LAPACK Summary

Prefixes

Each routine has a prefix, denoted by a hypen - in this guide, made of 3 letters xyy, where x is the data type, and yy is the matrix type.

Fortran data type	C data type	Abbreviation
real	float	S
double precision	double	d
complex	float complex double complex	c
complex*16	double complex	z

Matrix type	full	packed	RFP	banded	tridiag	generalized problem
general	ge			gb	gt	gg
symmetric	sy	sp	sf	sb	st	
Hermitian	he	hp	hf	hb		
SPD / HPD	po	pp	pf	pb	pt	
triangular	tr	tp	tf	tb		tg
upper Hessenberg	hs					hg
trapezoidal	tz					
orthogonal	or	op				
unitary	un	up				
diagonal					di	
bidiagonal					bd	

Storage

Full matrices are stored column-wise (so-called "Fortran" order). For symmetric, Hermition, and triangular matrices, elements below/above the diagonal (for upper/lower respectively) are not accessed. Similarly for upper Hessenberg, elements below the subdiagonal are not accessed.

Packed storage for triangular or symmetric matrices is by columns. For example, a 3×3 upper triangular matrix is stored as

$$\boldsymbol{U} = \begin{bmatrix} 1 & 2 & 4 \\ \cdot & 3 & 5 \\ \cdot & \cdot & 6 \end{bmatrix} \Longrightarrow \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ \cdot & \cdot & 6 \end{bmatrix}$$

and a 3×3 lower triangular matrix is stored as

$$\mathbf{L} = \begin{bmatrix} 1 & \cdot & \cdot \\ 2 & 4 & \cdot \\ 3 & 5 & 6 \end{bmatrix} \Longrightarrow \begin{bmatrix} \underbrace{1 \ 2 \ 3}_{\text{column 1 column 2 column 3}} \underbrace{4 \ 5}_{\text{column 3}} \underbrace{6}_{\text{column 3}} \end{bmatrix}$$

Rectangular full packed (RFP) for triangular or symmetric matrices reuses fast routines for full matrices, but with half the storage and avoiding the inefficient indexing of packed storage. It divides the matrix into 4 quadrants, transposes one of the triangles and packs it next to the other triangle; see LAPACK Working Note 199. For example,

$$L = \begin{bmatrix} L_{11} & \cdot \\ L_{21} & L_{22} \end{bmatrix} \Longrightarrow \begin{bmatrix} L_{11} \text{ and } L_{22}^T \\ L_{21} \end{bmatrix}$$

$$L = \begin{bmatrix} a_{11} & \cdot & \cdot & | & \cdot & \cdot & \cdot \\ a_{12} & a_{22} & \cdot & | & \cdot & \cdot & \cdot \\ a_{13} & a_{23} & a_{33} & | & \cdot & \cdot & \cdot \\ a_{14} & a_{24} & a_{34} & | & a_{44} & | & \cdot & \cdot \\ a_{15} & a_{25} & a_{35} & | & a_{45} & a_{55} & | \\ a_{16} & a_{26} & a_{36} & | & a_{46} & a_{56} & a_{66} \end{bmatrix} \implies \begin{bmatrix} \mathbf{a_{44}} & \mathbf{a_{45}} & \mathbf{a_{46}} \\ a_{11} & \mathbf{a_{55}} & \mathbf{a_{56}} \\ a_{12} & a_{22} & \mathbf{a_{66}} \\ a_{13} & a_{23} & a_{33} \\ \hline a_{14} & a_{24} & a_{34} \\ a_{15} & a_{25} & a_{35} \\ a_{16} & a_{26} & a_{36} \end{bmatrix}$$

There are 4 versions depending on whether n is even or odd and whether the upper or lower triangle is stored. Conversion routines are provided.

Banded storage puts columns of the matrix in corresponding columns of the array, and diagonals in rows of the array, for example:

$$\begin{bmatrix} a_{11} & a_{12} & \cdot & \cdot & \cdot \\ a_{21} & a_{22} & a_{23} & \cdot & \cdot \\ a_{31} & a_{32} & a_{33} & a_{34} & \cdot \\ \cdot & a_{42} & a_{43} & a_{44} & a_{45} \\ \cdot & \cdot & a_{53} & a_{54} & a_{55} \end{bmatrix} \Longrightarrow \begin{bmatrix} * & a_{12} & a_{23} & a_{34} & a_{45} \\ a_{11} & a_{22} & a_{33} & a_{44} & a_{55} \\ a_{21} & a_{32} & a_{43} & a_{54} & * \\ a_{31} & a_{42} & a_{53} & * & * \end{bmatrix}$$
 1st diagonal 2nd (main) diagonal 3rd diagonal 3rd diagonal 4th diagonal

Bi- and tri-diagonal matrices are stored as 2 or 3 vectors of length n and n-1.

Drivers

Drivers are higher level routines that solve an entire problem.

Linear system, solve Ax = b.

-sv — solve

-svx — expert; also $A^Tx = b$ or $A^Hx = b$, condition number, error bounds, scaling Matrix types [General ge, gb, gt; SPD po, pp, pb, pt; Symmetric sy, sp, he, hp]

Linear least squares, minimize $||b - Ax||_2$.

