## trf (getrf)

compute an LU factorization of a general  $M\times N$  matrix A using partial pivoting with row interchanges

## Synopsis

```
template <typename FS>
    int
    trf(GeMatrix<FS> &A, DenseVector<Array<int> > &P);
```

### Purpose

computes an LU factorization of a general  $M \times N$  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).

### Arguments

| А | (input/output)<br>On entry, the $M \times N$ matrix to be factored. On exit, the factors $L$ and $U$ from the factorization $A = PLU$ ; the unit diagonal elements of $L$ |
|---|---|
| Ρ | are not stored.<br>(output)<br>The pivot indices; for $1 \le i \le \min\{M, N\}$ , row <i>i</i> of the matrix was<br>interchanged with row $P(i)$ .                       |

### Returns

i > 0 then U(i, i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and division by zero will occur if it is used to solve a system of equations.

# tri (getri)

compute the inverse of a matrix using the LU factorization computed by trf

## Synopsis

```
template <typename FS>
    int
    tri(GeMatrix<FS> &A, DenseVector<Array<int> > &P);
```

### Purpose

tri computes the inverse of a matrix using the LU factorization computed by trf. This function inverts U and then computes  $A^{-1}$  by solving the system  $A^{-1} * L = U^{-1}$  for  $A^{-1}$ .

### Arguments

| A | (input/output)<br>On entry, the factors $L$ and $U$ from the factorization $A = PLU$ as<br>computed by trf. On successful exit, the inverse of the original matrix<br>A. |
|---|--|
| Ρ | (input)<br>The pivot indices from trf; for $1 \leq i \leq N$ , row <i>i</i> of the matrix was interchanged with row $P(i)$ .   |

### Returns

| i = 0 | successful exit  |
|-------|--|
| i > 0 | then $U(i, i)$ is exactly zero; the matrix is singular and its inverse could |
|       | not be computed.   |

### trf (gbtrf)

compute an LU factorization of a real  $M\times N$  band matrix A using partial pivoting with row interchanges

### Synopsis

```
template <typename BS>
    int
    trf(GbMatrix<BS> &A, DenseVector<Array<int> > &P);
```

### Purpose

trf computes an LU factorization of a real  $M \times N$  band matrix A using partial pivoting with row interchanges. This is the blocked version of the algorithm, calling Level 3 BLAS.

### Arguments

| A | (input/output)<br>On entry, the matrix $A$ in band storage and on exit overwritten with the $LU$ factorization. Matrix $A$ is required to have a total of $k_l$ subdiagonals and $k_l + k_u$ superdiagonals where on entry only the elements within the $k_l$ subdiagonals and $k_u$ superdiagonals need to be set (See Further Details). |
|---|---|
| Ρ | (input) The pivot indices; for $1 \le i \le N$ , row <i>i</i> of the matrix was interchanged with row $P(i)$ .  |

### Returns

i > 0 then U(i, i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and division by zero will occur if it is used to solve a system of equations.

## Further Details

Assume non-zero elements of A reside within a band of  $k_l$  subdiagonals and  $k_u$  superdiagonals. Then storing its LU factorization requires a band of  $k_l$  subdiagonals and  $k_l + k_u$  superdiagonals. Hence, the GbMatrix holding the matrix A needs to have  $k_l$  subdiagonals and  $k_l + k_u$  superdiagonals allocated; but only the elements within its  $k_l$  subdiagonals and  $k_u$  superdiagonals must be set.

If, for example, A is a tridiagonal matrix (i.e.  $k_l = k_u = 1$ ), then matrix U will have in general two super-diagonals. This requires the GbMatrix storing A has

allocated an additional superdiagonal (as indicated by '\*'):

$$A = \begin{pmatrix} a_{1,1} & a_{1,2} & * & 0 & 0 \\ a_{2,1} & a_{2,2} & a_{2,3} & * & 0 \\ 0 & a_{3,2} & a_{3,3} & a_{3,4} & * \\ 0 & 0 & a_{4,3} & a_{4,4} & a_{4,5} \\ 0 & 0 & 0 & a_{5,4} & a_{5,5} \end{pmatrix} \quad \rightsquigarrow \quad A_{LU} = \begin{pmatrix} u_{1,1} & u_{1,2} & u_{1,3} & 0 & 0 \\ m_{2,1} & u_{2,2} & u_{2,3} & u_{2,4} & 0 \\ 0 & m_{3,2} & u_{3,3} & u_{3,4} & u_{3,5} \\ 0 & 0 & m_{4,3} & u_{4,4} & u_{4,5} \\ 0 & 0 & 0 & m_{5,4} & u_{5,5} \end{pmatrix}.$$

Elements of L are stored (in general rearranged due to pivoting) on the sub-diagonal of  $A_{LU}$ .

### trs (getrs)

solve a system of linear equations AX = B or  $A^TX = B$  with a general  $N \times N$  matrix A using the LU factorization computed by trf

### Synopsis

```
template <typename MA, typename MB>
    int
    trs(Transpose trans, const GeMatrix<MA> &A,
        const DenseVector<Array<int> > &P, GeMatrix<MB> &B);
template <typename MA, typename VB>
    int
    trs(Transpose trans, const GeMatrix<MA> &A,
        const DenseVector<Array<int> > &P,
        DenseVector<VB> &B);
```

## Purpose

trs solves a system of linear equations AX = B or  $A^TX = B$  with a general  $N \times N$  matrix A using the LU factorization computed by trf.

