75

Lapack

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75.1 Introduction

LAPACK (linear algebra package) is an open source library of programs for solving the most commonly occurring numerical linear algebra problems [LUG99]. Original codes of LAPACK are written in Fortran 77. Complete documentation as well as source codes are available online at the Netlib repository [LAP]. LAPACK provides driver routines for solving complete problems such as linear equations, linear least squares problems, eigenvalue problems, and singular value problems. Each driver routine calls a sequence of computational routines, each of which performs a distinct computational task. In addition, LAPACK provides comprehensive error bounds for most computed quantities. LAPACK is designed to be portable for sequential and shared memory machines with deep memory hierarchies, in which most performance issues could be reduced to providing optimized versions of the Basic Linear Algebra Subroutines (BLAS). (See Chapter 74).

There have been a number of extensions of LAPACK. LAPACK95 is a Fortran 95 interface to the Fortran 77 LAPACK [LAP95]. CLAPACK and JLAPACK libraries are built using the Fortran to C (f2c) and Fortran to Java (f2j) conversion utilities, respectively [CLA], [JLA]. LAPACK++ is implemented in C++ and includes a subset of the features in LAPACK with emphasis on solving linear systems with nonsymmetric matrices, symmetric positive definite systems, and linear least squares systems [LA+]. ScaLAPACK is a portable implementation of some of the core routines in LAPACK for parallel distributed computing [Sca]. ScaLAPACK is designed for distributed memory machines with very powerful homogeneous sequential processors and with homogeneous network interconnections.

The purpose of this Chapter is to acquaint the reader with 10 essential numerical linear algebra problems and LAPACK's way of solving those problems. The reader may find it helpful to consult Chapter 74, where some of the terms used here are defined. The following table summarizes these problems and sections that are treated in version 3.0 of LAPACK.

Type of Problem	Acronyms	Section
Linear system of equations	SV	75.2
Linear least squares problems	LLS	75.3
Linear equality-constrained least squares problem	LSE	75.4
General linear model problem	GLM	75.5
Symmetric eigenproblems	SEP	75.6
Nonsymmetric eigenproblems	NEP	75.7
Singular value decomposition	SVD	75.8
Generalized symmetric definite eigenproblems	GSEP	75.9
Generalized nonsymmetric eigenproblems	GNEP	75.10
Generalized (or quotient) singular value decomposition	GSVD (QSVD)	75.11

Sections have been subdivided into the following headings: (1) Definition: Defines the problem, (2) Background: Discusses the background of the problem and references to the related sections in this handbook, (3) Driver Routines: Describes different types of driver routines available that solve the same problem, (4) Example: Specifies the calling sequence for a driver routine that solves the problem followed by numerical examples.

Data structures and naming conventions. All LAPACK routines are available in four data types, as indicated by the initial letter "x" of each subroutine name: x = "S" means real single precision, x = "D", real double precision, x = "C", complex single precision, x = "Z", complex*16 or double complex precision. In single precision (and complex single precision), the computation are performed with an unit roundoff of 5.96×10^{-8}. In double precision (and complex double precision) the computation are performed with an unit roundoff of 1.11×10^{-16}.

All matrices are assumed to be stored in column-major format. The software can also handle submatrices of matrices, even though these submatrices may not be stored in consecutive memory locations. For example, to specify the 10–by–10 submatrix lying in rows and columns 11 through 20 of a 30–by–30 matrix A, one must specify

- `A(11, 11)`, the upper left corner of the submatrix,
- `30` = Leading dimension of `A` in its declaration (often denoted `LDA` in calling sequences)
- `10` = Number of rows of the submatrix (often denoted `M`, can be at most `LDA`)
- `10` = Number of columns of submatrix (often denoted `N`)

All matrix arguments require these 4 parameters (some subroutines may have fewer inputs if, for example, the submatrix is assumed square so that M = N). (See Chapter 74, for more details.)

Most of the LAPACK routines require from the users to provide them a workspace (`WORK`) and its dimension (`LWORK`). The *optimal* workspace dimension refers to the workspace dimension, which enables the code to have the best performance on the targeted machine. The computation of the optimal workspace dimension is often complex so that most of LAPACK routines have the ability to compute it. If an LAPACK routine is called with `LWORK=-1`, then a workspace query is assumed. The routine only calculates the optimal size of the `WORK` array and returns this value as the first entry of the `WORK` array. If a larger workspace is provided, the extra part is not used, so that the code runs at the optimal performance. A *minimal* workspace dimension is provided in the document of routines. If a routine is called with a workspace dimension smaller than the minimal workspace dimension, the computation cannot be performed.

75.2   Linear System of Equations

Definitions:

The problem of linear equations is to compute a solution X of the system of linear equations

$$AX = B, \qquad\qquad (75.1)$$

where A is an n–by–n matrix and X and B are n–by–m matrices.

Backgrounds:

The theoretical and algorithmic background of the solution of linear equations are discussed extensively in Chapter 37 through Chapter 41, especially Chapter 38.

Driver Routines:

There are two types of driver routines for solving the systems of linear equations — simple driver and expert driver. The expert driver solves the system (Equation 75.1), allows A be replaced by A^T or A^* and provides error bounds, condition number estimate, scaling, and can refine the solution. Each of these types of drivers has different implementations that take advantage of the special properties or storage schemes of the matrix A, as listed in the following table.

	Routine Names	
Data Structure (Matrix Storage Scheme)	Simple Driver	Expert Driver
General dense	xGESV	xGESVX
General band	xGBSV	xGBSVX
General tridiagonal	xGTSV	xGTSVX
Symmetric/Hermitian positive definite	xPOSV	xPOSVX
Symmetric/Hermitian positive definite (packed storage)	xPPSV	xPPSVX
Banded symmetric positive definite	xPBSV	xPBSVX
Tridiagonal symmetric positive definite	xPTSV	xPTSVX
Symmetric/Hermitian indefinite	xSYSV/xHESV	xSYSVX/xHESVX
Symmetric/Hermitian indefinite (packed storage)	xSPSV/xHPSV	xSPSVX/xHPSVX
Complex symmetric	CSYSV/ZSYSV	CSYSVX/ZSYSVX

The prefix GE (for general dense), GB (for general band), etc., have standard meanings for all the BLAS and LAPACK routines.

Examples:

Let us show how to use the simple driver routine SGESV to solve a general linear system of equations. SGESV computes the solution of a real linear Equation 75.1 in single precision by first computing the LU decomposition with row partial pivoting of the coefficient matrix A, followed by the back and forward substitutions. SGESV has the following calling sequence:

```
CALL SGESV( N, NRHS, A, LDA, IPIV, B, LDB, INFO )
```

Input to SGESV:

> N: The number of linear equations, i.e., the order of A. N $\geq$ 0.

> NRHS: The number of right-hand sides, i.e., the number of columns of B. NRHS $\geq$ 0.

> A, LDA: The N–by–N coefficient matrix A and the leading dimension of the array A. LDA $\geq$ max(1, N).

> B, LDB: The N–by–NRHS matrix B and the leading dimension of the array B. LDB $\geq$ max(1, N).

Output from SGESV:

> A: The factors L and U from factorization $A = PLU$; the unit diagonal elements of L are not stored.

> IPIV: The pivot indices that define the permutation matrix P; row i of the matrix was interchanged with row IPIV(i).

> B: If INFO = 0, the N–by–NRHS solution X.

> INFO: = 0, successful exit. If INFO $= -j$, the jth argument had an illegal value. If INFO $= j$, $U(j, j)$ is exactly zero. The factorization has been completed, but the factor U is singular, so the solution could not be computed.

Consider a 4–by–4 linear system of Equation (75.1), where

$$A = \begin{bmatrix} 5 & 7 & 6 & 5 \\ 7 & 10 & 8 & 7 \\ 6 & 8 & 10 & 9 \\ 5 & 7 & 9 & 10 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 23 \\ 32 \\ 33 \\ 31 \end{bmatrix}.$$

The exact solution is $\mathbf{x} = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}^T$. Upon calling SGESV, the program successfully exits with $\text{INFO} = 0$ and the solution X of (75.1) resides in the array B

$$X = \begin{bmatrix} 0.9999998 \\ 1.0000004 \\ 0.9999998 \\ 1.0000001 \end{bmatrix}.$$

Since SGESV performs the computation in single precision arithmetic, it is normal to have an error of the order of 10^{-6} in the solution X. By reading the lower diagonal entries in the array A and filling the diagonal entries with ones, we recover the lower unit triangular matrix L of the LU factorization with row partial pivoting of A as follows:

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0.8571429 & 1 & 0 & 0 \\ 0.7142857 & 0.2500000 & 1 & 0 \\ 0.7142857 & 0.2500000 & -0.2000000 & 1 \end{bmatrix}.$$

The upper triangular matrix U is recovered by reading the diagonal and upper diagonal entries in A. That is:

$$U = \begin{bmatrix} 7.0000000 & 10.0000000 & 8.0000000 & 7.0000000 \\ 0 & -0.5714293 & 3.1428566 & 2.9999995 \\ 0 & 0 & 2.5000000 & 4.2500000 \\ 0 & 0 & 0 & 0.1000000 \end{bmatrix}.$$

Finally, the permutation matrix P is the identity matrix that exchanges its i-th row with row IPIV(i), for $i = n, \dots, 1$. Since

$$\text{IPIV} = \begin{bmatrix} 2 & 3 & 4 & 4 \end{bmatrix},$$

we have

$$P = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

75.3   Linear Least Squares Problems

Definitions:

The linear least squares (LLS) problem is to find

$$\min_{\mathbf{x}} \|\mathbf{b} - A\mathbf{x}\|_2, \tag{75.2}$$

where A is an m–by–n matrix and $\mathbf{b}$ is an m element vector.

