

NAG Toolbox for MATLAB

f04be

1 Purpose

f04be computes the solution to a real system of linear equations $AX = B$, where A is an n by n symmetric positive-definite matrix, stored in packed format, and X and B are n by r matrices. An estimate of the condition number of A and an error bound for the computed solution are also returned.

2 Syntax

```
[ap, b, rcond, errbnd, ifail] = f04be(uplo, ap, b, 'n', n, 'nrhs_p',
nrhs_p)
```

3 Description

The Cholesky factorization is used to factor A as $A = U^T U$, if **uplo** = 'U', or $A = LL^T$, if **uplo** = 'L', where U is an upper triangular matrix and L is a lower triangular matrix. The factored form of A is then used to solve the system of equations $AX = B$.

4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D 1999 *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia URL: <http://www.netlib.org/lapack/lug>

Higham N J 2002 *Accuracy and Stability of Numerical Algorithms* (2nd Edition) SIAM, Philadelphia

5 Parameters

5.1 Compulsory Input Parameters

1: **uplo** – string

If **uplo** = 'U', the upper triangle of the matrix A is stored.

If **uplo** = 'L', the lower triangle of the matrix A is stored.

Constraint: **uplo** = 'U' or 'L'.

2: **ap**(*) – double array

Note: the dimension of the array **ap** must be at least $\max(1, n \times (n + 1)/2)$.

The n by n symmetric matrix A . The upper or lower triangular part of the symmetric matrix is packed column-wise in a linear array. The j th column of A is stored in the array **ap** as follows:

if **uplo** = 'U', $\mathbf{ap}(i + (j - 1)j/2) = a_{ij}$ for $1 \leq i \leq j$;
if **uplo** = 'L', $\mathbf{ap}(i + (j - 1)(2n - j)/2) = a_{ij}$ for $j \leq i \leq n$.

See Section 8 below for further details.

3: **b(ldb,*)** – double array

The first dimension of the array **b** must be at least $\max(1, n)$

The second dimension of the array must be at least $\max(1, \mathbf{nrhs_p})$. To solve the equations $Ax = b$, where b is a single right-hand side, **b** may be supplied as a one-dimensional array with length **ldb** = $\max(1, n)$

The n by r matrix of right-hand sides B .

5.2 Optional Input Parameters

1: **n** – int32 scalar

The number of linear equations n , i.e., the order of the matrix A .

Constraint: $n \geq 0$.

2: **nrhs_p** – int32 scalar

Default: The second dimension of the array **b**.

The number of right-hand sides r , i.e., the number of columns of the matrix B .

Constraint: **nrhs_p** ≥ 0 .

5.3 Input Parameters Omitted from the MATLAB Interface

ldb

5.4 Output Parameters

1: **ap**(*) – double array

Note: the dimension of the array **ap** must be at least $\max(1, n \times (n + 1)/2)$.

If **ifail** = 0 or $Np1$, the factor U or L from the Cholesky factorization $A = U^T U$ or $A = LL^T$, in the same storage format as A .

2: **b**(ldb,*) – double array

The first dimension of the array **b** must be at least $\max(1, n)$

The second dimension of the array must be at least $\max(1, \mathbf{nrhs_p})$. To solve the equations $Ax = b$, where b is a single right-hand side, **b** may be supplied as a one-dimensional array with length **ldb** = $\max(1, n)$

If **ifail** = 0 or $Np1$, the n by r solution matrix X .

3: **rcond** – double scalar

If **ifail** = 0 or $Np1$, an estimate of the reciprocal of the condition number of the matrix A , computed as $\mathbf{rcond} = 1 / (\|A\|_1 \|A^{-1}\|_1)$.

4: **errbnd** – double scalar

If **ifail** = 0 or $Np1$, an estimate of the forward error bound for a computed solution \hat{x} , such that $\|\hat{x} - x\|_1 / \|x\|_1 \leq \mathbf{errbnd}$, where \hat{x} is a column of the computed solution returned in the array **b** and x is the corresponding column of the exact solution X . If **rcond** is less than *machine precision*, then **errbnd** is returned as unity.

5: **ifail** – int32 scalar

0 unless the function detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail < 0 and **ifail** \neq -999

If **ifail** = $-i$, the i th argument had an illegal value.

ifail = -999

Allocation of memory failed. The integer allocatable memory required is **n**, and the double allocatable memory required is $3 \times \mathbf{n}$. Allocation failed before the solution could be computed.

ifail > 0 and **ifail** ≤ *N*

If **ifail** = *i*, the leading minor of order *i* of *A* is not positive-definite. The factorization could not be completed, and the solution has not been computed.

ifail = *N* + 1

rcond is less than *machine precision*, so that the matrix *A* is numerically singular. A solution to the equations $AX = B$ has nevertheless been computed.

7 Accuracy

The computed solution for a single right-hand side, \hat{x} , satisfies an equation of the form

$$(A + E)\hat{x} = b,$$

where

$$\|E\|_1 = O(\epsilon)\|A\|_1$$

and ϵ is the *machine precision*. An approximate error bound for the computed solution is given by

$$\frac{\|\hat{x} - x\|_1}{\|x\|_1} \leq \kappa(A) \frac{\|E\|_1}{\|A\|_1},$$

where $\kappa(A) = \|A^{-1}\|_1 \|A\|_1$, the condition number of *A* with respect to the solution of the linear equations. f04be uses the approximation $\|E\|_1 = \epsilon \|A\|_1$ to estimate **errbnd**. See Section 4.4 of Anderson *et al.* 1999 for further details.

8 Further Comments

The packed storage scheme is illustrated by the following example when $n = 4$ and **uplo** = 'U'. Two-dimensional storage of the symmetric matrix *A*:

$$\begin{array}{cccc} a_{11} & a_{12} & a_{13} & a_{14} \\ & a_{22} & a_{23} & a_{24} \\ & & a_{33} & a_{34} \\ & & & a_{44} \end{array} \quad (a_{ij} = a_{ji})$$

Packed storage of the upper triangle of *A*:

$$\mathbf{ap} = [a_{11}, a_{12}, a_{22}, a_{13}, a_{23}, a_{33}, a_{14}, a_{24}, a_{34}, a_{44}]$$

The total number of floating-point operations required to solve the equations $AX = B$ is proportional to $(\frac{1}{3}n^3 + n^2r)$. The condition number estimation typically requires between four and five solves and never more than eleven solves, following the factorization.

In practice the condition number estimator is very reliable, but it can underestimate the true condition number; see Section 15.3 of Higham 2002 for further details.

The complex analogue of f04be is f04ce.

9 Example

```
uplo = 'U';
ap = [4.16;
      -3.12;
       5.03;
```

```
0.56000000000000001;  
-0.83;  
0.76;  
-0.1;  
1.18;  
0.34;  
1.18];  
b = [8.699999999999999, 8.300000000000001;  
-13.35, 2.13;  
1.89, 1.61;  
-4.14, 5];  
[apOut, bOut, rcond, errbnd, ifail] = f04be(uplo, ap, b)
```

```
apOut =  
2.0396  
-1.5297  
1.6401  
0.2746  
-0.2500  
0.7887  
-0.0490  
0.6737  
0.6617  
0.5347  
bOut =  
1.0000    4.0000  
-1.0000    3.0000  
2.0000    2.0000  
-3.0000    1.0000  
rcond =  
0.0103  
errbnd =  
1.0816e-14  
ifail =  
0
```