### Arguments

| trans | (input)   |
|-------|---|
|       | Specifies the form of the system of equations:                              |
|       | trans = NoTrans $AX = B$ (No transpose)                                     |
|       | trans = Trans $A^T X = B$ (Transpose)                                       |
|       | trans = ConjTrans $A^H X = B$ (Conjugate transpose = Transpose)             |
| А     | (input)   |
|       | The factors L and U from the factorization $A = PLU$ as computed by         |
|       | trf.  |
| Р     | (input)   |
|       | The pivot indices from trf; for $1 \leq i \leq N$ , row i of the matrix was |
|       | interchanged with row $P(i)$ .  |
| В     | (input/output)  |
|       | On entry, the right hand side matrix B. On exit, the solution matrix        |
|       | <i>X</i> .  |
|       |   |

### Returns

### trs (gbtrs)

solve a system of linear equations AX = B or  $A^TX = B$  with a general band matrix A using the LU factorization computed by trf

## Synopsis

```
template <typename MA, typename MB>
    int
    trs(Transpose trans, const GbMatrix<MA> &LU,
        const DenseVector<Array<int> > &P, GeMatrix<MB> &B);
template <typename MA, typename VB>
    int
    trs(Transpose trans, const GbMatrix<MA> &LU,
        const DenseVector<Array<int> > &P,
        DenseVector<VB> &B);
```

## Purpose

trs solves a system of linear equations AX = B or  $A^TX = B$  with a general band matrix A using the LU factorization computed by trf.

## Arguments

| trans | (input)<br>Specifies the form of the system of equations:                    |
|-------|--|
|       | trans = NoTrans $AX = B$ (No transpose)                                      |
|       | trans = Trans $A^T X = B$ (Transpose)  |
|       | trans = ConjTrans $A^H X = B$ (Conjugate transpose = Transpose)              |
| А     | (input)  |
|       | Details of the $LU$ factorization of the band matrix $A$ , as computed by    |
|       | trf. $U$ is stored as an upper triangular band matrix in the diagonal and    |
|       | the $k_l + k_u$ superdiagonals of A; the multipliers (i.e. the elements of L |
|       | rearranged due to pivoting) used during the factorization are stored in      |
|       | the $k_l$ subdiagonals of $A$ .  |
| Р     | (input)  |
|       | The pivot indices from trf; for $1 \leq i \leq N$ , row i of the matrix was  |
|       | interchanged with row $P(i)$ .   |
| В     | (input/output)   |
|       | On entry, the right hand side matrix $B$ . On exit, the solution matrix      |
|       | Χ.   |

### Returns

## sv (gesv)

compute the solution to a real system of linear equations AX = B

### Synopsis

```
template <typename MA, typename MB>
    int
    sv(GeMatrix<MA> &A, DenseVector<Array<int> > &P, GeMatrix<MB> &B);
template <typename MA, typename VB>
    int
    sv(GeMatrix<MA> &A, DenseVector<Array<int> > &P, DenseVector<VB> &B);
```

### Purpose

computes the solution to a real or complex system of linear equations AX = B, where A is an  $N \times N$  matrix and X and B are  $N \times R$  matrices.

The LU decomposition 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.

### Arguments

| А | (input/output)   |
|---|--|
|   | On entry, the $N \times N$ coefficient matrix A. On exit, the factors L and U        |
|   | from the factorization $A = PLU$ ; the unit diagonal elements of L are               |
|   | not stored.  |
| Р | (output)   |
|   | The pivot indices; for $1 \leq i \leq \min\{M, N\}$ , row <i>i</i> of the matrix was |
|   | interchanged with row $P(i)$ .   |
| В | (input/output)   |
|   | On entry, the $N \times R$ matrix of right hand side matrix B. On exit, if           |
|   | function returned 0, the $N \times R$ solution matrix X.                             |

#### Returns

i = 0 successful exit

i > 0 then U(i, i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, so the solution could not be computed.

### sv (gbsv)

compute the solution to a real system of linear equations AX = B, where A is a band matrix of order N with  $k_l$  subdiagonals and  $k_u$  superdiagonals, and X and B are  $N \times R$  matrices

## Synopsis

```
template <typename MA, typename MB>
    int
    sv(GbMatrix<MA> &A, DenseVector<Array<int> > &P, GeMatrix<MB> &B);
template <typename MA, typename VB>
    int
    sv(GbMatrix<MA> &A, DenseVector<Array<int> > &P, DenseVector<VB> &B);
```

## Purpose

sv computes the solution to a real system of linear equations AX = B, where A is a band matrix of order N with  $k_l$  subdiagonals and  $k_u$  superdiagonals, and X and B are  $N \times R$  matrices. The LU decomposition with partial pivoting and row interchanges is used to factor A as A = LU, where L is a product of permutation and unit lower triangular matrices with  $k_l$  subdiagonals, and U is upper triangular with  $k_l + k_u$  superdiagonals. The factored form of A is then used to solve the system of equations AX = B.

