

NAG Fortran Library Routine Document

F01BUF

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of *bold italicised* terms and other implementation-dependent details.

1 Purpose

F01BUF performs a $ULDL^T U^T$ decomposition of a real symmetric positive-definite band matrix.

2 Specification

```
SUBROUTINE F01BUF(N, M1, K, A, IA, W, IFAIL)
  INTEGER          N, M1, K, IA, IFAIL
  real           A(IA,N), W(M1)
```

3 Description

The symmetric positive-definite matrix A , of order n and bandwidth $2m + 1$, is divided into the leading principal sub-matrix of order k and its complement, where $m \leq k \leq n$. A UDU^T decomposition of the latter and an LDL^T decomposition of the former are obtained by means of a sequence of elementary transformations, where U is unit upper triangular, L is unit lower triangular and D is diagonal. Thus if $k = n$, an LDL^T decomposition of A is obtained.

This routine is specifically designed to precede F01BVF for the transformation of the symmetric-definite eigenproblem $Ax = \lambda Bx$ by the method of Crawford where A and B are of band form. In this context, k is chosen to be close to $n/2$ and the decomposition is applied to the matrix B .

4 References

Wilkinson J H (1965) *The Algebraic Eigenvalue Problem* Oxford University Press, Oxford

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

5 Parameters

- 1: N – INTEGER *Input*
On entry: n , the order of the matrix A .
- 2: M1 – INTEGER *Input*
On entry: $m + 1$, where m is the number of non-zero super-diagonals in A . Normally $M1 \ll N$.
- 3: K – INTEGER *Input*
On entry: k , the change-over point in the decomposition.
Constraint: $M - 1 \leq K \leq N$.
- 4: A(IA,N) – *real* array *Input/Output*
On entry: the upper triangle of the n by n symmetric band matrix A , with the diagonal of the matrix stored in the $(m + 1)$ th row of the array, and the m super-diagonals within the band stored in the first m rows of the array. Each column of the matrix is stored in the corresponding column of the array. For example, if $n = 6$ and $m = 2$, the storage scheme is

```

*      *      a13 a24 a35 a46
*      a12 a23 a34 a45 a56
a11 a22 a33 a44 a55 a66

```

Elements in the top left corner of the array are not used. The following code assigns the matrix elements within the band to the correct elements of the array:

```

      DO 20 J = 1, N
        DO 10 I = MAX(1,J-M1+1), J
          A(I-J+M1,J) = matrix (I,J)
10      CONTINUE
20 CONTINUE

```

On exit: A is overwritten by the corresponding elements of L, D and U.

5: IA – INTEGER *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which F01BUF is called.

Constraint: IA ≥ M1.

6: W(M1) – *real* array *Workspace*

7: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, for users not familiar with this parameter the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

6 Error Indicators and Warnings

If on entry IFAIL = 0 or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL = 1

On entry, $K < M$ or $K > N$.

IFAIL = 2

The matrix A is not positive-definite, perhaps as a result of rounding errors, giving an element of D which is zero or negative. IFAIL=3 when the failure occurs in the leading principal sub-matrix of order K and IFAIL = 2 when it occurs in the complement.

7 Accuracy

The Cholesky decomposition of a positive-definite matrix is known for its remarkable numerical stability (see Wilkinson (1965)). The computed U , L and D satisfy the relation $ULDL^T U^T = A + E$ where the 2-norms of A and E are related by $\|E\| \leq c(m+1)^2 \epsilon \|A\|$ where c is a constant of order unity and ϵ is the *machine precision*. In practice, the error is usually appreciably smaller than this.


```
      STOP
*
99999 FORMAT (1X,8F9.4)
      END
```

9.2 Program Data

F01BUF Example Program Data

```
 7  3
   3
  -9  31
   6  -2  123
  -4 -66  145
  15 -24  61
   4 -74  98
 -18  24   6
```

9.3 Program Results

F01BUF Example Program Results

Computed upper triangular matrix

```
 3.0000
-3.0000  4.0000
 2.0000  4.0000  2.0000
-1.0000  5.0000  3.0000
 3.0000 -4.0000  5.0000
 2.0000 -1.0000  2.0000
-3.0000  4.0000  6.0000
```
