F08HEF (SSBTRD/DSBTRD) - NAG Fortran Library Routine Document

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

2 Specification

```
SUBROUTINE FO8HEF(VECT, UPLO, N, KD, AB, LDAB, D, E, Q, LDQ, WORK, 1 INFO)

ENTRY ssbtrd(VECT, UPLO, N, KD, AB, LDAB, D, E, Q, LDQ, WORK, 1 INFO)

INTEGER N, KD, LDAB, LDQ, INFO
real AB(LDAB,*), D(*), E(*), Q(LDQ,*), WORK(*)

CHARACTER*1 VECT, UPLO
```

The ENTRY statement enables the routine to be called by its LAPACK name.

3 Description

The symmetric band matrix A is reduced to symmetric tridiagonal form T by an orthogonal similarity transformation: $T = Q^T A Q$. 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 vectorisable form of the reduction, due to Kaufman [1].

4 References

- [1] Kaufman L (1984) Banded eigenvalue solvers on vector machines ACM Trans. Math. Software 10 73–86
- [2] Parlett B N (1980) The Symmetric Eigenvalue Problem Prentice-Hall

5 Parameters

```
1: VECT — CHARACTER*1
```

Input

On entry: indicates whether Q is to be returned as follows:

```
if VECT = 'V', then Q is returned (and the array Q must contain a matrix on entry); if VECT = 'U', then Q is updated (and the array Q must contain a matrix on entry); if VECT = 'N', then 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 as follows:

```
if UPLO = 'U', then the upper triangular part of A is stored; if UPLO = 'L', then 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: $N \geq 0$.

4: KD — INTEGER Input

On entry: k, the number of super-diagonals of the matrix A if UPLO = 'U', or the number of sub-diagonals if UPLO = 'L'.

Constraint: $KD \geq 0$.

5: AB(LDAB,*) - real array

Input/Output

Note: the second dimension of the array AB must be at least max(1,N).

On entry: the n by n symmetric band matrix A, stored in rows 1 to k+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 AB(k+1+i-j,j) for $\max(1,j-k) \le i \le j$; if UPLO = 'L', the elements of the lower triangle of A within the band must be stored with element a_{ij} in AB(1+i-j,j) for $j \le i \le \min(n,j+k)$.

On exit: A is overwritten.

6: LDAB — INTEGER

Input

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

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

7: $D(*) - real \operatorname{array}$

Output

Note: the dimension of the array D must be at least max(1,N).

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

8: E(*) — real array

Output

Note: the dimension of the array E must be at least max(1,N-1).

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

9: Q(LDQ,*) - real array

Output

Note: the second dimension of the array Q must be at least max(1,N) if VECT = 'V', and at least 1 if VECT = 'N'.

On exit: the n by n orthogonal matrix Q if VECT = 'V'.

Q is not referenced if VECT = 'N'.

10: LDQ — INTEGER

Input

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

Constraints:

 $LDQ \ge max(1,N)$ if VECT = V' or U';

 $LDQ \ge 1 \text{ if VECT} = 'N'.$

11: WORK(*) — real array

Workspace

Note: the dimension of the array WORK must be at least max(1,N).

12: INFO — INTEGER

Output

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

6 Error Indicators and Warnings

INFO < 0

If INFO = -i, the *i*th parameter 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

$$||E||_2 \le c(n)\epsilon ||A||_2$$

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

$$\parallel E \parallel_2 = O(\epsilon),$$

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 (CHBTRD/ZHBTRD).

9 Example

To compute 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 (SSBTRD/DSBTRD) to reduce A to tridiagonal form T, and to form the orthogonal matrix Q; the results are then passed to F08JEF (SSTEQR/DSTEQR) which computes the eigenvalues and eigenvectors of A.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

- * FO8HEF Example Program Text
- * Mark 16 Release. NAG Copyright 1992.
- * .. Parameters ..

INTEGER NIN, NOUT
PARAMETER (NIN=5,NOUT=6)

INTEGER NMAX, KMAX, LDAB, LDQ

PARAMETER (NMAX=8, KMAX=8, LDAB=KMAX+1, LDQ=NMAX)

* .. Local Scalars ..

INTEGER I, IFAIL, INFO, J, KD, N

CHARACTER UPLO

* .. Local Arrays ..

```
real
                       AB(LDAB, NMAX), D(NMAX), E(NMAX-1), Q(LDQ, NMAX),
                       WORK(2*NMAX-2)
      .. External Subroutines ..
     EXTERNAL
                       ssbtrd, ssteqr, XO4CAF
      .. Intrinsic Functions ...
      INTRINSIC
                      MAX, MIN
      .. Executable Statements ..
      WRITE (NOUT,*) 'FO8HEF Example Program Results'
      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, KD
      IF (N.LE.NMAX .AND. KD.LE.KMAX) THEN
         Read A from data file
         READ (NIN,*) UPLO
         IF (UPLO.EQ.'U') THEN
            DO 20 I = 1, N
               READ (NIN,*) (AB(KD+1+I-J,J),J=I,MIN(N,I+KD))
   20
            CONTINUE
         ELSE IF (UPLO.EQ.'L') THEN
            DO 40 I = 1, N
               READ (NIN,*) (AB(1+I-J,J),J=MAX(1,<math>I-KD),I)
   40
            CONTINUE
         END IF
         Reduce A to tridiagonal form T = (Q**T)*A*Q (and form Q)
         CALL ssbtrd('V', UPLO, N, KD, AB, LDAB, D, E, Q, LDQ, WORK, INFO)
         Calculate all the eigenvalues and eigenvectors of A
         CALL ssteqr('V', N, D, E, Q, LDQ, WORK, INFO)
         WRITE (NOUT,*)
         IF (INFO.GT.O) THEN
            WRITE (NOUT,*) 'Failure to converge.'
         ELSE
            Print eigenvalues and eigenvectors
            WRITE (NOUT,*) 'Eigenvalues'
            WRITE (NOUT,99999) (D(I),I=1,N)
            WRITE (NOUT, *)
            IFAIL = 0
            CALL X04CAF('General',' ',N,N,Q,LDQ,'Eigenvectors',IFAIL)
         END IF
      END IF
      STOP
99999 FORMAT (3X, (8F8.4))
      END
```

9.2 Program Data

```
FO8HEF 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

FO8HEF 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
```