### Arguments

| A | (input/output)  |
|---|---|
|   | On entry, the matrix $A$ in band storage and on exit overwritten with the             |
|   | $LU$ factorization. Matrix <b>A</b> is required to have a total of $k_l$ subdiagonals |
|   | and $k_l + k_u$ superdiagonals where on entry only the elements within                |
|   | the $k_l$ subdiagonals and $k_u$ superdiagonals need to be set (See Further           |
|   | Details).   |
| Р | (input)   |
|   | The pivot indices; for $1 \le i \le N$ , row <i>i</i> of the matrix was interchanged  |
|   | with row $P(i)$ .   |
| В | (input/output)  |
|   | On entry, the right hand side matrix $B$ . On exit, the solution matrix               |
|   | X.  |

### Returns

i > 0 then U(i, i) is exactly zero. The factorization has been completed, but the factor U is exactly singular, and division by zero will occur if it is used to solve a system of equations.

#### **Further Details**

Assume non-zero elements of A reside within a band of  $k_l$  subdiagonals and  $k_u$  superdiagonals. Then storing its LU factorization requires a band of  $k_l$  subdiagonals and  $k_l + k_u$  superdiagonals. Hence, the GbMatrix holding the matrix A needs to have  $k_l$  subdiagonals and  $k_l + k_u$  superdiagonals allocated; but only the elements within its  $k_l$  subdiagonals and  $k_u$  superdiagonals must be set.

If, for example, A is a tridiagonal matrix (i.e.  $k_l = k_u = 1$ ), then matrix U will have in general two super-diagonals. This requires the GbMatrix storing A has allocated an additional superdiagonal (as indicated by '\*'):

$$A = \begin{pmatrix} a_{1,1} & a_{1,2} & * & 0 & 0 \\ a_{2,1} & a_{2,2} & a_{2,3} & * & 0 \\ 0 & a_{3,2} & a_{3,3} & a_{3,4} & * \\ 0 & 0 & a_{4,3} & a_{4,4} & a_{4,5} \\ 0 & 0 & 0 & a_{5,4} & a_{5,5} \end{pmatrix} \quad \rightsquigarrow \quad A_{LU} = \begin{pmatrix} u_{1,1} & u_{1,2} & u_{1,3} & 0 & 0 \\ m_{2,1} & u_{2,2} & u_{2,3} & u_{2,4} & 0 \\ 0 & m_{3,2} & u_{3,3} & u_{3,4} & u_{3,5} \\ 0 & 0 & m_{4,3} & u_{4,4} & u_{4,5} \\ 0 & 0 & 0 & m_{5,4} & u_{5,5} \end{pmatrix}$$

Elements of L are stored (in general rearranged due to pivoting) on the subdiagonal of  $A_{LU}$ .

### trs (trtrs)

solve a triangular system of the form AX = B or  $A^T X = B$ 

## Synopsis

```
template <typename MA, typename MB>
    int
    trs(Transpose trans, const TrMatrix<MA> &A, GeMatrix<MB> &B);
template <typename MA, typename VB>
    int
    trs(Transpose trans, const TrMatrix<MA> &A, DenseVector<VB> &B);
```

### Purpose

trs solves a triangular system of the form AX = B or  $A^TX = B$ , where A is a triangular matrix of order N, and B is an  $N \times R$  matrix. A check is made to verify that A is nonsingular.

### Arguments

| trans | (input)  |
|-------|--|
|       | Specifies the form of the system of equations:                             |
|       | trans = NoTrans $AX = B$ (No transpose)                                    |
|       | trans = Trans $A^T X = B$ (Transpose)                                      |
|       | trans = ConjTrans $A^H X = B$ (Conjugate transpose = Transpose)            |
| А     | (input)  |
|       | The (unit or non-unit) triangular matrix A.                                |
| В     | (input/output)   |
|       | On entry, the $N \times R$ matrix of right hand side matrix B. On exit, if |
|       | function returned 0, the $N \times R$ solution matrix X.                   |
|       |  |

### Returns

| i = 0 successful exit |
|-----------------------|
|-----------------------|

i > 0 then A(i, i) is zero, indicating that the matrix is singular and the solutions X have not been computed.

# qrf (geqrf)

compute a QR factorization of a real  $M\times N$  matrix A

### Synopsis

```
template <typename MA, typename VT>
    int
    qrf(GeMatrix<MA> &A, DenseVector<VT> &tau);
```

### Purpose

**qrf** computes a QR factorization of a real  $M \times N$  matrix A:

$$A = QR$$
.

### Arguments

| А   | (input/output)  |
|-----|---|
|     | On entry, the $M \times N$ matrix A. On exit, the elements on and above the   |
|     | diagonal of the array contain the $\min\{M, N\} \times N$ upper trapezoidal   |
|     | matrix R (R is upper triangular if $m \ge n$ ); the elements below the        |
|     | diagonal, with the array tau, represent the orthogonal matrix $Q$ as a        |
|     | product of $\min\{m, n\}$ elementary reflectors (see Further Details).        |
| tau | (output)  |
|     | The scalar factors $\tau$ of the elementary reflectors (see Further Details). |

### Returns

i = 0 successful exit

### Further Details

The matrix Q is represented as a product of elementary reflectors

$$Q = H_1 H_2 \cdots H_k, \text{ where } k = \min\{m, n\}.$$

Each  $H_i$  has the form

$$H_i = I - \tau * v * v'$$

where  $\tau$  is a real scalar, and v is a real vector with  $v_1 = \ldots v_{i-1} = 0$  and  $v_i = 1$ ;  $(v_{i+1}, \ldots, v_m)$  is stored on exit in A(i+1,i), ..., A(m,i) and  $\tau$  in tau(i).