Backgrounds:

The most usual case is $m \geq n$ and rank$(A) = n$. In this case, the solution to the LLS problem (75.2) is unique, and the problem is also referred to as finding a least squares solution to an overdetermined system of linear equations. When $m < n$ and rank$(A) = m$, there are an infinite number of solutions $\mathbf{x}$ that exactly satisfy $\mathbf{b} - A\mathbf{x} = 0$. In this case, it is often useful to find the unique solution $\mathbf{x}$ that minimizes $\|\mathbf{x}\|_2$, and the problem is referred to as finding a *minimum norm solution* to an underdetermined system of linear equations. (See Chapter 5.8 and Chapter 39 for more information on linear least squares problems.)

Driver Routines:

There are four types of driver routines that solve the LLS problem (75.2) and also allow A be replaced by A^*. In the general case when rank$(A) < \min(m, n)$, we seek the *minimum norm least squares* solution $\mathbf{x}$ that minimizes both $\|\mathbf{x}\|_2$ and $\|\mathbf{b} - A\mathbf{x}\|_2$. The types of driver routines are categorized by the methods used to solve the LLS problem, as shown in the following table.

Type of Matrix	Algorithm	Routine Names
General dense	QR or LQ factorization	xGELS
General dense	Complete orthogonal factorization	xGELSY
General dense	SVD	xGELSS
General dense	Divide-and-conquer SVD	xGELSD

xGELSD is significantly faster than xGELSS, but it demands somewhat more workspace depending on the matrix dimensions. Among these routines, only xGELS requires A to be full rank while xGELSY, xGELSS, and xGELSD allow less than full rank.

Note that all driver routines allow several right-hand side vectors $\mathbf{b}$, and corresponding solutions $\mathbf{x}$ to be handled in a single call, storing these vectors as columns of matrices B and X, respectively. However, the LLS problem (75.2) is solved for each right-hand side independently; that is not the same as finding a matrix X which minimizes $\|B - AX\|_2$.

Examples:

Let us show how to use the simple driver routine SGELS to solve the LLS problem (75.2). SGELS computes the QR decomposition of the matrix A, updates the vector $\mathbf{b}$ and then computes the solution $\mathbf{x}$ by back substitution. SGELS has the following calling sequence:

```
CALL SGELS( TRANS, M, N, NRHS, A, LDA, B, LDB, WORK, LWORK, INFO )
```

Input to SGELS:

TRANS: = 'N' or 'T', solves the LLS with A or A^T.

M, N: The numbers of rows and columns of the matrix A. M $\geq$ 0 and N $\geq$ 0.

M, NRHS: The number of rows and columns of the matrices B and X. NRHS $\geq$ 0.

A, LDA: The M–by–N matrix A and the leading dimension of the array A, LDA $\geq$ max(1, M).

B, LDB: The matrix B and the leading dimension of the array B, LDB $\geq$ max(1, M, N).
If TRANS = 'N', then B is M–by–NRHS. If TRANS = 'T'. then B is N–by–NRHS.

WORK, LWORK: The workspace array and its dimension. LWORK $\geq$ min(M, N) + max(1, M, N, NRHS).
If LWORK $= -1$, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, and returns this value as the first entry of the WORK array.

Output from SGELS:

B: It is overwritten by the solution vectors, stored columnwise.

- If TRANS = 'N' and M $\geq$ N, rows 1 to N of B contain the solution vectors of the LLS problem $\min_{\mathbf{x}} \|\mathbf{b} - A\mathbf{x}\|_2$; the residual sum of squares in each column is given by the sum of squares of elements N $+$ 1 to M in that column;

- If TRANS = 'N' and M < N, rows 1 to N of B contain the minimum norm solution vectors of the underdetermined system $AX = B$;
- If TRANS = 'T' and M ≥ N, rows 1 to M of B contain the minimum norm solution vectors of the underdetermined system $A^T X = B$;
- If TRANS = 'T' and M < N, rows 1 to M of B contain the solution vectors of the LLS problem $\min_{\mathbf{x}} \|\mathbf{b} - A^T\mathbf{x}\|_2$; the residual sum of squares for the solution in each column is given by the sum of the squares of elements M+1 to N in that column.

WORK : If INFO = 0, WORK(1) returns the optimal LWORK.

INFO : INFO = 0 if successful exit. If INFO = $-j$, the jth input argument had an illegal value.

Consider an LLS problem (75.2) with a 6–by–5 matrix A and a 6–by–1 matrix $\mathbf{b}$:

$$A = \begin{bmatrix} -74 & 80 & 18 & -11 & -4 \\ 14 & -69 & 21 & 28 & 0 \\ 66 & -72 & -5 & 7 & 1 \\ -12 & 66 & -30 & -23 & 3 \\ 3 & 8 & -7 & -4 & 1 \\ 4 & -12 & 4 & 4 & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 51 \\ -61 \\ -56 \\ 69 \\ 10 \\ -12 \end{bmatrix}.$$

The exact solution of the LLS problem is $\mathbf{x} = \begin{bmatrix} 1 & 2 & -1 & 3 & -4 \end{bmatrix}^T$ with residual $\|\mathbf{b} - A\mathbf{x}\|_2 = 0$. Upon calling SGELS, the first 5 elements of B are overwritten by the solution vector $\mathbf{x}$

$$\mathbf{x} = \begin{bmatrix} 1.0000176 \\ 2.0000196 \\ -0.9999972 \\ 3.0000386 \\ -4.0000405 \end{bmatrix},$$

while the sixth element of B contains the residual sum of squares 0.0000021. With M = 6, N = 5, NRHS = 1, LWORK has been set to 11. For such a small matrices, the minimal workspace is also the optimal workspace.

75.4   The Linear Equality-Constrained Least Squares Problem

Definitions:

The linear equality-constrained least squares (LSE) problem is

$$\min_{\mathbf{x}} \|\mathbf{c} - A\mathbf{x}\|_2 \quad \text{subject to} \quad B\mathbf{x} = \mathbf{d}, \tag{75.3}$$

where A is an m–by–n matrix and B is a p–by–n matrix, $\mathbf{c}$ is an m-vector, and $\mathbf{d}$ is a p-vector, with $p \le n \le m + p$.

Backgrounds:

Under the assumptions that B has full row rank p and the matrix $\begin{bmatrix} A \\ B \end{bmatrix}$ has full column rank n, the LSE problem (75.3) has a unique solution $\mathbf{x}$.

Driver Routines:

The driver routine for solving the LSE is xGGLSE, which uses a generalized QR factorization of the matrices A and B.

Examples:

Let us show how to use the driver routine SGGLSE to solve the LSE problem (75.3). SGGLSE first computes a generalized QR decomposition of A and B, and then computes the solution by back substitution. SGGLSE has the following calling sequence:

```
CALL SGGLSE( M, N, P, A, LDA, B, LDB, C, D, X, WORK, LWORK, INFO )
```

Input to SGGLSE:

  M, P: The numbers of rows of the matrices A and B, respectively. M $\geq$ 0 and P $\geq$ 0.

  N: The number of columns of the matrices A and B. N $\geq$ 0. Note that $0 \leq$ P $\leq$ N $\leq$ M+P.

  A, LDA: The M–by–N matrix A and the leading dimension of the array A. LDA $\geq$ max(1,M).

  B, LDB: The P–by–N matrix B and the leading dimension of the array B. LDB $\geq$ max(1,P).

  C, D: The right-hand side vectors for the least squares part, and the constrained equation part of the LSE, respectively.

  WORK, LWORK: The workspace array and its dimension. LWORK $\geq$ max(1, M + N + P).

    If LWORK $= -1$, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, returns this value as the first entry of the WORK array.

Output from SGGLSE:

  C: The residual sum of squares for the solution is given by the sum of squares of elements N–P+1 to M of vector C.

  X: The solution of the LSE problem.

  WORK: If INFO = 0, WORK(1) returns the optimal LWORK.

  INFO: $= 0$ if successful exit. If INFO $= -j$, the jth argument had an illegal value.

Let us demonstrate the use of SGGLSE to solve the LSE problem (75.3), where

$$A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 3 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix}, \quad \mathbf{d} = \begin{bmatrix} 7 \\ 4 \end{bmatrix}.$$

The unique exact solution is $\mathbf{x} = \frac{1}{8}[46 \quad -2 \quad 12]^T$. Upon calling SGGLSE with this input data and M $= 4$, N $= 3$, P $= 2$, LWORK $= 9$, an approximate solution of the LSE problem is returned in X:

$$X = [5.7500000 \quad -0.2500001 \quad 1.4999994]^T.$$

The array C is overwritten by the residual sum of squares for the solution:

$$C = [4.2426405 \quad 8.9999981 \quad 2.1064947 \quad 0.2503501]^T.$$

75.5   A general Linear Model Problem

Definitions:

The general linear model (GLM) problem is

$$\min_{\mathbf{x},\mathbf{y}} \|\mathbf{y}\|_2 \quad \text{subject to} \quad \mathbf{d} = A\mathbf{x} + B\mathbf{y}, \tag{75.4}$$

where A is an n–by–m matrix, B is an n–by–p matrix, and $\mathbf{d}$ is a n-vector, with $m \leq n \leq m + p$.