-1s — full rank, rank(A) = min(m, n), uses QR.

-lsy — rank deficient, uses complete orthogonal factorization.

-1sd — rank deficient, uses SVD.

Matrix types [General ge]

Generalized linear least squares.

Minimize $||c - Ax||_2$ subject to Bx = d.

-lse — B full row rank, matrix $\begin{bmatrix} A \\ B \end{bmatrix}$ full col rank.

Minimize $||y||_2$ subject to d = Ax + By.

-glm - A full col rank, matrix $\begin{bmatrix} A & B \end{bmatrix}$ full row rank.

Matrix types [General gg]

SVD singular value decomposition, $A = U\Sigma V^H$

-svd — singular values, [left, right vectors]

-sdd — divide-and-conquer; faster but more memory

Matrix types [General ge]

Generalized SVD, $A = U\Sigma_1 Q^T$ and $B = V\Sigma_2 Q^T$

-svd — singular values, [left, right vectors]

Matrix types [General gg]

Conversion routines

-tfttp — RFP to Packed

-tfttr — RFP to Triangular full

-trttp — Triangular full to Packed -trttf — Triangular full to RFP

-tpttr — Packed to Triangular full

-tpttf — Packed to RFP

Eigenvalues, solve $Ax = \lambda x$.

Symmetric

-ev — all eigenvalues, [eigenvectors]

-evx — expert; also subset

-evd — divide-and-conquer; faster but more memory

-evr — relative robust; fastest and least memory

Matrix types [Symmetric sy, sp, sb, st, he, hp, hb]

Nonsymmetric

-ev — eigenvalues, [left, right eigenvectors]

-evx — expert; also balance matrix, condition numbers

-es — Schur factorization

-esx — expert; also condition numbers

Matrix types [General ge]

Generalized eigenvalue, solve $Ax = \lambda Bx$

Symmetric, B SPD

-gv — all eigenvalues, [eigenvectors]

-gvx — expert; also subset

-gvd — divide-and-conquer, faster but more memory

Matrix types [Symmetric sy, sp, sb, he, hp, hb]

Nonsymmetric

-ev — eigenvalues, [left, right eigenvectors]

-evx — expert; also balance matrix, condition numbers

-es — Schur factorization

-esx — expert; also condition numbers

Matrix types [General gg]

Computational routines

Computational routines perform one step of solving the problem. Drivers call a sequence of computational routines.

Triangular factorization

- -trf factorize: General LU, Cholesky LL^T, tridiag LDL^T, sym. indefinite LDL^T
- -trs solve using factorization
- -con condition number estimate
- -rfs error bounds, iterative refinement
- -tri inverse (not for band)
- -equ equilibrate *A* (not for tridiag, symmetric indefinite, triangular)

Matrix types [General ge, gb, gt; SPD po, pp, pf, pb, pt; Symmetric sy, sp, he, hp, Triangular tr, tp, tf, tb]

Orthogonal factorization

- -qp3 QR factorization, with pivoting
- -grf *QR* factorization
- -rgf RQ factorization
- -qlf *QL* factorization
- -lqf LQ factorization
- -tzrqf RQ factorization
- -tzrzf RZ trapezoidal factorization

Matrix types [General ge, some Trapezoidal tz]

- -gqr generate Q after -qrf
- -grq generate Q after -rqf
- -gql generate Q after -qlf
- -glq generate Q after -lqf
- -mqr multiply by Q after -qrf
- -mrq multiply by Q after -rqf
- -mql multiply by Q after -qlf
- -mlq multiply by Q after -lqf
- -mrz multiply by Q after -tzrzf
- Matrix types [Orthogonal or, un]

Generalized orthogonal factorization

- $-qrf QR \text{ of } A, \text{ then } RQ \text{ of } Q^TB$
- $-\text{rqf} RQ \text{ of } A, \text{ then } QR \text{ of } BQ^T$

Matrix types [General gg]

Eigenvalue

- -trd tridiagonal reduction
- Matrix types [Symmetric sy, he, sp, hp]
- -gtr generate matrix after -trd
- -mtr multiply matrix after -trd
- Matrix types [Orthogonal or, op, un, up]

Symmetric tridiagonal eigensolvers

- -eqr using implicitly shifted QR
- -pteqr using Cholesky and bidiagonal QR
- -erf using square-root free QR
- -edc using divide-and-conquer
- -egr using relatively robust representation
- -ebz eigenvalues using bisection
- -ein eigenvectors using inverse iteration
- Matrix types [Symmetric tridiag st, one SPD pt]

Nonsymmetric

- -hrd Hessenberg reduction
- -bal balance
- -bak back transforming
- Matrix types [General ge]
- -ghr generate matrix after -hrd
- -mhr multiply matrix after -hrd
- Matrix types [Orthogonal or, un]
- -egr Schur factorization
- -ein eigenvectors using inverse iteration
- Matrix types [upper Hessenberg hs]
- -evc eigenvectors
- -exc reorder Schur factorization
- -syl Sylvester equation
- -sna condition numbers
- -sen condition numbers of eigenvalue cluster/subspace

Matrix types [Triangular tr]