# orgqr (orgqr)

generate an  $M \times N$  real matrix Q with orthonormal columns

### Synopsis

```
template <typename MA, typename VT>
    int
    orgqr(GeMatrix<MA> &A, const DenseVector<VT> &tau);
```

### Purpose

orgqr generates an  $M \times N$  real matrix Q with orthonormal columns, which is defined as the first N columns of a product of k elementary reflectors of order M

$$Q = H_1 H_2 \cdot \dots \cdot H_k$$

as returned by **qrf**.

### Arguments

| А   | (input/output)  |
|-----|---|
|     | On entry, the $i$ -th column must contain the vector which defines the      |
|     | elementary reflector $H_i$ , for $i = 1, 2,, k$ , as returned by qrf in the |
|     | first k columns of its matrix argument A. On exit, the $M \times N$ matrix  |
|     | Q.  |
| tau | (input)   |
|     | TAU(i) must contain the scalar factor of the elementary reflector $H_i$ ,   |
|     | as returned by qrf.   |
|     |   |

### Returns

# ormqr (ormqr)

### Synopsis

```
template <typename MA, typename VT, typename MC>
    int
    ormqr(BlasSide side, Transpose trans,
        const GeMatrix<MA> &A, const DenseVector<VT> &tau,
        GeMatrix<MC> &C);
```

## Purpose

ormqr overwrites the general real  $M \times N$  matrix C as follows:

$$C \leftarrow \begin{cases} QC & \text{if side=Left and trans=NoTrans} \\ Q^TC & \text{if side=Left and trans=Trans} \\ CQ & \text{if side=Right and trans=NoTrans} \\ CQ^T & \text{if side=Right and trans=Trans} \end{cases}$$

where Q is a real orthogonal matrix defined as the product of k elementary reflectors

$$Q = H_1 H_2 \cdot \dots \cdot H_k$$

as returned by qrf. Q is of order M if side=Left and of order N if side=Right.

### Arguments

| side  | (input)<br>side = Left apply $Q$ or $Q^T$ from left<br>side = Right apply $Q$ or $Q^T$ from right |
|-------|---|
| trans | (input)   |
|       | trans=NoTrans No transpose, apply $Q$   |
|       | trans=Trans Transpose, apply $Q^T$  |
| А     | (input)   |
|       | On entry, the <i>i</i> -th column must contain the vector which defines the                       |
|       | elementary reflector $H_i$ , for $i = 1, 2, \ldots, k$ , as returned by <b>qrf</b> in the         |
|       | first $k$ columns of its matrix argument $A$ . $A$ is modified by the routine                     |
|       | but restored on exit.   |
| tau   | (input)   |
|       | TAU(i) must contain the scalar factor of the elementary reflector $H_i$ ,                         |
|       | as returned by qrf.   |
| С     | (input/output)  |
|       | On entry, the $M \times N$ matrix C.  |
|       | On exit, C is overwritten by $QC$ or $Q^TC$ or $CQ^T$ or $CQ$ .                                   |
|       |   |

# Returns

### ls (gels)

solve overdetermined or under determined real linear systems involving an  $M\times N$  matrix A, or its transpose, using a QR or LQ factorization of A

## Synopsis

template <typename MA, typename MB>
 int
 ls(Transpose trans, GeMatrix<MA> &A, GeMatrix<MB> &B);

### Purpose

Is solves overdetermined or underdetermined real linear systems involving an  $M \times N$  matrix A, or its transpose, using a QR or LQ factorization of A. It is assumed that A has full rank. The following options are provided:

1. If trans = NoTrans and  $M \ge N$ : find the least squares solution of an overdetermined system, i. e. , solve the least squares problem

$$||B - AX|| \to \min.$$

- 2. If trans = NoTrans and M < N: find the minimum norm solution of an underdetermined system AX = B.
- 3. If trans = Trans and  $M \ge N$ : find the minimum norm solution of an undetermined system  $A^T X = B$ .
- 4. If trans = Trans and M < N: find the least squares solution of an overdetermined system, i.e., solve the least squares problem

$$||B - A^T * X|| \to \min.$$

Several right hand side vectors b and solution vectors x can be handled in a single call; they are stored as the columns of the  $M \times R$  right hand side matrix B and the  $N \times R$  solution matrix X.

### Arguments

| trans | (input)   |
|-------|---|
|       | trans = NoTrans the linear system involves $A$ ;                              |
|       | trans = Trans the linear system involves $A^T$ .                              |
| А     | (input/output)  |
|       | On entry, the $M \times N$ matrix A. On exit, if $M \ge N$ , A is overwritten |
|       | by details of its $QR$ factorization as returned by qrf; if $M < N$ , A is    |
|       | overwritten by details of its $LQ$ factorization as returned by lqf.          |

#### (input/output)

On entry, the matrix B of right hand side vectors, stored column-wise; B is  $M \times R$  if trans=NoTrans, or  $N \times R$  if trans=Trans.