Backgrounds:

When $B = I$, the problem reduces to an ordinary linear least squares problem (75.2). When B is square and nonsingular, the GLM problem is equivalent to the *weighted linear least squares problem*:

$$\min_{\mathbf{x}} \|B^{-1}(\mathbf{d} - A\mathbf{x})\|_2.$$

Note that the GLM is equivalent to the LSE problem

$$\min_{\mathbf{x},\mathbf{y}} \left\| 0 - \begin{bmatrix} 0 & I \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} \right\|_2 \quad \text{subject to} \quad \begin{bmatrix} A & B \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \mathbf{d}.$$

Therefore, the GLM problem has a unique solution of the matrix $\begin{bmatrix} 0 & I \\ A & B \end{bmatrix}$ has full column rank $m + p$.

Driver Routines:

The driver routine for solving the GLM problem (75.4) is xGGGLM, which uses a generalized QR factorization of the matrices A and B.

Examples:

Let us show how to use the driver routine SGGGLM to solve the GLM problem (75.4). SGGGLM computes a generalized QR decomposition of the matrices A and B, and then computes the solution by back substitution. SGGGLM has the following calling sequence:

```
CALL SGGGLM( N, M, P, A, LDA, B, LDB, D, X, Y, WORK, LWORK, INFO )
```

Input to SGGGLM:

  N: The number of rows of the matrices A and B. N $\geq$ 0.

  M, P: The number of columns of the matrices A and B, respectively. 0 $\leq$ M $\leq$ N and P $\geq$ N-M.

  A, LDA: The N–by–M matrix A and the leading dimension of the array A. LDA $\geq$ max(1,N).

  B, LDB: The N–by–P matrix B and the leading dimension of the array B. LDB $\geq$ max(1,N).

  D: The left-hand side of the GLM equation.

  WORK, LWORK: The workspace array and its dimension. LWORK $\geq$ max(1,N+M+P).

   If LWORK = -1, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, and returns this value as the first entry of the WORK array.

Output from SGGGLM:

> X, Y: Solution vectors.
>
> WORK: If INFO = 0, WORK(1) returns the optimal LWORK.
>
> INFO: INFO = 0 if successful exit. If INFO $= -j$, the jth argument had an illegal value.

Let us demonstrate the use of SGGGLM for solving the GLM problem (75.4), where

$$A = \begin{bmatrix} 1 & 2 & 1 & 4 \\ -1 & 1 & 1 & 1 \\ -1 & -2 & -1 & 1 \\ -1 & 2 & -1 & -1 \\ 1 & 1 & 1 & 2 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 2 & 2 \\ -1 & 1 & -2 \\ 3 & 1 & 6 \\ 2 & -2 & 4 \\ 1 & -1 & 2 \end{bmatrix}, \quad \mathbf{d} = \begin{bmatrix} 7.99 \\ 0.98 \\ -2.98 \\ 3.04 \\ 4.02 \end{bmatrix}.$$

Upon calling SGGGLM with this input data, N = 5, M = 4, P = 3, LWORK = 12, the program successfully exits and returns the following solution vectors:

$$X = [1.002950 \quad 2.001435 \quad -0.987797 \quad 0.009080]^T$$

and

$$Y = [0.003435 \quad -0.004417 \quad 0.006871]^T.$$

75.6 Symmetric Eigenproblems

Definitions:

The symmetric eigenvalue problem (SEP) is to find the eigenvalues, λ, and corresponding eigenvectors, $\mathbf{x} \neq 0$, such that

$$A\mathbf{x} = \lambda\mathbf{x}, \tag{75.5}$$

where A is real and symmetric. If A is complex and Hermitian, i.e., $A^* = A$, then it is referred to as the *Hermitian eigenvalue problem*.

Backgrounds:

When all eigenvalues and eigenvectors have been computed, we write

$$A = X\Lambda X^*, \tag{75.6}$$

where Λ is a diagonal matrix whose diagonal elements are real and are the eigenvalues, and X is an orthogonal (or unitary) matrix whose columns are the eigenvectors. This is the classical *spectral decomposition* of A. The theoretical and algorithmic background of the solution of the symmetric eigenvalue problem are discussed in Chapter 42.

Driver Routines:

There are four types of driver routines for solving the SEP (75.5) and each has its own variations that take advantage of the special structure or storage of the matrix A, as summarized in the following table.

Types of Matrix	Routine Names			
(Storage Scheme)	Simple Driver	Divide-and-Conquer	Expert Driver	RRR Driver
General symmetric	xSYEV	xSYEVD	xSYEVX	xSYEVR
General symmetric				
(packed storage)	xSPEV	xSPEVD	xSPEVX	–
Band matrix	xSBEV	xSBEVD	xSBEVX	–
Tridiagonal matrix	xSTEV	xSTEVD	xSTEVX	xSTEVR

The simple drivers compute all eigenvalues and (optionally) eigenvectors. The expert drivers compute all or a selected subset of the eigenvalues and (optionally) eigenvectors. The divide-and-conquer drivers have the same functionality as, yet outperform, the simple driver, but it requires more workspace. The relative robust representation (RRR) drivers compute all or a subset of the eigenvalues and (optionally) the eigenvectors. The last one is generally faster than any other types of driver routines and uses the least amount of workspace.

Examples:

Let us show how to use the simple driver SSYEV to solve the SEP (75.5) by computing the spectral decomposition (75.6). SSYEV first reduces A to a tridiagonal form, and then uses the implicit QL or QR algorithm to compute eigenvalues and optionally eigenvectors. SSYEV has the following calling sequence:

```
CALL SSYEV( JOBZ, UPLO, N, A, LDA, W, WORK, LWORK, INFO )
```

Input to SSYEV:

 JOBZ: = 'N', compute eigenvalues only;

   = 'V', compute eigenvalues and eigenvectors.

 UPLO: = 'U', the upper triangle of A is stored in the array A; if UPLO = 'L', the lower triangle of A is stored.

 N: The order of the matrix A. N $\geq$ 0.

 A, LDA: The symmetric matrix A and the leading dimension of the array A. LDA $\geq$ max(1, N).

 WORK, LWORK: The workspace array and its dimension. LWORK $\geq$ max(1, 3 ∗ N − 1).

   If LWORK = −1, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, and returns this value as the first entry of the WORK array.

Output from SSYEV:

 A: The orthonormal eigenvectors X, if JOBZ = 'V'.

 W: The eigenvalues λ in ascending order.

 WORK: If INFO = 0, WORK(1) returns the optimal LWORK.

 INFO: = 0 if successful exit. If INFO = −j, the jth input argument had an illegal value. If INFO = j, the j off-diagonal elements of an intermediate tridiagonal form did not converge to zero.

Let us demonstrate the use of SSYEV to solve the SEP (75.5), where

$$A = \begin{bmatrix} 5 & 4 & 1 & 1 \\ 4 & 5 & 1 & 1 \\ 1 & 1 & 4 & 2 \\ 1 & 1 & 2 & 4 \end{bmatrix}.$$

The exact eigenvalues are 1, 2, 5, and 10. Upon calling SSYEV with the matrix A and $N = 4$, $LWORK = 3 * N - 1 = 11$, A is overwritten by its orthonormal eigenvectors X.

$$X = \begin{bmatrix} 0.7071068 & -0.0000003 & 0.3162279 & 0.6324555 \\ -0.7071068 & 0.0000001 & 0.3162278 & 0.6324555 \\ 0.0000002 & 0.7071069 & -0.6324553 & 0.3162278 \\ -0.0000001 & -0.7071066 & -0.6324556 & 0.3162278 \end{bmatrix}.$$

The eigenvalues that correspond to the eigenvectors in each columns of X are returned in W:

$$W = [0.9999996 \quad 1.9999999 \quad 4.9999995 \quad 10.0000000].$$

75.7 Nonsymmetric Eigenproblems

Definitions:

The nonsymmetric eigenvalue problem (NEP) is to find the eigenvalues, λ, and corresponding (right) eigenvectors, $\mathbf{x} \neq 0$, such that

$$A\mathbf{x} = \lambda\mathbf{x} \tag{75.7}$$

and, perhaps, the left eigenvectors, $\mathbf{y} \neq 0$, satisfying

$$\mathbf{y}^* A = \lambda\mathbf{y}^*. \tag{75.8}$$

Backgrounds:

The problem is solved by computing the *Schur decomposition* of A, defined in the real case as

$$A = ZTZ^T,$$

where Z is an orthogonal matrix and T is an upper quasi-triangular matrix with 1–by–1 and 2–by–2 diagonal blocks, the 2–by–2 blocks corresponding to complex conjugate pairs of eigenvalues of A. In the complex case, the Schur decomposition is

$$A = ZTZ^*,$$

where Z is unitary and T is a complex upper triangular matrix.

The columns of Z are called the *Schur vectors*. For each k ($1 \leq k \leq n$), the first k columns of Z form an orthonormal basis for the invariant subspace corresponding to the first k eigenvalues on the diagonal of T. It is possible to order the Schur factorization so that any desired set of k eigenvalues occupy the k leading positions on the diagonal of T. The theoretical and algorithmic background of the solution of the nonsymmetric eigenvalue problem is discussed in Chapter 43.

Driver Routines:

Both the simple drivers xGEEV and expert drivers xGEEVX are provided. The simple drivers compute all the eigenvalues of A and (optionally) the right or left eigenvectors (or both). The expert drivers perform the same task as the simple drivers plus the additional feature that it balances the matrix to try to improve the conditioning of the eigenvalues and eigenvectors, and it computes the condition numbers for the eigenvalues or eigenvectors (or both).

Examples:

Let us show how to use the simple driver SGEEV to solve the NEP (75.7). SGEEV first reduces A to an upper Hessenberg form (a Hessenberg matrix is a matrix where all entries below the first lower subdiagonal are

zeros), and then uses the implicit QR algorithm to compute the Schur decomposition, and finally computes eigenvectors of the upper quasi-triangular matrix. SGEEV has the following calling sequence:

```
CALL SGEEV( JOBVL, JOBVR, N,A, LDA,WR, WI, VL, LDVL, VR, LDVR,WORK,
LWORK, INFO )
```

Input to SGEEV:

JOBVL, JOBVR: = 'V', the left and/or right eigenvectors are computed;

= 'N', the left and/or right eigenvectors are not computed.

