NAG Toolbox for MATLAB

f01bu

1 Purpose

f01bu performs a $ULDL^{\mathrm{T}}U^{\mathrm{T}}$ decomposition of a real symmetric positive-definite band matrix.

2 Syntax

```
[a, ifail] = f01bu(m1, k, a, 'n', n)
```

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 function is specifically designed to precede f01bv 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

5.1 Compulsory Input Parameters

1: **m1 – int32 scalar**

$m+1$, where m is the number of nonzero superdiagonals in A. Normally $\mathbf{m1} \ll \mathbf{n}$.

2: **k – int32 scalar**

k, the change-over point in the decomposition.

Constraint: $\mathbf{m1} - 1 \leq \mathbf{k} \leq \mathbf{n}$.

3: **a(lda,n) – double array**

lda, the first dimension of the array, must be at least **m1**.

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

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

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:

```
for j=1:n
  for i=max(1,j-m1+1):j
    a(i-j+m1,j) = matrix (i,j);
  end
end
```

5.2 Optional Input Parameters

1: **n – int32 scalar**

Default: The dimension of the array **a**.

n, the order of the matrix A.

5.3 Input Parameters Omitted from the MATLAB Interface

lda, w

5.4 Output Parameters

1: **a(lda,n) – double array**

A contains the corresponding elements of L, D and U.

2: **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 $= 1$

On entry, $\mathbf{k} < \mathbf{m1}$ or $\mathbf{k} > \mathbf{n}$.

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 $ULDL^{\mathrm{T}}U^{\mathrm{T}} = A + E$ 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.

8 Further Comments

The time taken by f01bu is approximately proportional to $nm^2 + 3nm$.

This function is specifically designed for use as the first stage in the solution of the generalized symmetric eigenproblem $Ax = \lambda Bx$ by Crawford's method which preserves band form in the transformation to a similar standard problem. In this context, for maximum efficiency, k should be chosen as the multiple of m nearest to $n/2$.

The matrix U is such that $U^{-1}AU^{-\mathrm{T}}$ is diagonal in its last $n-k$ rows and columns, L is such that $L^{-1}U^{-1}AU^{-\mathrm{T}}L^{-\mathrm{T}} = D$ and D is diagonal. To find U, L and D where $A = ULDL^{\mathrm{T}}U^{\mathrm{T}}$ requires $nm(m+3)/2 - m(m+1)(m+2)/3$ multiplications and divisions which, is independent of k.

9 Example

```
m1 = int32(3);
k = int32(4);
a = [0, 0, 6, -4, 15, 4, -18;
     0, -9, -2, -66, -24, -74, 24;
     3, 31, 123, 145, 61, 98, 6];
[aOut, ifail] = f01bu(m1, k, a)
```

```
aOut =
     0     0     2    -1     3     2    -3
     0    -3     4     5    -4    -1     4
     3     4     2     3     5     2     6
ifail =
           0
```