On exit, B is overwritten by the solution vectors, stored column-wise:

- 1. if trans=NoTrans and  $M \ge N$ , rows 1 to N of B contain the least squares solution vectors; the residual sum of squares for the solution in each column is given by the sum of squares of elements N + 1 to M in that column;
- 2. if trans=NoTrans and M < N, rows 1 to N of B contain the minimum norm solution vectors;
- 3. if trans=Trans and  $M \ge N$ , rows 1 to M of B contain the minimum norm solution vectors;
- 4. if trans=Trans and M < N, rows 1 to M of B contain the least squares solution vectors; the residual sum of squares for the solution in each column is given by the sum of squares of elements M + 1 to N in that column.

#### Returns

### lss (gelss)

compute the minimum norm solution to a real linear least squares problem using a singular value decomposition (SVD)

### Synopsis

```
template <typename MA, typename MB>
    int
    lss(GeMatrix<MA> &A, GeMatrix<MB> &B);
```

### Purpose

lss computes the minimum norm solution to a real linear least squares problem:

$$||b - Ax||_2 \to \min$$

using the singular value decomposition (SVD) of A. A is an  $M \times N$  matrix which may be rank-deficient.

Several right hand side vectors b and solution vectors x can be handled in a single call; they are stored as the columns of the  $M \times R$  right hand side matrix B and the  $N \times R$  solution matrix X.

The effective rank of A is determined by treating as zero those singular values which are less than RCOND times the largest singular value.

## Arguments

| А | (input/output)  |
|---|---|
|   | On entry, the $M \times N$ matrix A. On exit, the first min $\{m, n\}$ rows of A              |
|   | are overwritten with its right singular vectors, stored row-wise.                             |
| В | (input/output)  |
|   | On entry, the $M \times R$ right hand side matrix $B$ .                                       |
|   | On exit, B is overwritten by the $N \times R$ solution matrix X. If $M \ge N$                 |
|   | and $\operatorname{rank}(A) = N$ , the residual sum-of-squares for the solution in the        |
|   | <i>i</i> -th column is given by the sum of squares of elements $B_{N+1,i}, \ldots, B_{M,i}$ . |

### Returns

| i = 0 | successful exit   |
|-------|---|
| i > 0 | the algorithm for computing the SVD failed to converge; more precise-     |
|       | ly, $i$ off-diagonal elements of an intermediate bi-diagonal form did not |
|       | converge to zero.   |

## To-do

- 1. Provide a version of lss for a single right-hand side, i. e. handle the case where B would be a  $M \times 1$  matrix (as was done for sv).
- 2. In this form the wrapper for gelss suppresses some of the output computed by its underlying LAPACK routine (e.g. the singular values).

### ev (geev,real)

compute for an  $N \times N$  real non-symmetric matrix A, the eigenvalues and, optionally, the left and/or right eigenvectors

### Synopsis

```
template <typename MA, typename WR, typename WI, typename VL, typename VR>
    int
    ev(bool leftEV, bool rightEV,
        GeMatrix<MA> &A, DenseVector<WR> &wr, DenseVector<WI> &wi,
        GeMatrix<VL> &vl, GeMatrix<VR> &vr);
```

### Purpose

ev computes for an  $N \times N$  real non-symmetric matrix A, the eigenvalues and, optionally, the left and/or right eigenvectors. The right eigenvector  $v_j$  of A satisfies

$$Av_j = \lambda_j v_j$$

where  $\lambda_j$  is its eigenvalue.

The left eigenvector  $u_j$  of A satisfies

$$u_j^H A = \lambda_j u_j^H$$

where  $u_j^H$  denotes the conjugate transpose of  $u_j$ .

The computed eigenvectors are normalized to have Euclidean norm equal to 1 and largest component real.

#### Arguments

| leftEV  | (input)  |
|---------|--|
|         | specifies whether left eigenvectors of $A$ are computed.             |
| rightEV | (input)  |
|         | specifies whether right eigenvectors of $A$ are computed.            |
| А       | (input/output)   |
|         | On entry, the $N \times N$ matrix A.                                 |
|         | On exit, $A$ has been overwritten.                                   |
| wr,wi   | (output)   |
|         | wr and wi contain the real and imaginary parts, respectively, of the |
|         | computed eigenvalues. Complex conjugate pairs of eigenvalues appear  |
|         | consecutively with the eigenvalue having the positive imaginary part |
|         | first.   |
| vl      | (output)   |

If leftEV=true, the left eigenvectors  $u_j$  are stored one after another in the columns of vl, in the same order as their eigenvalues. If leftEV=false, then vl is not referenced.

If the *j*-th eigenvalue is real, then  $u_j$  is stored in the *j*-th column of vl. If the *j*-th and (j + 1)-th eigenvalues form a complex conjugate pair, then

$$u_j = vl(_,j) + i * vl(_,j+1)$$

and

$$u_{j+1} = vl(_,j) - i * vl(_,j+1)$$

(output)

If rightEV=true, the left eigenvectors  $u_j$  are stored one after another in the columns of vr, in the same order as their eigenvalues. If rightEV=false, then vr is not referenced.