N: The order of the matrix A. N $\geq$ 0.

A, LDA: The matrix A and the leading dimension of the array A. LDA $\geq$ max(1, N).

LDVL, LDVR: The leading dimensions of the arrays VL and VR if the left and right eigenvectors are computed. LDVL, LDVR $\geq$ N.

WORK, LWORK: The workspace array and its dimension. LWORK $\geq$ max(1, 3 * N). If eigenvectors are computed, LWORK $\geq$ 4 * N. For good performance, LWORK must generally be larger.

If LWORK = −1, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, and returns this value as the first entry of the WORK array.

Output from SGEEV:

WR, WI: The real and imaginary parts of the computed eigenvalues. Complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having the positive imaginary part first.

VL: If the jth eigenvalue λ_j is real, then the jth left eigenvector $\mathbf{y}_j$ is stored in VL(:, j). If the jth and $(j + 1)$-st eigenvalues λ_j and λ_{j+1} form a complex conjugate pair, then VL(:, j) + $i \cdot$ VL(:, $j + 1$) and VL(:, j) − $i \cdot$ VL(:, $j + 1$) are the corresponding left eigenvectors $\mathbf{y}_j$ and $\mathbf{y}_{j+1}$.

VR: If the jth eigenvalue λ_j is real, then the jth right eigenvector $\mathbf{x}_j$ is stored in VR(:, j). If the jth and $(j + 1)$-st eigenvalues λ_j and λ_{j+1} form a complex conjugate pair, then VR(:, j) + $i \cdot$ VR(:, $j + 1$) and VR(:, j) − $i \cdot$ VR(:, $j + 1$) are the corresponding right eigenvectors $\mathbf{x}_j$ and $\mathbf{x}_{j+1}$.

WORK: If INFO = 0, WORK(1) returns the optimal LWORK.

INFO: = 0 if successful exit. If INFO = −j, the jth argument had an illegal value. If INFO = j, the QR algorithm failed to compute all the eigenvalues, and no eigenvectors have been computed; elements $j + 1 : N$ of WR and WI contain eigenvalues, which have converged.

Let us demonstrate the use of SGEEV for solving the NEP (75.7), where

$$A = \begin{bmatrix} 4 & -5 & 0 & 3 \\ 0 & 4 & -3 & -5 \\ 5 & -3 & 4 & 0 \\ 3 & 0 & 5 & 4 \end{bmatrix}.$$

The exact eigenvalues are $12, 1 + i \cdot 5, 1 - i \cdot 5$ and 2. Upon calling SGEEV with this matrix and N = 4, LWORK = 4 * N = 16, each eigenvalue, λ_j, is retrieved by combining the jth entry in WR and WI

such that $\lambda_j = \text{WR}(j) + i \cdot \text{WI}(j)$. If $\text{WI}(j)$ is 0, then the jth eigenvalue is real. For this example, we have

$$\lambda_1 = 12.0000000$$
$$\lambda_2 = 1.000000 + i \cdot 5.0000005$$
$$\lambda_3 = 1.000000 - i \cdot 5.0000005$$
$$\lambda_4 = 1.9999999.$$

The left eigenvectors are stored in VL. Since the first and fourth eigenvalues are real, their eigenvectors are the corresponding columns in VL, that is, $\mathbf{y}_1 = \text{VL}(:,1)$ and $\mathbf{y}_4 = \text{VL}(:,4)$. Since the second and third eigenvalues form a complex conjugate pair, the second eigenvector, $\mathbf{y}_2 = \text{VL}(:,2) + i \cdot \text{VL}(:,3)$ and the third eigenvector, $\mathbf{y}_3 = \text{VL}(:,2) - i \cdot \text{VL}(:,3)$. If we place all the eigenvectors in a matrix Y where $Y = [\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3, \mathbf{y}_4]$, we have

$$Y = \begin{bmatrix} -0.5000001 & 0.0000003 - i \cdot 0.4999999 & 0.0000003 + i \cdot 0.4999999 & 0.5000000 \\ 0.4999999 & -0.5000002 & -0.5000002 & 0.5000001 \\ -0.5000000 & -0.5000000 - i \cdot 0.0000002 & -0.5000000 + i \cdot 0.0000002 & -0.4999999 \\ -0.5000001 & -0.0000003 + i \cdot 0.5000000 & -0.0000003 - i \cdot 0.5000000 & 0.5000001 \end{bmatrix}.$$

The right eigenvectors $\mathbf{x}_j$ can be recovered from VR in the way similar to the left eigenvectors. The right eigenvector matrix X is

$$X = \begin{bmatrix} -0.5000000 & 0.5000002 & 0.5000002 & 0.5000001 \\ 0.4999999 & -0.0000001 - i \cdot 0.5000000 & -0.0000001 + i \cdot 0.5000000 & 0.5000000 \\ -0.5000000 & -0.0000001 - i \cdot 0.4999999 & -0.0000001 + i \cdot 0.4999999 & -0.5000000 \\ -0.5000001 & -0.5000001 & -0.5000001 & 0.5000000 \end{bmatrix}.$$

75.8 Singular Value Decomposition

Definitions:

The singular value decomposition (SVD) of an m–by–n matrix A is

$$A = U\Sigma V^T \quad (A = U\Sigma V^* \quad \text{in the complex case}), \tag{75.9}$$

where U and V are orthogonal (unitary) and Σ is an m–by–n diagonal matrix with real diagonal elements, σ_j, such that

$$\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{\min(m,n)} \geq 0.$$

The σ_j are the singular values of A and the first $\min(m,n)$ columns of U and V are the left and right singular vectors of A.

Backgrounds:

The singular values σ_j and the corresponding left singular vectors $\mathbf{u}_j$ and right singular vectors $\mathbf{v}_j$ satisfy

$$A\mathbf{v}_j = \sigma_j \mathbf{u}_j \quad \text{and} \quad A^T\mathbf{u}_j = \sigma_j \mathbf{v}_j \quad (\text{or} \quad A^*\mathbf{u}_j = \sigma_j \mathbf{v}_j \quad \text{in complex case}),$$

where $\mathbf{u_j}$ and $\mathbf{v_j}$ are the jth columns of U and V respectively. (See Chapter 17 and Chapter 45 for more information on singular value decompositions.)

Driver Routines:

Two types of driver routines are provided in LAPACK. The simple drivers xGESVD compute all the singular values and (optionally) left and/or right singular vectors. The divide and conquer drivers xGESDD have the same functionality as the simple drivers except that they are much faster for larger matrices, but use more workspace.

Examples:

Let us show how to use the simple driver SGESVD to compute the SVD (75.9). SGESVD first reduces A to a bidiagonal form, and then uses an implicit QR-type algorithm to compute singular values and optionally singular vectors. SGESVD has the following calling sequence:

```
CALL SGESVD( JOBU, JOBVT, M, N, A, LDA, S, U, LDU, VT, LDVT, WORK,
LWORK, INFO )
```

Input to SGESVD:

 JOBU: Specifies options for computing all or part of the left singular vectors U:

  = 'A', all M columns of U are returned in the array U:

  = 'S', the first $\min(M,N)$ columns of U are returned;

  = 'O', the first $\min(M,N)$ columns of U are overwritten on the array A;

  = 'N', no left singular vectors are computed. *Note that* JOBVT *and* JOBU *cannot both be* 'O'.

 JOBVT: Specifies options for computing all or part of the right singular vectors V^T:

  = 'A', all N rows of V^T are returned in the array VT;

  = 'S', the first $\min(M,N)$ rows of V^T are returned;

  = 'O', the first $\min(M,N)$ rows of V^T are overwritten on the array A;

  = 'N', no right singular vectors are computed.

 M, N: The number of rows and columns of the matrix A. M, N $\geq$ 0.

 A, LDA: The M–by–N matrix A and the leading dimension of the array A. LDA $\geq$ $\max(1,M)$.

 LDU, LDVT: The leading dimension of the arrays U and VT. LDU, LDVT $\geq$ 1;

  If JOBU = 'S' or 'A', LDU $\geq$ M.

  If JOBVT = 'A', LDVT $\geq$ N; If JOBVT = 'S', LDVT $\geq$ $\min(M,N)$.

 WORK, LWORK: The workspace array and its dimension. LWORK $\geq$ $\max(3\min(M,N) + \max(M,N), 5\min(M,N))$.

  If LWORK = -1, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array and returns this value as the first entry of the WORK array.

Output from SGESVD:

 A: If JOBU = 'O', A is overwritten with the first $\min(M, N)$ columns of U (the left singular vectors, stored columnwise);

  If JOBVT = 'O', A is overwritten with the first $\min(M,N)$ rows of V^T (the right singular vectors, stored rowwise);

 S: Singular values of A, sorted so that $S(i) \geq S(i+1)$.

 U: If JOBU = 'A', U contains M–by–M orthogonal matrix U. If JOBU = 'S', U contains the first $\min(M,N)$ columns of U. If JOBU = 'N' or 'O', U is not referenced.

VT: If JOBVT = 'A', VT contains right N–by–N orthogonal matrix V^T. If JOBVT = 'S', VT contains the first min(M,N) rows of V^T (the right singular vectors stored rowwise). If JOBVT = 'N' or 'O', VT is not referenced.

WORK: If INFO = 0, WORK(1) returns the optimal LWORK.

