, n
REAL*8               a(lda, n), work(n)
REAL*8               anorm, DLANSY
anorm = DLANSY(norm, uplo, n, a, lda, work)

CHARACTER*1          norm, uplo
INTEGER*4            lda, n
REAL*4               rwork(n)
COMPLEX*8            a(lda, n)
REAL*4               anorm, CLANHE
anorm = CLANHE(norm, uplo, n, a, lda, rwork)
```

```
CHARACTER*1        norm, uplo
INTEGER*4          lda, n
REAL*4             rwork(n)
COMPLEX*8          a(lda, n)
REAL*4             anorm, CLANSY
anorm = CLANSY(norm, uplo, n, a, lda, rwork)

CHARACTER*1        norm, uplo
INTEGER*4          lda, n
REAL*8             rwork(n)
COMPLEX*16         a(lda, n)
REAL*8             anorm, ZLANHE
anorm = ZLANHE(norm, uplo, n, a, lda, rwork)

CHARACTER*1        norm, uplo
INTEGER*4          lda, n
REAL*8             rwork(n)
COMPLEX*16         a(lda, n)
REAL*8             anorm, ZLANSY
anorm = ZLANSY(norm, uplo, n, a, lda, rwork)
```

LAPACK8:

```
CHARACTER*1        norm, uplo
INTEGER*8          lda, n
REAL*8             a(lda, n), work(n)
REAL*8             anorm, SLANSY
anorm = SLANSY(norm, uplo, n, a, lda, work)

CHARACTER*1        norm, uplo
INTEGER*8          lda, n
REAL*8             rwork(n)
COMPLEX*16         a(lda, n)
REAL*8             anorm, CLANHE
anorm = CLANHE(norm, uplo, n, a, lda, rwork)

CHARACTER*1        norm, uplo
INTEGER*8          lda, n
REAL*8             rwork(n)
COMPLEX*16         a(lda, n)
REAL*8             anorm, CLANSY
anorm = CLANSY(norm, uplo, n, a, lda, rwork)
```

Input

norm Specifies which norm is to be computed, as follows:

norm = 'F', 'f', 'E', or 'e':	Compute $\|A\|_F$ = the Frobenius norm.
norm = 'I' or 'i':	Compute $\|A\|_\infty$ = maximum row sum.

	norm = 'I', 'O', or 'o':	Compute $\|\|A\|\|_1$ = maximum column sum.
	norm = 'M' or 'm':	Compute $max(\|A_{ij}\|)$.
uplo	Specifies whether the upper or lower triangular part of the symmetric or Hermitian matrix A is stored, as follows:	
	uplo = 'U' or 'u':	The upper triangular part of A is stored.
	uplo = 'L' or 'l':	The lower triangular part of A is stored.
n	The order of the matrix A. **n** ≥ 0.	
a	The symmetric or Hermitian matrix A, as follows:	
	If **uplo** = 'U' or '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' or '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	The leading dimension of array **a** in the calling program unit. **lda** ≥ max(1,**n**).	

Working Storage

work, rwork	Arrays used for work space. Not referenced unless **norm** = 'I' or 'I' or 'i' or 'O' or 'o'.

Output

anorm	The function value is the value of the requested norm of A.

Notes

Actual character arguments in a subroutine call may be longer than the corresponding dummy arguments. Therefore, readability of the **CALL** statement may be improved by coding the **norm** argument as 'Frobenius' for 'F', 'Infinity-Norm' for 'I', 'One-norm' or '1-norm' for 'O', or 'Max-Element' for 'M'.

NAME

XERBLA – Error Handler

Purpose

This subprogram is the error handler for many LAPACK subprograms, as indicated in the "Notes" section in the applicable subprogram descriptions. As supplied in LAPACK, XERBLA writes the following error message onto the standard error file:

```
********************************************************************************
* XERBLA: subprogram name called with invalid value of argument number iarg *
********************************************************************************
```

where *name* is the name of the subprogram in which the error was detected, and *iarg* is the argument number of the offending argument. For example, in SGBSV, **n** is argument number 1 and **kl** is argument number 2. If the main program is in Fortran and is executed under SPP-UX, a call traceback is also written onto the standard error file (XERBLA does not write a call traceback when used on HP-UX systems). XERBLA then terminates execution with a nonzero exit status.

You may supply a version of XERBLA that alters this action. All LAPACK subprograms that call XERBLA have a **RETURN** statement after the **CALL XERBLA** statement, so if your version of XERBLA exits with a **RETURN** statement, you could detect the error by examining the **info** flag after each LAPACK subprogram call. Other subprograms, such as the Level 2 and 3 BLAS, also call XERBLA. All BLAS, VECLIB, and SCILIB subprograms that call XERBLA also follow the **CALL XERBLA** statement with a **RETURN** statement. However, many of those subprograms do not have a status response variable such as **info** in their argument list to alert the caller. If you write an XERBLA that does not end with a **STOP** statement, you need some other mechanism to detect errors occurring in non-LAPACK subprograms. One such mechanism is a flag in a common block that is set by your XERBLA and tested by the calling program after calls where errors could be detected.

Usage

LAPACK:

```
CHARACTER*6        name
INTEGER*4          iarg
CALL XERBLA(name, iarg)
```

LAPACK8:

```
CHARACTER*6        name
INTEGER*8          iarg
CALL XERBLA(name, iarg)
```

Input

name	The name of the subprogram in which the error was detected.
iarg	The number of the argument that was found to be in error.

Notes

This subprogram conforms to specifications of the Level 2 and 3 BLAS and LAPACK.

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