If the *j*-th eigenvalue is real, then  $u_j$  is stored in the *j*-th column of vr. If the *j*-th and (j + 1)-th eigenvalues form a complex conjugate pair, then

$$u_j = vr(,j) + i * vr(,j+1)$$

and

$$u_{j+1} = vr(,j) - i * vr(,j+1)$$

#### Returns

vr

- i = 0 successful exit
- i > 0 the QR algorithm failed to compute all the eigenvalues, and no eigenvectors have been computed; elements i + 1 to N of wr and wi contain eigenvalues which have converged.

### ev (geev,complex)

compute for an  $N \times N$  complex non-symmetric matrix A, the eigenvalues and, optionally, the left and/or right eigenvectors

### Synopsis

template <typename MA, typename W, typename VL, typename VR>
 int
 ev(bool leftEv, bool rightEv,
 GeMatrix<MA> &A, DenseVector<W> &w, GeMatrix<VL> &vl, GeMatrix<VR> &vr);

### Purpose

ev computes for an  $N \times N$  complex non-symmetric matrix A, the eigenvalues and, optionally, the left and/or right eigenvectors. The right eigenvector  $v_j$  of A satisfies

$$Av_j = \lambda_j v_j$$

where  $\lambda_j$  is its eigenvalue.

The left eigenvector  $u_j$  of A satisfies

$$u_j^H A = \lambda_j u_j^H$$

where  $u_j^H$  denotes the conjugate transpose of  $u_j$ .

The computed eigenvectors are normalized to have Euclidean norm equal to 1 and largest component real.

### Arguments

| leftEV  | (input)  |
|---------|--|
|         | specifies whether left eigenvectors of $A$ are computed.                 |
| rightEV | (input)  |
|         | specifies whether right eigenvectors of $A$ are computed.                |
| А       | (input/output)   |
|         | On entry, the $N \times N$ matrix $A$ .                                  |
|         | On exit, $A$ has been overwritten.                                       |
| W       | (output)   |
|         | contains the computed eigenvalues.                                       |
| vl      | (output)   |
|         | If leftEV=true, the left eigenvectors $u_j$ are stored one after ano-    |
|         | ther in the columns of $vl$ , in the same order as their eigenvalues. If |
|         | leftEV=false, then vl is not referenced.                                 |
| vr      | (output)   |
|         | If rightEV=true, the left eigenvectors $u_j$ are stored one after ano-   |
|         | ther in the columns of vr, in the same order as their eigenvalues. If    |
|         | rightEV=false, then vr is not referenced.                                |

# Returns

i > 0 the QR algorithm failed to compute all the eigenvalues, and no eigenvectors have been computed; elements i + 1 to N of wr and wi contain eigenvalues which have converged.

# ev (syev)

compute all eigenvalues and, optionally, eigenvectors of a real symmetric matrix  ${\cal A}$ 

## Synopsis

```
template <typename MA, typename VW>
    int
    ev(bool compEV, SyMatrix<MA> &A, DenseVector<VW> &w);
```

## Purpose

 $\operatorname{ev}$  computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix A.

## Arguments

| compEV | (input)   |
|--------|---|
|        | specifies whether eigenvectors of $A$ are computed.                     |
| А      | (input/output)  |
|        | On entry, the symmetric matrix $A$ .                                    |
|        | On successful exit and if compEV=true, then the underlying full storage |
|        | scheme of $A$ contains the orthonormal eigenvectors of the matrix $A$ . |
|        | If compEV=false, then on exit the referenced triangle of the underlying |
|        | full storage scheme is destroyed.                                       |
| W      | (output)  |
|        | On successful exit, the eigenvalues in ascending order.                 |

### Returns

| i = 0 | successful exit  |
|-------|--|
| i > 0 | the algorithm failed to converge; $i$ off-diagonal elements of an interme- |
|       | diate tridiagonal form did not converge to zero.                           |

# ev (sbev)

compute all the eigenvalues and, optionally, eigenvectors of a real symmetric band matrix  ${\cal A}$ 

## Synopsis

```
template <typename MA, typename VW, typename MZ>
    int
    ev(bool compEV, SbMatrix<MA> &A, DenseVector<VW> &w, GeMatrix<MZ> &Z);
```

## Purpose

ev computes all the eigenvalues and, optionally, eigenvectors of a real symmetric band matrix A.

## Arguments

| compEV | (input)  |
|--------|--|
|        | specifies whether eigenvectors of $A$ are computed.                              |
| А      | (input/output)   |
|        | On entry, the symmetric band matrix $A$ .  |
|        | On exit, $A$ is overwritten by values generated during the reduction to          |
|        | tridiagonal form.  |
| W      | (output)   |
|        | On successful exit, the eigenvalues in ascending order.                          |
| Z      | If $compEV=true$ , then on successful exit, Z contains the                       |
|        | orthonormal eigenvectors of the matrix $A$ , with the <i>i</i> -th column of $Z$ |
|        | holding the eigenvector associated with $w(i)$ .                                 |
|        | If $compEV=false$ , then Z is not referenced.                                    |

### Returns

| i | = 0 | successful exit  |  |
|---|-----|------------------|--|
|   | ~   | Saccossiai ollic |  |

i > 0 the algorithm failed to converge; *i* off-diagonal elements of an intermediate tridiagonal form did not converge to zero.