INFO: = 0 if successful exit. If INFO $= -j$, the jth argument had an illegal value. If INFO > 0, the QR-type algorithm (subroutine SBDSQR) did not converge. INFO specifies how many superdiagonals of an intermediate bidiagonal form B did not converge to zero. WORK(2:min(M,N)) contains the unconverged superdiagonal elements of an upper bidiagonal matrix B whose diagonal is in S (not necessarily sorted). B satisfies $A = UBV^T$, so it has the same singular values as A, and singular vectors related by U and V^T.

Let us show the numerical results of SGESVD in computing the SVD by a 8–by–5 matrix A as follows

$$A = \begin{bmatrix} 22 & 10 & 2 & 3 & 7 \\ 14 & 7 & 10 & 0 & 8 \\ -1 & 13 & -1 & -11 & 3 \\ -3 & -2 & 13 & -2 & 4 \\ 9 & 8 & 1 & -2 & 4 \\ 9 & 1 & -7 & 5 & -1 \\ 2 & -6 & 6 & 5 & 1 \\ 4 & 5 & 0 & -2 & 2 \end{bmatrix}.$$

The exact singular singular values are $\sqrt{1248}, 20, \sqrt{384}, 0, 0$. The rank of the matrix A is 3. Upon calling SGESVD with M = 8, N = 5, LWORK = 25, the computed singular values of A are returned in S:

$$\text{S} = [35.3270454 \quad 20.0000038 \quad 19.5959187 \quad 0.0000007 \quad 0.0000004].$$

The columns in U contain the left singular vectors U of A:

$$U = \begin{bmatrix} -7.0711e\text{-}001 & 1.5812e-001 & -1.7678e-001 & 2.4818e-001 & -4.0289e-001 & -3.2305e-001 & -3.3272e-001 & -6.9129e-002 \\ -5.3033e\text{-}001 & 1.5811e-001 & 3.5355e-001 & -6.2416e-001 & 2.5591e-001 & -3.9178e-002 & 3.0548e-001 & -1.3725e-001 \\ -1.7678e\text{-}001 & -7.9057e-001 & 1.7677e-001 & 3.0146e-001 & 1.9636e-001 & -3.1852e-001 & 2.3590e-001 & -1.6112e-001 \\ 0 & 1.5811e-001 & 7.0711e-001 & 2.9410e-001 & 3.1907e-001 & 4.7643e-002 & -5.2856e-001 & 7.1055e-002 \\ -3.5355e\text{-}001 & -1.5811e-001 & -1.0000e-006 & 2.3966e-001 & -7.8607e-002 & 8.7800e-001 & 1.0987e-001 & -5.8528e-002 \\ -1.7678e\text{-}001 & 1.5812e-001 & -5.3033e-001 & 1.7018e-001 & 7.9071e-001 & -7.0484e-003 & -9.0913e-002 & -8.3220e-004 \\ 0 & 4.7434e-001 & 1.7678e-001 & 5.2915e-001 & -1.5210e-002 & -1.3789e-001 & 6.6193e-001 & 7.9763e-002 \\ -1.7678e\text{-}001 & -1.5811e-001 & -1.0000e-006 & -7.1202e-002 & 1.3965e-002 & -2.0712e-002 & 4.9676e-002 & 9.6726e-001 \end{bmatrix}.$$

The rows in VT contain the right singular vectors V^T of A:

$$V^T = \begin{bmatrix} -8.0064e-001 & -4.8038e-001 & -1.6013e-001 & 0 & -3.2026e-001 \\ 3.1623e-001 & -6.3246e-001 & 3.1622e-001 & 6.3246e-001 & -1.8000e-006 \\ -2.8867e-001 & -3.9000e-006 & 8.6603e-001 & -2.8867e-001 & 2.8868e-001 \\ -4.0970e-001 & 3.4253e-001 & -1.2426e-001 & 6.0951e-001 & 5.7260e-001 \\ 8.8224e-002 & -5.0190e-001 & -3.3003e-001 & -3.8100e-001 & 6.9730e-001 \end{bmatrix}.$$

75.9 Generalized Symmetric Definite Eigenproblems

Definitions:

The generalized symmetric definite eigenvalue problem (GSEP) is to find the eigenvalues, λ, and corresponding eigenvectors, $\mathbf{x} \neq 0$, such that

$$A\mathbf{x} = \lambda B\mathbf{x} \quad \text{(type 1)} \tag{75.10}$$

or

$$AB\mathbf{x} = \lambda\mathbf{x} \quad \text{(type 2)} \tag{75.11}$$

or

$$BA\mathbf{x} = \lambda\mathbf{x} \quad \text{(type 3)} \tag{75.12}$$

where A and B are symmetric or Hermitian and B is positive definite.

Backgrounds:

For all these problems the eigenvalues λ are real. The matrix Z of the computed eigenvectors satisfy $Z^*AZ = \Lambda$ (problem types 1 and 3) or $Z^{-1}AZ^{-*} = I$ (problem type 2), where Λ is a diagonal matrix with the eigenvalues on the diagonal. Z also satisfies $Z^*BZ = I$ (problem types 1 and 2) or $Z^*B^{-1}Z = I$ (problem type 3). These results are consequences of spectral theory for symmetric matrices. For example, the GSEP type 1 can be rearranged as

$$B^{-\frac{1}{2}}AB^{-\frac{1}{2}}\mathbf{y} = \lambda\mathbf{y},$$

where $\mathbf{y} = B^{\frac{1}{2}}\mathbf{x}$.

Driver Routines:

There are three types of driver routines for solving the GSEP, and each has variations that take advantage of the special structure or storage of the matrices A and B, as shown in the following table:

Types of Matrix	Routine Names		
(Storage Scheme)	Simple Driver	Divide-and-Conquer	Expert Driver
General dense	xSYGV/xHEGV	xSYGVD/xHEGVD	xSYGVX/xHEGVX
General dense			
(packed storage)	xSPGV/xHPGV	xSPGVD/xHPGVD	xSPGVX/xHPGVX
Band matrix	xSBGV/xHBGV	xSBBVD/xHBGVD	xSBGVX/xHBGVX

The simple driver computes all the eigenvalues and (optionally) the eigenvectors. The expert driver computes all or a selected subset of the eigenvalues and (optionally) eigenvectors. The divide-and-conquer driver solves the same problem as the simple driver. It is much faster than the simple driver, but uses more workspace.

Examples:

Let us show how to use the simple driver SSYGV to compute the GSEP (75.10), (75.11) and (75.12). SSGYV first reduces each of these problems to a standard symmetric eigenvalue problem, using a Cholesky decomposition of B, and then computes eigenvalues and eigenvectors of the standard symmetric eigenvalue problem by an implicit QR-type algorithm. SSYGV has the following calling sequence: CALL SSYGV(

ITYPE, JOBZ, UPLO, N, A, LDA, B, LDB, W, WORK, LWORK, INFO) Input to SSYGV:

ITYPE: Specifies the problem type to be solved:

JOBZ: = 'N', compute eigenvalues only;

    = 'V', compute eigenvalues and eigenvectors.

UPLO: = 'U', the upper triangles of A and B are stored;

    = 'L', the lower triangles of A and B are stored.

N: The order of the matrices A and B. N $\geq$ 0.

A, LDA: The symmetric matrix A and the leading dimension of the array A. LDA $\geq$ max(1,N).

B: The symmetric positive definite matrix B and the leading dimension of the array B. LDB $\geq$ max(1,N).

WORK, LWORK: The workspace array and its length. LWORK $\geq$ max(1, 3 * N - 1).

If LWORK $= -1$, then a workspace query is assumed; the routine only calculates the optimal size of the WORK array, and returns this value as the first entry of the WORK array.

Output from SSYGV:

A: Contains the normalized eigenvector matrix Z if requested.

B: If INFO $\leq$ N, the part of B containing the matrix is overwritten by the triangular factor U or L from the Cholesky factorization $B = U^T U$ or $B = L L^T$.

W: The eigenvalues in ascending order.

WORK: If INFO $= 0$, WORK(1) returns the optimal LWORK.

INFO: $= 0$, then successful exit. If INFO $= -j$, then the jth argument had an illegal value. If INFO > 0, then SSYGV returned an error code:

- INFO $\leq$ N: if INFO $= j$, the algorithm failed to converge;
- INFO $>$ N: if INFO $= N + j$, for $1 \leq j \leq N$, then the leading minor of order j of B is not positive definite. The factorization of B could not be completed and no eigenvalues or eigenvectors were computed.

Let us show the use of SSYGV to solve the type 1 GSEP (75.10) for the following 5–by–5 matrices A and B:

$$A = \begin{bmatrix} 10 & 2 & 3 & 1 & 1 \\ 2 & 12 & 1 & 2 & 1 \\ 3 & 1 & 11 & 1 & -1 \\ 1 & 2 & 1 & 9 & 1 \\ 1 & 1 & -1 & 1 & 15 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 12 & 1 & -1 & 2 & 1 \\ 1 & 14 & 1 & -1 & 1 \\ -1 & 1 & 16 & -1 & 1 \\ 2 & -1 & -1 & 12 & -1 \\ 1 & 1 & 1 & -1 & 11 \end{bmatrix}.$$

Upon calling SSYGV with N $= 5$, LWORK $= 3 * N - 1 = 14$, A is overwritten by the eigenvector matrix Z:

$$Z = \begin{bmatrix} -0.1345906 & 0.0829197 & -0.1917100 & 0.1420120 & -0.0763867 \\ 0.0612948 & 0.1531484 & 0.1589912 & 0.1424200 & 0.0170980 \\ 0.1579026 & -0.1186037 & -0.0748390 & 0.1209976 & -0.0666645 \\ -0.1094658 & -0.1828130 & 0.1374690 & 0.1255310 & 0.0860480 \\ 0.0414730 & 0.0035617 & -0.0889779 & 0.0076922 & 0.2894334 \end{bmatrix}.$$

The corresponding eigenvalues are returned in W:

$$W = \begin{bmatrix} 0.4327872 & 0.6636626 & 0.9438588 & 1.1092844 & 1.4923532 \end{bmatrix}.$$

75.10 Generalized Nonsymmetric Eigenproblems

Definitions:

The generalized nonsymmetric eigenvalue problem (GNEP) is to find the eigenvalues, λ, and corresponding (right) eigenvectors, $\mathbf{x} \neq 0$, such that

$$A\mathbf{x} = \lambda B\mathbf{x} \tag{75.13}$$

and optionally, the corresponding left eigenvectors $\mathbf{y} \neq 0$, such that

$$\mathbf{y}^* A = \lambda \mathbf{y}^* B, \tag{75.14}$$

where A and B are n–by–n matrices.

