NAG Library Routine Document

F08HEF (DSBTRD)

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

F08HEF (DSBTRD) reduces a real symmetric band matrix to tridiagonal form.

2 Specification

```
SUBROUTINE F08HEF (VECT, UPLO, N, KD, AB, LDAB, D, E, Q, LDQ, WORK, INFO)

INTEGER            N, KD, LDAB, LDQ, INFO
REAL (KIND=nag_wp) AB(LDAB,*), D(N), E(N-1), Q(LDQ,*), WORK(N)
CHARACTER(1)       VECT, UPLO
```

The routine may be called by its LAPACK name ***dsbtrd***.

3 Description

F08HEF (DSBTRD) reduces a symmetric band matrix A to symmetric tridiagonal form T by an orthogonal similarity transformation:

$$T = Q^{\mathrm{T}} A Q.$$

The orthogonal matrix Q is determined as a product of Givens rotation matrices, and may be formed explicitly by the routine if required.

The routine uses a vectorizable form of the reduction, due to Kaufman (1984).

4 References

Kaufman L (1984) Banded eigenvalue solvers on vector machines *ACM Trans. Math. Software* **10** 73–86

Parlett B N (1998) *The Symmetric Eigenvalue Problem* SIAM, Philadelphia

5 Parameters

1: VECT – CHARACTER(1) *Input*

On entry: indicates whether Q is to be returned.

VECT = 'V'
: Q is returned.

VECT = 'U'
: Q is updated (and the array Q must contain a matrix on entry).

VECT = 'N'
: Q is not required.

Constraint: VECT = 'V', 'U' or 'N'.

2: UPLO – CHARACTER(1) *Input*

On entry: indicates whether the upper or lower triangular part of A is stored.

UPLO = 'U'
: The upper triangular part of A is stored.

UPLO = 'L'
The lower triangular part of A is stored.

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

3: N – INTEGER *Input*

On entry: n, the order of the matrix A.

Constraint: N ≥ 0.

4: KD – INTEGER *Input*

On entry: if UPLO = 'U', the number of superdiagonals, k_d, of the matrix A.

If UPLO = 'L', the number of subdiagonals, k_d, of the matrix A.

Constraint: KD ≥ 0.

5: AB(LDAB,$*$) – REAL (KIND=nag_wp) array *Input/Output*

Note: the second dimension of the array AB must be at least $\max(1, \mathrm{N})$.

On entry: the upper or lower triangle of the n by n symmetric band matrix A.

The matrix is stored in rows 1 to $k_d + 1$, more precisely,

if UPLO = 'U', the elements of the upper triangle of A within the band must be stored with element A_{ij} in $\mathrm{AB}(k_d + 1 + i - j, j)$ for $\max(1, j - k_d) \leq i \leq j$;

if UPLO = 'L', the elements of the lower triangle of A within the band must be stored with element A_{ij} in $\mathrm{AB}(1 + i - j, j)$ for $j \leq i \leq \min(n, j + k_d)$.

On exit: AB is overwritten by values generated during the reduction to tridiagonal form.

The first superdiagonal or subdiagonal and the diagonal of the tridiagonal matrix T are returned in AB using the same storage format as described above.

6: LDAB – INTEGER *Input*

On entry: the first dimension of the array AB as declared in the (sub)program from which F08HEF (DSBTRD) is called.

Constraint: LDAB $\geq \max(1, \mathrm{KD} + 1)$.

7: D(N) – REAL (KIND=nag_wp) array *Output*

On exit: the diagonal elements of the tridiagonal matrix T.

8: E(N $-$ 1) – REAL (KIND=nag_wp) array *Output*

On exit: the off-diagonal elements of the tridiagonal matrix T.

9: Q(LDQ,$*$) – REAL (KIND=nag_wp) array *Input/Output*

Note: the second dimension of the array Q must be at least $\max(1, \mathrm{N})$ if VECT = 'V' or 'U' and at least 1 if VECT = 'N'.

On entry: if VECT = 'U', Q must contain the matrix formed in a previous stage of the reduction (for example, the reduction of a banded symmetric-definite generalized eigenproblem); otherwise Q need not be set.

On exit: if VECT = 'V' or 'U', the n by n matrix Q.

If VECT = 'N', Q is not referenced.

10: LDQ – INTEGER *Input*

On entry: the first dimension of the array Q as declared in the (sub)program from which F08HEF (DSBTRD) is called.

Constraints:

if VECT = 'V' or 'U', $\text{LDQ} \geq \max(1, \text{N})$;
if VECT = 'N', $\text{LDQ} \geq 1$.