# ev (spev)

compute all the eigenvalues and, optionally, eigenvectors of a real symmetric matrix in packed storage

## Synopsis

```
template <typename MA, typename VW, typename MZ>
    int
    ev(bool compEV, SpMatrix<MA> &A, DenseVector<VW> &w, GeMatrix<MZ> &Z);
```

## Purpose

ev computes all the eigenvalues and, optionally, eigenvectors of a real symmetric matrix in packed storage.

## Arguments

| compEV | (input)  |
|--------|--|
|        | specifies whether eigenvectors of $A$ are computed.                              |
| А      | (input/output)   |
|        | On entry, the symmetric matrix $A$ in packed storage format.                     |
|        | On exit, $A$ is overwritten by values generated during the reduction to          |
|        | tridiagonal form.  |
| W      | (output)   |
|        | On successful exit, the eigenvalues in ascending order.                          |
| Z      | If $compEV=true$ , then on successful exit, Z contains the                       |
|        | orthonormal eigenvectors of the matrix $A$ , with the <i>i</i> -th column of $Z$ |
|        | holding the eigenvector associated with $w(i)$ .                                 |
|        | If $compEV=false$ , then Z is not referenced.                                    |

### Returns

| i | = 0 | successful exit  |  |
|---|-----|------------------|--|
|   | ~   | Saccossiai ollic |  |

i > 0 the algorithm failed to converge; *i* off-diagonal elements of an intermediate tridiagonal form did not converge to zero.

# ev (heev)

compute all eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix  ${\cal A}$ 

# Synopsis

```
template <typename MA, typename VW>
    int
    ev(bool compEV, HeMatrix<MA> &A, DenseVector<VW> &w);
```

## Purpose

 $\operatorname{ev}$  computes all eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix A.

## Arguments

| compEV | (input)   |
|--------|---|
|        | specifies whether eigenvectors of $A$ are computed.                   |
| А      | (input/output)  |
|        | On entry, the Hermitian matrix A.                                     |
|        | On successful exit and if $compEV=true$ , A contains the orthonormal  |
|        | eigenvectors of the matrix A. If compEV=false, then on exit the refe- |
|        | renced triangle of the underlying full storage scheme is destroyed.   |
| W      | (output)  |
|        | On successful exit, the eigenvalues in ascending order.               |

### Returns

| i = 0 | successful exit  |
|-------|--|
| i > 0 | the algorithm failed to converge; $i$ off-diagonal elements of an interme- |
|       | diate tridiagonal form did not converge to zero.                           |

## ev (hbev)

compute all the eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix  ${\cal A}$ 

## Synopsis

```
template <typename MA, typename VW, typename MZ>
    int
    ev(bool compEV, HbMatrix<MA> &A, DenseVector<VW> &w, GeMatrix<MZ> &Z);
```

# Purpose

ev computes all the eigenvalues and, optionally, eigenvectors of a complex Hermitian band matrix A.

### Arguments

| compEV | (input)  |
|--------|--|
|        | specifies whether eigenvectors of $A$ are computed.                              |
| А      | (input/output)   |
|        | On entry, the Hermitian band matrix $A$ .  |
|        | On exit, $A$ is overwritten by values generated during the reduction to          |
|        | tridiagonal form.  |
| W      | (output)   |
|        | On successful exit, the eigenvalues in ascending order.                          |
| Z      | If $compEV=true$ , then on successful exit, Z contains the                       |
|        | orthonormal eigenvectors of the matrix $A$ , with the <i>i</i> -th column of $Z$ |
|        | holding the eigenvector associated with $w(i)$ .                                 |
|        | If $compEV=false$ , then Z is not referenced.                                    |

### Returns

| i | = 0 | successful exit  |  |
|---|-----|------------------|--|
|   | ~   | Saccossiai ollic |  |

i > 0 the algorithm failed to converge; *i* off-diagonal elements of an intermediate tridiagonal form did not converge to zero.

# ev (hpev)

compute all the eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix in packed storage

# Synopsis

```
template <typename MA, typename VW, typename MZ>
    int
    ev(bool compEV, HpMatrix<MA> &A, DenseVector<VW> &w, GeMatrix<MZ> &Z);
```

# Purpose

ev computes all the eigenvalues and, optionally, eigenvectors of a complex Hermitian matrix in packed storage.