Backgrounds:

Sometimes an equivalent notation is used to refer to the GNEP of the pair (A, B). The GNEP can be solved via the generalized Schur decomposition of the pair (A, B), defined in the real case as

$$A = QSZ^T, \quad B = QTZ^T,$$

where Q and Z are orthogonal matrices, T is upper triangular, and S is an upper quasi-triangular matrix with 1-by-1 and 2-by-2 diagonal blocks, the 2-by-2 blocks corresponding to complex conjugate pairs of eigenvalues. In the complex case, the generalized Schur decomposition is

$$A = QSZ^*, \quad B = QTZ^*$$

where Q and Z are unitary and S and T are both upper triangular. The columns of Q and Z are called left and right generalized Schur vectors and span pairs of deflating subspaces of A and B. Deflating subspaces are a generalization of invariant subspaces: For each k, $1 \leq k \leq n$, the first k columns of Z span a right deflating subspace mapped by both A and B into a left deflating subspace spanned by the first k columns of Q. It is possible to order the generalized Schur form so that any desired subset of k eigenvalues occupy the k leading position on the diagonal of (S, T). (See Chapter 43 and Chapter 15 for more information on generalized eigenvalue problems.)

Driver Routines:

Both the simple and expert drivers are provided in LAPACK. The simple drivers xGGEV compute all eigenvalues of the pair (A, B), and optionally the left and/or right eigenvectors. The expert drivers xGGEVX perform the same task as the simple driver routines; in addition, they also balance the matrix pair to try to improve the conditioning of the eigenvalues and eigenvectors, and compute the condition numbers for the eigenvalues and/or left and right eigenvectors.

Examples:

Let us show how to use the simple driver SGGEV to solve the GNEP (75.13) and (75.14). SGGEV first reduces the pair (A, B) to generalized upper Hessenberg form (H, R), where H is upper Hessenberg (zero below the first lower subdiagonal) and R is upper triangular. Then SGGEV computes the generalized Schur form (S, T) of the generalized upper Hessenberg form (H, R), using an QZ algorithm. The eigenvalues are computed from the diagonals of (S, T). Finally, SGGEV computes left and/or right eigenvectors if requested. SGGEV has the following calling sequence:

```
  CALL SGGEV( JOBVL, JOBVR, N, A, LDA, B, LDB, ALPHAR, ALPHAI, BETA, VL,
LDVL,
            VR, LDVR, WORK, LWORK, INFO )
```

Input to SGGEV:

        JOBVL, JOBVR: = 'N', do not compute the left and/or right eigenvectors;

            = 'V', compute the left and/or right eigenvectors.

        N: The order of the matrices A and B. N $\geq$ 0.

        A, LDA: The matrix A and the leading dimension of the array A. LDA $\geq$ max(1, N).

        B, LDB: The matrix B and the leading dimension of the array B. LDB $\geq$ max(1, N).

LDVL, LDVR: The leading dimensions of the eigenvector matrices VL and VR. LDVL, LDVR $\geq$ 1. If eigenvectors are required, then LDVL, LDVR $\geq$ N.

WORK, LWORK: The workspace array and its length. LWORK $\geq$ max$(1, 8 * N)$. For good performance, LWORK must generally be larger.

If LWORK $= -1$, then a workspace query is assumed; the routine only calculates the optimal size of WORK, returns this value in WORK(1) on return.

Output from SGGEV:

ALPHAR, ALPHAI, BETA: $(\text{ALPHAR}(j) + i \cdot \text{ALPHAI}(j))/\text{BETA}(j)$ for $j = 1, 2, \ldots, $N, are the generalized eigenvalues. If ALPHAI(j) is zero, then the jth eigenvalue is real; if positive, then the jth and $(j + 1)$-st eigenvalues are a complex conjugate pair, with ALPHAI($j + 1$) negative.

VL: If JOBVL $=$ 'V', the left eigenvectors $\mathbf{y}_j$ are stored in the columns of VL, in the same order as their corresponding eigenvalues. If the jth eigenvalue is real, then $\mathbf{y}_j = $ VL$(:, j)$, the jth column of VL. If the jth and $(j+1)$th eigenvalues form a complex conjugate pair, then $\mathbf{y}_j = $ VL$(:, j) + i \cdot $ VL$(:, j+1)$ and $\mathbf{y}_{j+1} = $ VL$(:, j) - i \cdot $ VL$(:, j+1)$.

VR: If JOBVR $=$ 'V', the right eigenvectors $\mathbf{x}_j$ are stored one after another in the columns of VR, in the same order as their eigenvalues. If the jth eigenvalue is real, then $\mathbf{x}_j = $ VR$(:, j)$, the jth column of VR. If the jth and $(j + 1)$th eigenvalues form a complex conjugate pair, then $\mathbf{x}_j = $ VR$(:, j) + i \cdot $ VR$(:, j+1)$ and $\mathbf{x}_{j+1} = $ VR$(:, j) - i \cdot $ VR$(:, j+1)$.

WORK: If INFO $= 0$, WORK(1) returns the optimal LWORK.

INFO: INFO $= 0$ if successful exit. If INFO $= -j$, the jth argument had an illegal value. If INFO $= 1, \ldots, $N, then the QZ iteration failed. No eigenvectors have been calculated, but ALPHAR(j), ALPHAI(j), and BETA(j) should be correct for $j = $ INFO $+ 1, \ldots, $N. If INFO $= $ N+1, then other than QZ iteration failed in SHGEQZ. If INFO $= $ N+2, then error return from STGEVC.

Note that the quotients ALPHAR(j)/BETA(j) and ALPHAI(j)/BETA(j) may easily over- or underflow, and BETA(j) may even be zero. Thus, the user should avoid naively computing the ratio. However, ALPHAR and ALPHAI will be always less than and usually comparable to $\| A \|$ in magnitude, and BETA always less than and usually comparable to $\| B \|$.

Let us demonstrate the use of SGGEV in solving the GNEP of the following 6–by–6 matrices A and B:

$$A = \begin{bmatrix} 50 & -60 & 50 & -27 & 6 & 6 \\ 38 & -28 & 27 & -17 & 5 & 5 \\ 27 & -17 & 27 & -17 & 5 & 5 \\ 27 & -28 & 38 & -17 & 5 & 5 \\ 27 & -28 & 27 & -17 & 16 & 5 \\ 27 & -28 & 27 & -17 & 5 & 16 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 16 & 5 & 5 & 5 & -6 & 5 \\ 5 & 16 & 5 & 5 & -6 & 5 \\ 5 & 5 & 16 & 5 & -6 & 5 \\ 5 & 5 & 5 & 16 & -6 & 5 \\ 5 & 5 & 5 & 5 & -6 & 16 \\ 6 & 6 & 6 & 6 & -5 & 6 \end{bmatrix}.$$

The exact eigenvalues are $\frac{1}{2} + i \cdot \frac{\sqrt{3}}{2}, \frac{1}{2} + i \cdot \frac{\sqrt{3}}{2}, \frac{1}{2} - i \cdot \frac{\sqrt{3}}{2}, \frac{1}{2} - i \cdot \frac{\sqrt{3}}{2}, \infty, \infty$. Upon calling SGGEV with N $= 6$, LWORK $= 48$, on exit, arrays ALPHAR, ALPHAI and BETA are

$$\text{ALPHAR} = \begin{bmatrix} -25.7687130 & 6.5193458 & 5.8156629 & 5.8464251 & 5.5058141 & 11.2021322 \end{bmatrix},$$

$$\text{ALPHAI} = \begin{bmatrix} 0.0000000 & 11.2832556 & -10.0653677 & 10.1340599 & -9.5436525 & 0.0000000 \end{bmatrix},$$

$$\text{BETA} = \begin{bmatrix} 0.0000000 & 13.0169611 & 11.6119413 & 11.7124090 & 11.0300474 & 0.0000000 \end{bmatrix}.$$

Therefore, there are two infinite eigenvalues corresponding to $\text{BETA}(1) = \text{BETA}(6) = 0$ and four finite eigenvalues $\lambda_j = (\text{ALPHAR}(j) + i \cdot \text{ALPHAI}(j))/\text{BETA}(j)$ for $j = 2, 3, 4, 5$.

$$(\text{ALPHAR}(2:5) + i \cdot \text{ALPHAI}(2:5))/\text{BETA}(2:5) = \begin{bmatrix} 0.50083 + i \cdot 0.86681 \\ 0.50083 - i \cdot 0.86681 \\ 0.49917 + i \cdot 0.86524 \\ 0.49917 - i \cdot 0.86524 \end{bmatrix}.$$

