NAG Toolbox for MATLAB

f01ab

1 Purpose

f01ab calculates the accurate inverse of a real symmetric positive-definite matrix, using a Cholesky factorization and iterative refinement.

2 Syntax

```
[a, b, ifail] = f01ab(a, 'n', n)
```

3 Description

To compute the inverse X of a real symmetric positive-definite matrix A, f01ab first computes a Cholesky factorization of A as $A = LL^{\mathrm{T}}$, where L is lower triangular. An approximation to X is found by computing L^{-1} and then the product $L^{-\mathrm{T}}L^{-1}$. The residual matrix $R = I - AX$ is calculated using ***additional precision***, and a correction D to X is found by solving $LL^{\mathrm{T}}D = R$. X is replaced by $X + D$, and this iterative refinement of the inverse is repeated until full machine accuracy has been obtained.

4 References

Wilkinson J H and Reinsch C 1971 *Handbook for Automatic Computation II, Linear Algebra* Springer–Verlag

5 Parameters

5.1 Compulsory Input Parameters

1: **a(lda,n) – double array**

lda, the first dimension of the array, must be at least $\mathbf{n} + 1$.

The upper triangle of the n by n positive-definite symmetric matrix A. The elements of the array below the diagonal need not be set.

5.2 Optional Input Parameters

1: **n – int32 scalar**

Default: The dimension of the arrays **a**, **b**. (An error is raised if these dimensions are not equal.)

n, the order of the matrix A.

Constraint: $\mathbf{n} \geq 1$.

5.3 Input Parameters Omitted from the MATLAB Interface

lda, ldb, z

5.4 Output Parameters

1: **a(lda,n) – double array**

The lower triangle of the inverse matrix X is stored in the elements of the array below the diagonal, in rows 2 to $n + 1$; x_{ij} is stored in $\mathbf{a}(i + 1, j)$ for $i \geq j$. The upper triangle of the original matrix is unchanged.

2: **b(ldb,n) – double array**

The lower triangle of the inverse matrix X, with x_{ij} stored in $\mathbf{b}(i,j)$, for $i \geq j$.

3: **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 $= 1$

The matrix A is not positive-definite, possibly due to rounding errors.

ifail $= 2$

The refinement process fails to converge, i.e., the matrix A is ill-conditioned.

ifail $= 3$

n < 1, or **lda** $<$ **n** $+ 1$, or **ldb** $<$ **n**.

7 Accuracy

The computed inverse should be correct to full machine accuracy. For a detailed error analysis see page 40 of Wilkinson and Reinsch 1971.

8 Further Comments

The time taken by f01ab is approximately proportional to n^3.

9 Example

```
a = [5, 7, 6, 5;
     7, 10, 8, 7;
     6, 8, 10, 9;
     5, 7, 9, 10;
     0, -0.01238964498066066, 0, 0];
[aOut, b, ifail] = f01ab(a)
```

```
aOut =
     5     7     6     5
    68    10     8     7
   -41    25    10     9
   -17    10     5    10
    10    -6    -3     2
b =
    68     0     0     0
   -41    25     0     0
   -17    10     5     0
    10    -6    -3     2
ifail =
           0
```