

NAG 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, LDA, W, IFAIL)
```

```
INTEGER N, M1, K, LDA, IFAIL
```

```
REAL (KIND=nag_wp) A(LDA,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 | <i>Input</i> |
| | <i>On entry:</i> n , the order of the matrix A . | |
| 2: | M1 – INTEGER | <i>Input</i> |
| | <i>On entry:</i> $m + 1$, where m is the number of nonzero superdiagonals in A . Normally $M1 \ll N$. | |
| 3: | K – INTEGER | <i>Input</i> |
| | <i>On entry:</i> k , the change-over point in the decomposition. | |
| | <i>Constraint:</i> $M1 - 1 \leq K \leq N$. | |
| 4: | A(LDA,N) – REAL (KIND=nag_wp) array | <i>Input/Output</i> |
| | <i>On entry:</i> 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 superdiagonals 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: LDA – INTEGER *Input*

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

Constraint: $LDA \geq M1$.

6: W(M1) – REAL (KIND=nag_wp) array *Workspace*

7: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction for details.

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, if you are 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.**

On exit: IFAIL = 0 unless the routine detects an error or a warning has been flagged (see Section 6).

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, $K < M1$ or $K > N$.

IFAIL = 2

IFAIL = 3

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 $ULLD^T U^T = A + E$ 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.


```
      Write (nout,99999)(a(j,i),j=max(1,m1+1-i),m1)
      End Do

99999 Format (1X,8F9.4)
      End Program f01bufe
```

9.2 Program Data

```
F01BUF Example Program Data
  7  3          : n, m1
  3
  -9   31
  6   -2  123
  -4  -66  145
  15  -24   61
  4   -74   98
 -18  24    6   : a
```

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
```