The left eigenvectors $\mathbf{y}_j$ are stored in VL. Since $\text{ALPHAI}(1) = \text{ALPHAI}(6) = 0$, $\mathbf{y}_1 = \text{VL}(:,1)$ and $\mathbf{y}_6 = \text{VL}(:,6)$. The second and third eigenvalues form a complex conjugate pair, the $\mathbf{y}_2 = \text{VL}(:,2) + i \cdot \text{VL}(:,3)$ and $\mathbf{y}_3 = \text{VL}(:,2) - i \cdot \text{VL}(:,3)$. Similarly, $\mathbf{y}_4 = \text{VL}(:,4) + i \cdot \text{VL}(:,5)$ and $\mathbf{y}_5 = \text{VL}(:,4) + i \cdot \text{VL}(:,5)$. If we place all the left eigenvectors in a matrix Y, where $Y = [\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3, \mathbf{y}_4, \mathbf{y}_5, \mathbf{y}_6]$, we have

$$Y = \begin{bmatrix} -0.1666666 & 0.2632965 + i \cdot 0.3214956 & 0.2632965 - i \cdot 0.3214956 & -0.4613968 + i \cdot 0.1902102 & -0.4613968 - i \cdot 0.1902102 & 0.1666667 \\ -0.1666666 & -0.2834885 - i \cdot 0.7165115 & -0.2834885 + i \cdot 0.7165115 & 0.9231794 - i \cdot 0.0765849 & 0.9231794 + i \cdot 0.0765849 & 0.1666667 \\ -0.1666666 & 0.1623165 + i \cdot 0.7526108 & 0.1623165 - i \cdot 0.7526108 & -0.9240005 - i \cdot 0.0759995 & -0.9240005 + i \cdot 0.0759995 & 0.1666667 \\ -0.1666666 & 0.0396326 - i \cdot 0.4130635 & 0.0396326 + i \cdot 0.4130635 & 0.4619284 + i \cdot 0.1907958 & 0.4619284 - i \cdot 0.1907958 & 0.1666666 \\ -0.1666671 & -0.0605860 + i \cdot 0.0184893 & -0.0605860 - i \cdot 0.0184893 & 0.0000969 - i \cdot 0.0761408 & 0.0000969 + i \cdot 0.0761408 & 0.1666666 \\ 1.0000000 & -0.0605855 + i \cdot 0.0184900 & -0.0605855 - i \cdot 0.0184900 & 0.0000959 - i \cdot 0.0761405 & 0.0000959 + i \cdot 0.0761405 & -1.0000000 \end{bmatrix}.$$

The right eigenvectors can be recovered from VR in a way similar to the left eigenvectors. If we place all the right eigenvectors in a matrix X, where $X = [\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5, \mathbf{x}_6]$, we have

$$U = \begin{bmatrix} 0.1666672 & -0.2039835 - i \cdot 0.5848466 & -0.2039835 + i \cdot 0.5848466 & 0.5722237 - i \cdot 0.0237538 & 0.5722237 + i \cdot 0.0237538 & 0.1666672 \\ 0.1666664 & -0.7090308 - i \cdot 0.2908980 & -0.7090308 + i \cdot 0.2908980 & 0.4485306 - i \cdot 0.5514694 & 0.4485306 + i \cdot 0.5514694 & 0.1666664 \\ 0.1666666 & -0.7071815 + i \cdot 0.2928185 & -0.7071815 - i \cdot 0.2928185 & -0.0709520 - i \cdot 0.7082051 & -0.0709520 + i \cdot 0.7082051 & 0.1666666 \\ 0.1666666 & -0.2013957 + i \cdot 0.5829236 & -0.2013957 - i \cdot 0.5829236 & -0.4667411 - i \cdot 0.3361499 & -0.4667411 + i \cdot 0.3361499 & 0.1666666 \\ 1.0000000 & -0.2023994 + i \cdot 0.0000001 & -0.2023994 - i \cdot 0.0000001 & 0.0536732 - i \cdot 0.1799536 & 0.0536732 + i \cdot 0.1799536 & 1.0000000 \\ 0.1666666 & -0.2023991 - i \cdot 0.0000002 & -0.2023991 + i \cdot 0.0000002 & 0.0536734 - i \cdot 0.1799532 & 0.0536734 + i \cdot 0.1799532 & 0.1666664 \end{bmatrix}.$$

75.11   Generalized Singular Value Decomposition

Definitions:

The generalized (or quotient) singular value decomposition (GSVD or QSVD) of an *m*–by–*n* matrix A and a *p*–by–*n* matrix B is given by the pair of factorizations

$$A = U\Sigma_1 \begin{bmatrix} 0 & R \end{bmatrix} Q^T \quad \text{and} \quad B = V\Sigma_2 \begin{bmatrix} 0 & R \end{bmatrix} Q^T. \tag{75.15}$$

The matrices in these factorizations have the following properties:

- U is *m*-by-*m*, V is *p*-by-*p*, Q is *n*-by-*n*, and all three matrices are orthogonal. If A and B are complex, these matrices are unitary instead of orthogonal, and Q^T should be replaced by Q^* in the pair of factorizations.

- R is r-by-r, upper triangular and nonsingular. $\begin{bmatrix} 0 & R \end{bmatrix}$ is r-by-n (in other words, the 0 is an r-by-$(n-r)$ zero matrix). The integer r is the rank of $\begin{bmatrix} A \\ B \end{bmatrix}$.

- Σ_1 is *m*-by-*r* and Σ_2 is *p*-by-*r*. Both are real, nonnegative and diagonal, satisfying $\Sigma_1^T \Sigma_1 + \Sigma_2^T \Sigma_2 = I$. Write $\Sigma_1^T \Sigma_1 = \text{diag}(\alpha_1^2, \ldots, \alpha_r^2)$ and $\Sigma_2^T \Sigma_2 = \text{diag}(\beta_1^2, \ldots, \beta_r^2)$. The ratios α_j/β_j for $j = 1, 2, \ldots, r$ are called the *generalized singular values*.

Σ_1 and Σ_2 have the following detailed structures, depending on whether $m - r \geq 0$ or $m - r < 0$.

- In the first case, when $m - r \geq 0$,

$$\Sigma_1 = \begin{array}{c} \\ k \\ \ell \\ m-k-\ell \end{array} \overset{\begin{array}{cc} k & \ell \end{array}}{\begin{pmatrix} I & 0 \\ 0 & C \\ 0 & 0 \end{pmatrix}} \quad \text{and} \quad \Sigma_2 = \begin{array}{c} \\ \ell \\ p-\ell \end{array} \overset{\begin{array}{cc} k & \ell \end{array}}{\begin{pmatrix} 0 & S \\ 0 & 0 \end{pmatrix}}. \tag{75.16}$$

Here $k + \ell = r$, and ℓ is the rank of B. C and S are diagonal matrices satisfying $C^2 + S^2 = I$, and S is nonsingular. Let c_j and s_j are the diagonal entries of C and S, respectively. Then we have $\alpha_1 = \cdots = \alpha_k = 1$, $\alpha_{k+j} = c_j$ for $j = 1, \ldots, \ell$, $\beta_1 = \cdots = \beta_k = 0$, and $\beta_{k+j} = s_j$ for $j = 1, \ldots, \ell$. Thus, the first k generalized singular values $\alpha_1/\beta_1, \ldots, \alpha_k/\beta_k$ are infinite and the remaining ℓ generalized singular values are finite.

- In the second case, when $m - r < 0$,

$$\Sigma_1 = \begin{array}{c} \\ k \\ m-k \end{array} \overset{\begin{array}{ccc} k & m-k & k+\ell-m \end{array}}{\begin{pmatrix} I & 0 & 0 \\ 0 & C & 0 \end{pmatrix}} \quad \text{and} \quad \Sigma_2 = \begin{array}{c} \\ m-k \\ k+\ell-m \\ p-\ell \end{array} \overset{\begin{array}{ccc} k & m-k & k+\ell-m \end{array}}{\begin{pmatrix} 0 & S & 0 \\ 0 & 0 & I \\ 0 & 0 & 0 \end{pmatrix}}.$$
$$\tag{75.17}$$

Again, $k + \ell = r$, and ℓ is the rank of B. C and S are diagonal matrices satisfying $C^2 + S^2 = I$, and S is nonsingular. Let c_j and s_j are the diagonal entries of C and S, respectively. Then we have $\alpha_1 = \cdots = \alpha_k = 1$, $\alpha_{k+j} = c_j$ for $j = 1, \ldots, m - k$, $\alpha_{m+1} = \cdots = \alpha_r = 0$, and $\beta_1 = \cdots = \beta_k = 0$, $\beta_{k+j} = s_j$ for $j = 1, \ldots, m - k$, $\beta_{m+1} = \cdots = \beta_r = 1$. Thus, the first k generalized singular values $\alpha_1/\beta_1, \ldots, \alpha_k/\beta_k$ are infinite, and the remaining ℓ generalized singular values are finite.