## Arguments

| compEV | (input)  |
|--------|--|
|        | specifies whether eigenvectors of $A$ are computed.                              |
| А      | (input/output)   |
|        | On entry, the Hermitian matrix $A$ in packed storage format.                     |
|        | On exit, $A$ is overwritten by values generated during the reduction to          |
|        | tridiagonal form.  |
| W      | (output)   |
|        | On successful exit, the eigenvalues in ascending order.                          |
| Z      | If $compEV=true$ , then on successful exit, Z contains the                       |
|        | orthonormal eigenvectors of the matrix $A$ , with the <i>i</i> -th column of $Z$ |
|        | holding the eigenvector associated with $w(i)$ .                                 |
|        | If $compEV=false$ , then Z is not referenced.                                    |

## Returns

| i | = 0 | successful | $\operatorname{exit}$ |
|---|-----|------------|-----------------------|
|   | *   |            |                       |

i > 0 the algorithm failed to converge; *i* off-diagonal elements of an intermediate tridiagonal form did not converge to zero.

# svd (gesvd)

compute the singular value decomposition (SVD) of a complex or real  $M \times N$  matrix A, optionally computing the left and/or right singular vectors

### Synopsis

```
template <typename MA, typename VS, typename VU, typename VVT>
    int
    svd(SVectorsJob jobu, SVectorsJob jobvt, GeMatrix<MA> &A,
        DenseVector<VS> &S, GeMatrix<VU> &U, GeMatrix<VVT> &VT);
/* calls: svd(All,All,A,s,U,V) */
template <typename MA, typename VS, typename MU, typename MV>
    int
    svd(GeMatrix<MA> &A, DenseVector<VS> &s, GeMatrix<MU> &U, GeMatrix<MV> &VT);
```

## Purpose

svd computes the singular value decomposition (SVD) of a real (or complex)  $M \times N$  matrix A, optionally computing the left and/or right singular vectors. The SVD is written

$$A = U\Sigma V^T \quad (\text{or } A = U\Sigma V^H)$$

where  $\Sigma$  is an  $M \times N$  matrix which is zero except for its min $\{m, n\}$  diagonal elements, U is an  $M \times N$  orthogonal (or unitary) matrix, and V is an  $N \times N$ orthogonal (or unitary) matrix. The diagonal elements of  $\Sigma$  are the singular values of A; they are real and non-negative, and are returned in descending order. The first min $\{m, n\}$  columns of U and V are the left and right singular vectors of A. **Note** that the routine returns  $V^T$  (or  $V^H$ ), not V.

### Arguments

| jobu Specifies options for computing all or part of the matrix |                         | omputing all or part of the matrix $U$ :              |
|--|-------------------------|---|
| -  | jobu = All              | all $M$ columns of $U$ are returned in matrix $U$     |
|  | jobu = SmallDim         | the first $\min\{m, n\}$ columns of U (the left sin-  |
|  |                         | gular vectors) are returned in the matrix U           |
|  | jobu = Overwrite        | the first $\min\{m, n\}$ columns of U (the left sin-  |
|  |                         | gular vectors) are overwritten on the matrix A        |
|  | jobu = None             | no columns of $U$ (no left singular vectors) are      |
|  |                         | computed  |
| jobvt  | Specifies options for c | omputing all or part of the matrix $V^T$ (or $V^H$ ): |

|    | jobu = All  | all N rows of $V^T$ (or $V^H$ ) are returned in matrix  |
|----|---|---|
|    | U   | VT  |
|    | jobu = SmallDim   | the first $\min\{m, n\}$ rows of $V^T$ (or $V^H$ ) (the right singular vectors) are returned in the matrix VT   |
|    | jobu = Overwrite  | the first $\min\{m, n\}$ rows of $V^T$ (or $V^H$ ) (the right singular vectors) are overwritten on the matrix <b>A</b>  |
|    | jobu = None   | no rows of $V^T$ (or $V^H$ ) (no right singular vectors) are computed   |
|    | Note: jobu and jobu   | t can not both be set to be Overwrite.  |
| А  | (input/output)  |   |
|    | On entry, the $M \times N$                                  |   |
|    |   | Overwrite, $A$ is overwritten with the first  |
|    |   | f $U$ (the left singular vectors, stored columnwise);   |
|    | of $V^T$ (or $V^H$ ) (the r                                 | e, A is overwritten with the first $\min\{m, n\}$ rows<br>ight singular vectors, stored rowwise); if jobu $\neq$  |
| S  | (output)  | $\neq$ <b>Overwrite</b> , the contents of A are destroyed.  |
| 0  | ( - )   | f A, sorted so that $S(i) \ge S(i+1)$ .   |
| U  | (output)  | $\sum_{i=1}^{n} \sum_{i=1}^{n} \sum_{i$ |
| -  | ( - )   | tains the $M \times M$ orthogonal (or unitary) matrix   |
|    | <b>C</b>  | im, U contains the first $\min\{m, n\}$ columns of U  |
|    | (the left singular vect                                     | ors, stored columnwise); if jobu = None, then U   |
|    | is not referenced.  |   |
| VT | (output)  |   |
|    | $V^T$ (or $V^H$ ); if jobu =<br>of $V^T$ (or $V^H$ ) (the r | ontains the $N \times N$ orthogonal (or unitary) matrix<br>= SmallDim, VT contains the first min $\{m, n\}$ rows<br>ight singular vectors, stored rowwise); if jobu =   |
|    | None, then VT is not r                                      | ciciciiteu.   |

### Returns

- i = 0 successful exit
- i > 0 the algorithm failed to converge; *i* specifies how many superdiagonals of an intermediate bidiagonal form *B* did not converge to zero.