NAG Toolbox for MATLAB

f04bd

1 Purpose

f04bd computes the solution to a real system of linear equations AX = B, where A is an n by n symmetric positive-definite matrix 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

```
[a, b, rcond, errbnd, ifail] = f04bd(uplo, a, b, 'n', n, 'nrhs_p', nrhs_p)
```

3 Description

The Cholesky factorization is used to factor A as $A = U^{\mathrm{T}}U$, if **uplo** = 'U', or $A = LL^{\mathrm{T}}$, 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 $\mathbf{uplo} = 'L'$, the lower triangle of the matrix A is stored.

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

2: a(lda,*) - double array

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

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

The n by n symmetric matrix A.

If $\mathbf{uplo} = 'U'$, the leading \mathbf{n} by \mathbf{n} upper triangular part of \mathbf{a} contains the upper triangular part of the matrix A, and the strictly lower triangular part of \mathbf{a} is not referenced.

If $\mathbf{uplo} = 'L'$, the leading \mathbf{n} by \mathbf{n} lower triangular part of \mathbf{a} contains the lower triangular part of the matrix A, and the strictly upper triangular part of \mathbf{a} is not referenced.

3: 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, \mathbf{b} may be supplied as a one-dimensional array with length $\mathbf{ldb} = \max(1, \mathbf{n})$

[NP3663/21] f04bd.1

f04bd NAG Toolbox Manual

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 a.

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: $\mathbf{nrhs}_{\mathbf{p}} \geq 0$.

5.3 Input Parameters Omitted from the MATLAB Interface

lda, ldb

5.4 Output Parameters

1: a(lda,*) - double array

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

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 $A = U^{T}U$ or $A = LL^{T}$.

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 $\max(1, \mathbf{nrhs}_{\mathbf{p}})$. To solve the equations Ax = b, where b is a single right-hand side, \mathbf{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 $\mathbf{rcond} = 1/(\|A\|_1 \|A^{-1}\|_1)$.

4: errbnd – double scalar

If **ifail** = 0 or Np1, an estimate of the forward error bound for a computed solution \hat{x} , such that $\|\hat{x} - x\|_1 / \|x\|_1 \le \text{errbnd}$, 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 **roond** 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).

f04bd.2 [NP3663/21]

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 \mathbf{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

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

where $\kappa(A) = \|A^{-1}\|_1 \|A\|_1$, the condition number of A with respect to the solution of the linear equations. f04bd 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 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 f04bd is f04cd.

9 Example

[NP3663/21] f04bd.3

f04bd NAG Toolbox Manual

```
1.89, 1.61;
-4.14, 5];
[aOut, bOut, rcond, errbnd, ifail] = f04bd(uplo, a, b)
aOut =
               -1.5297 0.2746 -0.0490
1.6401 -0.2500 0.6737
0 0.7887 0.6617
             -1.5297
1.6401
    2.0396
          0
          0
                   0
                              0 0.5347
bOut =
              4.0000
    1.0000
   -1.0000
               3.0000
    2.0000 2.0000
   -3.0000 1.0000
rcond =
    0.0103
errbnd =
   1.0816e-14
ifail =
            0
```

f04bd.4 (last) [NP3663/21]