Backgrounds:

Here are some important special cases of the QSVD. First, when B is square and nonsingular, then $r = n$ and the QSVD of A and B is equivalent to the SVD of AB^{-1}, where the singular values of AB^{-1} are equal to the generalized singular values of A and B:

$$AB^{-1} = (U\Sigma_1 R Q^T)(V\Sigma_2 R Q^T)^{-1} = U(\Sigma_1 \Sigma_2^{-1})V^T .$$

Second, if the columns of $\begin{bmatrix} A^T & B^T \end{bmatrix}^T$ are orthonormal, then $r = n$, $R = I$ and the QSVD of A and B is equivalent to the CS (Cosine-Sine) decomposition of $\begin{bmatrix} A^T & B^T \end{bmatrix}^T$:

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} U & 0 \\ 0 & V \end{bmatrix} \begin{bmatrix} \Sigma_1 \\ \Sigma_2 \end{bmatrix} Q^T.$$

Third, the generalized eigenvalues and eigenvectors of the pencil $A^T A - \lambda B^T B$ can be expressed in terms of the QSVD of A and B, namely,

$$X^T A^T A X = \begin{bmatrix} 0 & 0 \\ 0 & \Sigma_1^T \Sigma_1 \end{bmatrix} \quad \text{and} \quad X^T B^T B X = \begin{bmatrix} 0 & 0 \\ 0 & \Sigma_2^T \Sigma_2 \end{bmatrix}.$$

where $X = Q \begin{bmatrix} I & 0 \\ 0 & R^{-1} \end{bmatrix}$. Therefore, the columns of X are the eigenvectors of $A^T A - \lambda B^T B$, and the "nontrivial" eigenvalues are the squares of the generalized singular values. "Trivial" eigenvalues are those corresponding to the leading $n - r$ columns of X, which span the common null space of $A^T A$ and $B^T B$.

The "trivial eigenvalues" are not well defined.[1] (See Chapter 15 for more information on generalized singular value problems.)

Driver Routines:

The driver routines xGGSVD compute the GSVD (75.15) of A and B.

Examples:

Let us show how to use the driver routine SGGSVD to compute the QSVD (75.15). SGGSVD first reduces the matrices A and B to a pair of triangular matrices, and then use a Jacobi-like method to compute the QSVD of the triangular pair. SGGSVD has the following calling sequence:

```
 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 )
```

Input to SGGSVD:

> JOBU, JOBV, JOBQ: , = 'U', orthogonal matrices U, V and Q are computed;
>> = 'N', these orthogonal matrices are not computed.
>
> M, N, P: The number of rows or columns of the matrices A and B as defined in (15)
>
> A, LDA: The M-by-N matrix A and the leading dimension of the array A. LDA $\geq$ max(1, M).
>
> B, LDB: The P-by-N matrix B and the leading dimension of the array B. LDB $\geq$ max(1, P).
>
> LDU, LDV, LDQ: The leading dimension of the arrays U, V, and Q if the orthogonal matrices U, V, and Q are computed, LDU $\geq$ max(1, M), LDV $\geq$ max(1, P), LDQ $\geq$ max(1, N).
>
> WORK: The real workspace array, dimension max(3N, M, P) + N.
>
> IWORK: The integer workspace array, dimension N.

Output from SGGSVD:

> K, L: The dimension of the subblocks described in the definition of GSVD. K + L is the effective numerical rank of the matrix $\begin{bmatrix} A^T & B^T \end{bmatrix}^T$.
>
> A: The entire triangular matrix R is stored in A(1:K+L, N–K–L+1:N) if $m - r \geq 0$. Otherwise, contains the subblock $R(1 : m, 1 : k + \ell)$ of R are stored in A(1:M, N–K–L+1:N).
>
> B: The subblock $R(m + 1 : k + \ell, m + 1 : k + \ell)$ of R are stored in B(M–K+1:L, N+M–K–L+1:N) if $m - r < 0$.
>
> ALPHA, BETA: The generalized singular value pairs;
>> ALPHA(1:K) = 1 and BETA(1:K) = 0.
>>
>> - If M–K–L $\geq$ 0, then ALPHA(K + 1 : K + L) = C and BETA(K + 1 : K + L) = S.
>> - If M–K–L < 0, then
>>> ALPHA(K + 1 : M) = C and   ALPHA(M + 1 : K + L) = 0,
>>>
>>> BETA(K + 1 : M) = S and   BETA(M + 1 : K + L) = 1;
>>
>> And ALPHA(K+L+1:N) = 0, BETA(K+L+1:N) = 0.

---

[1] If we tried to compute the trivial eigenvalues in the same way as the nontrivial ones, that is by taking ratios of the leading $n - r$ diagonal entries of $X^T A^T A X$ and $X^T B^T B X$, we would get 0/0.

U, V, Q: Contains computed orthogonal matrices U, V and Q if requested.

INFO: INFO = 0 if successful exit. If $\mathtt{INFO} = -j$, then the jth argument had an illegal value. If INFO = 1, the Jacobi-type procedure failed to converge.

Let us demonstrate the use of SGGSVD in computing the QSVD of the following 6–by–5 matrices A and B:

$$
A = \begin{bmatrix} 1 & 2 & 3 & 1 & 5 \\ 0 & 3 & 2 & 0 & 2 \\ 1 & 0 & 2 & 1 & 0 \\ 0 & 2 & 3 & 0 & -1 \\ 1 & 0 & 2 & 1 & 1 \\ 0 & 2 & 1 & 0 & 1 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 1 & -2 & 2 & 1 & 1 \\ 0 & 3 & 0 & 0 & 0 \\ 1 & -2 & 2 & 1 & 1 \\ 0 & 2 & 0 & 0 & 0 \\ 2 & -4 & 4 & 2 & 2 \\ 1 & 3 & 2 & 1 & 1 \end{bmatrix}.
$$

Upon calling SGGSVD with $\mathtt{M} = 6, \mathtt{P} = 6, \mathtt{N} = 5, \mathtt{LWORK} = 20$, we have $\mathtt{K} = 2$ and $\mathtt{L} = 2$. The QSVD (75.15) of A and B falls in the first case (75.16) since $\mathtt{M} - \mathtt{K} - \mathtt{L} = 6 - 2 - 2 = 2 > 0$. The arrays ALPHA and BETA are

$$
\mathtt{ALPHA} = \begin{bmatrix} 1.0000000 & 1.0000000 & 0.1537885 & 0.5788464 & 0.0000000 \end{bmatrix}
$$

$$
\mathtt{BETA} = \begin{bmatrix} 0.0000000 & 0.0000000 & 0.9881038 & 0.8154366 & 0.0000000 \end{bmatrix}
$$

Hence, Σ_1 and Σ_2 have the structure as described in (75.16), namely,

$$
\Sigma_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0.1537885 & 0 \\ 0 & 0 & 0 & 0.5788464 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{and} \quad \Sigma_2 = \begin{bmatrix} 0 & 0 & 0.9881038 & 0 \\ 0 & 0 & 0 & 0.8154366 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.
$$

The first two generalized singular values are infinite, $\alpha_1/\beta_1 = \alpha_2/\beta_2 = \infty$, and the remaining two generalized singular values are finite, $\alpha_3/\beta_3 = 0.15564$ and $\alpha_4/\beta_4 = 0.70986$.

Furthermore, the array A(1:4,2:5) contains the 4–by–4 upper triangular matrix R as defined in (75.15):

$$
R = \begin{bmatrix} 3.6016991 & -1.7135643 & -0.2843603 & 1.8104467 \\ 0 & -2.6087811 & -4.2943931 & 5.1107349 \\ 0 & 0 & 6.9692163 & 3.5063875 \\ 0 & 0 & 0 & 7.3144341 \end{bmatrix}.
$$

The orthogonal matrices U, V and Q are returned in the arrays U, V and Q, respectively,

$$
U = \begin{bmatrix} -0.6770154 & -0.4872811 & -0.4034495 & -0.2450049 & -0.2151961 & 0.1873468 \\ -0.0947438 & -0.5723576 & 0.4163284 & 0.1218751 & 0.0785425 & -0.6848933 \\ 0.2098812 & 0.0670342 & 0.2612190 & -0.7393155 & -0.5670457 & -0.1228532 \\ 0.6974092 & -0.5903998 & -0.3678919 & 0.0010751 & -0.0196356 & 0.1712235 \\ 0.0000000 & 0.0000001 & -0.0735656 & -0.6152450 & 0.7822418 & -0.0644937 \\ -0.0473719 & -0.2861788 & 0.6744684 & -0.0019711 & 0.1170180 & 0.6687696 \end{bmatrix},
$$

$$
V = \begin{bmatrix} -0.3017521 & -0.2581125 & 0.9018297 & -0.0002676 & -0.1695592 & -0.0166328 \\ 0.4354534 & -0.2679386 & 0.1028928 & 0.0704557 & 0.2595005 & -0.8097517 \\ -0.3017520 & -0.2581124 & -0.1784097 & -0.8828155 & -0.0002829 & -0.1764375 \\ 0.2903022 & -0.1786257 & -0.1298870 & -0.0008522 & -0.9259184 & -0.0980879 \\ -0.6035041 & -0.5162248 & -0.3568195 & 0.4625078 & -0.0224125 & -0.1660080 \\ 0.4240036 & -0.7046767 & -0.0097810 & -0.0419325 & 0.2146671 & 0.5250862 \end{bmatrix},
$$

$$
Q = \begin{bmatrix} -0.7071068 & -0.2073452 & -0.5604916 & -0.0112638 & -0.3777966 \\ 0.0000000 & 0.0000000 & 0.0000000 & 0.9995558 & -0.0298012 \\ 0.0000001 & 0.5853096 & 0.2932303 & -0.0225276 & -0.7555932 \\ 0.7071067 & -0.2073452 & -0.5604916 & -0.0112638 & -0.3777965 \\ -0.0000001 & -0.7559289 & 0.5345224 & -0.0112638 & -0.3777965 \end{bmatrix}.
$$

References

[CLA] http://www.netlib.org/clapack/

[JLA] http://www.netlib.org/java/f2j/

[LUG99] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen, *LAPACK Users' Guide*, 3rd ed., SIAM, Philadelphia, 1999.

[LAP] http://www.netlib.org/lapack/

[LAP95] http://www.netlib.org/lapack95/

[LA+] http://www.netlib.org/lapack++/

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