11: WORK(N) – REAL (KIND=nag_wp) array *Workspace*

12: INFO – INTEGER *Output*

On exit: $\text{INFO} = 0$ unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the routine:

$\text{INFO} < 0$

If $\text{INFO} = -i$, argument i had an illegal value. An explanatory message is output, and execution of the program is terminated.

7 Accuracy

The computed tridiagonal matrix T is exactly similar to a nearby matrix $(A + E)$, where

$$\|E\|_2 \leq c(n)\epsilon\|A\|_2,$$

$c(n)$ is a modestly increasing function of n, and ϵ is the ***machine precision***.

The elements of T themselves may be sensitive to small perturbations in A or to rounding errors in the computation, but this does not affect the stability of the eigenvalues and eigenvectors.

The computed matrix Q differs from an exactly orthogonal matrix by a matrix E such that

$$\|E\|_2 = O(\epsilon),$$

where ϵ is the ***machine precision***.

8 Further Comments

The total number of floating point operations is approximately $6n^2k$ if VECT = 'N' with $3n^3(k-1)/k$ additional operations if VECT = 'V'.

The complex analogue of this routine is F08HSF (ZHBTRD).

9 Example

This example computes all the eigenvalues and eigenvectors of the matrix A, where

$$A = \begin{pmatrix} 4.99 & 0.04 & 0.22 & 0.00 \\ 0.04 & 1.05 & -0.79 & 1.04 \\ 0.22 & -0.79 & -2.31 & -1.30 \\ 0.00 & 1.04 & -1.30 & -0.43 \end{pmatrix}.$$

Here A is symmetric and is treated as a band matrix. The program first calls F08HEF (DSBTRD) to reduce A to tridiagonal form T, and to form the orthogonal matrix Q; the results are then passed to F08JEF (DSTEQR) which computes the eigenvalues and eigenvectors of A.

9.1 Program Text

```
    Program f08hefe

!     F08HEF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: dsbtrd, dsteqr, nag_wp, x04caf
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
!     .. Local Scalars ..
      Integer                          :: i, ifail, info, j, kd, ldab, ldq, n
      Character (1)                    :: uplo
!     .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable  :: ab(:,:), d(:), e(:), q(:,:), work(:)
!     .. Intrinsic Procedures ..
      Intrinsic                        :: max, min
!     .. Executable Statements ..
      Write (nout,*) 'F08HEF Example Program Results'
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) n, kd
      ldab = kd + 1
      ldq = n
      Allocate (ab(ldab,n),d(n),e(n-1),q(ldq,n),work(2*n-2))

!     Read A from data file

      Read (nin,*) uplo
      If (uplo=='U') Then
        Do i = 1, n
          Read (nin,*)(ab(kd+1+i-j,j),j=i,min(n,i+kd))
        End Do
      Else If (uplo=='L') Then
        Do i = 1, n
          Read (nin,*)(ab(1+i-j,j),j=max(1,i-kd),i)
        End Do
      End If

!     Reduce A to tridiagonal form T = (Q**T)*A*Q (and form Q)
!     The NAG name equivalent of dsbtrd is f08hef
      Call dsbtrd('V',uplo,n,kd,ab,ldab,d,e,q,ldq,work,info)

!     Calculate all the eigenvalues and eigenvectors of A
!     The NAG name equivalent of dsteqr is f08jef
      Call dsteqr('V',n,d,e,q,ldq,work,info)

      Write (nout,*)
      If (info>0) Then
        Write (nout,*) 'Failure to converge.'
      Else

!       Print eigenvalues and eigenvectors

        Write (nout,*) 'Eigenvalues'
        Write (nout,99999) d(1:n)
        Write (nout,*)
        Flush (nout)

!       Standardize the eigenvectors so that first elements are non-negative.
        Do i = 1, n
          If (q(1,i)<0.0_nag_wp) q(1:n,i) = -q(1:n,i)
        End Do

!       ifail: behaviour on error exit
!              =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
        ifail = 0
```

```
        Call x04caf('General',' ',n,n,q,ldq,'Eigenvectors',ifail)

      End If

99999 Format (3X,(8F8.4))
    End Program f08hefe
```

9.2 Program Data

```
F08HEF Example Program Data
  4  2                        :Values of N and KD
  'L'                         :Value of UPLO
  4.99
  0.04   1.05
  0.22  -0.79  -2.31
         1.04  -1.30  -0.43   :End of matrix A
```

9.3 Program Results

```
 F08HEF Example Program Results

 Eigenvalues
    -2.9943 -0.7000  1.9974  4.9969

 Eigenvectors
          1       2       3       4
 1   0.0251  0.0162  0.0113  0.9995
 2  -0.0656 -0.5859  0.8077  0.0020
 3  -0.9002 -0.3135 -0.3006  0.0311
 4  -0.4298  0.7471  0.5070 -0.0071
```
