NAG Toolbox for MATLAB

f04bf

1 Purpose

f04bf computes the solution to a real system of linear equations $AX = B$, where A is an n by n symmetric positive-definite band matrix of band width $2k + 1$, 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

```
[ab, b, rcond, errbnd, ifail] = f04bf(uplo, kd, ab, 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 band matrix with k superdiagonals, and L is a lower triangular band matrix with k subdiagonals. 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: **kd – int32 scalar**

The number of superdiagonals k (and the number of subdiagonals) of the band matrix A.

Constraint: **kd** ≥ 0.

3: **ab(ldab,*) – double array**

The first dimension of the array **ab** must be at least **kd** $+ 1$

The second dimension of the array must be at least $\max(1, \mathbf{n})$

The n by n symmetric band matrix A. The upper or lower triangular part of the symmetric matrix is stored in the first **kd** $+ 1$ rows of the array. The jth column of A is stored in the jth column of the array **ab** as follows:

if **uplo** = 'U', $\mathbf{ab}(k + 1 + i - j, j) = a_{ij}$ for $\max(1, j - k) \leq i \leq j$;
if **uplo** = 'L', $\mathbf{ab}(1 + i - j, j) = a_{ij}$ for $j \leq i \leq \min(n, j + k)$.

See Section 8 below for further details.

4: **b(ldb,*) – double array**

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

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 $\mathbf{ldb} = \max(1, \mathbf{n})$

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

5.2 Optional Input Parameters

1: **n – int32 scalar**

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

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

Constraint: $\mathbf{n} \geq 0$.

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: $\mathbf{nrhs\_p} \geq 0$.

5.3 Input Parameters Omitted from the MATLAB Interface

ldab, ldb

5.4 Output Parameters

1: **ab(ldab,*) – double array**

The first dimension of the array **ab** must be at least $\mathbf{kd} + 1$

The second dimension of the array must be at least $\max(1, \mathbf{n})$

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

2: **b(ldb,*) – double array**

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

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 $\mathbf{ldb} = \max(1, \mathbf{n})$

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 $\mathbf{rcond} = 1/\left(\|A\|_1 \|A^{-1}\|_1\right)$.

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 ith 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 $3 \times$ **n**. Allocation failed before the solution could be computed.

ifail > 0 and **ifail** $\leq N$

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 $\kappa(A) = \left\|A^{-1}\right\|_1 \|A\|_1$, the condition number of A with respect to the solution of the linear equations. f04bf 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 band storage scheme for the array **ab** is illustrated by the following example, when $n = 6$, $k = 2$, and **uplo** = 'U':

On entry:

$$\begin{array}{cccccc} * & * & a_{13} & a_{24} & a_{35} & a_{46} \\ * & a_{12} & a_{23} & a_{34} & a_{45} & a_{56} \\ a_{11} & a_{22} & a_{33} & a_{44} & a_{55} & a_{66} \end{array}$$

On exit:

$$\begin{array}{cccccc} * & * & u_{13} & u_{24} & u_{35} & u_{46} \\ * & u_{12} & u_{23} & u_{34} & u_{45} & u_{56} \\ u_{11} & u_{22} & u_{33} & u_{44} & u_{55} & u_{66} \end{array}$$

Similarly, if **uplo** = 'L' the format of **ab** is as follows:

On entry:

$$\begin{array}{cccccc} a_{11} & a_{22} & a_{33} & a_{44} & a_{55} & a_{66} \\ a_{21} & a_{32} & a_{43} & a_{54} & a_{65} & * \\ a_{31} & a_{42} & a_{53} & a_{64} & * & * \end{array}$$

On exit:

$$\begin{array}{cccccc} l_{11} & l_{22} & l_{33} & l_{44} & l_{55} & l_{66} \\ l_{21} & l_{32} & l_{43} & l_{54} & l_{65} & * \\ l_{31} & l_{42} & l_{53} & l_{64} & * & * \end{array}$$

Array elements marked $*$ need not be set and are not referenced by the function.

Assuming that $n \gg k$, the total number of floating-point operations required to solve the equations $AX = B$ is approximately $n(k+1)^2$ for the factorization and $4nkr$ for the solution following the factorization. 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 f04bf is f04cf.

9 Example

```
uplo = 'U';
kd = int32(1);
ab = [5.495816452771857e+222, 2.68, -2.39, -2.22;
     5.49, 5.63, 2.6, 5.17];
b = [22.09, 5.1;
     9.31, 30.81;
     -5.24, -25.82;
     11.83, 22.9];
[abOut, bOut, rcond, errbnd, ifail] = f04bf(uplo, kd, ab, b)
```

```
abOut =
  1.0e+222 *
    5.4958    0.0000   -0.0000   -0.0000
    0.0000    0.0000    0.0000    0.0000
bOut =
    5.0000   -2.0000
   -2.0000    6.0000
   -3.0000   -1.0000
    1.0000    4.0000
rcond =
    0.0135
errbnd =
   8.2406e-15
ifail =
           0
```