NAG Library Routine Document

F08HSF (ZHBTRD)

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

F08HSF (ZHBTRD) reduces a complex Hermitian band matrix to tridiagonal form.

2 Specification

```
SUBROUTINE F08HSF(VECT, UPLO, N, KD, AB, LDAB, D, E, Q, LDQ, WORK, INFO)
INTEGER             N, KD, LDAB, LDQ, INFO
double precision    D(N), E(N-1)
complex*16          AB(LDAB,*), Q(LDQ,*), WORK(N)
CHARACTER*1         VECT, UPLO
```

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

3 Description

F08HSF (ZHBTRD) reduces a Hermitian band matrix A to real symmetric tridiagonal form T by a unitary similarity transformation:

$$T = Q^{\mathrm{H}}AQ.$$

The unitary 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,$*$) – ***complex*16*** 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 Hermitian 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 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 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 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 F08HSF (ZHBTRD) is called.

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

7: D(N) – ***double precision*** array *Output*

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

8: E(N $-$ 1) – ***double precision*** array *Output*

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

9: Q(LDQ,$*$) – ***complex*16*** 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 Hermitian-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 F08HSF (ZHBTRD) is called.

Constraints:

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

11: WORK(N) – ***complex*16*** array *Workspace*

12: INFO – INTEGER *Output*

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

6 Error Indicators and Warnings

Errors or warnings detected by the routine:

INFO < 0

If 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 unitary matrix by a matrix E such that

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

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

8 Further Comments

The total number of real floating-point operations is approximately $20n^2k$ if VECT = 'N' with $10n^3(k-1)/k$ additional operations if VECT = 'V'.

The real analogue of this routine is F08HEF (DSBTRD).

9 Example

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

$$A = \begin{pmatrix} -3.13 + 0.00i & 1.94 - 2.10i & -3.40 + 0.25i & 0.00 + 0.00i \\ 1.94 + 2.10i & -1.91 + 0.00i & -0.82 - 0.89i & -0.67 + 0.34i \\ -3.40 - 0.25i & -0.82 + 0.89i & -2.87 + 0.00i & -2.10 - 0.16i \\ 0.00 + 0.00i & -0.67 - 0.34i & -2.10 + 0.16i & 0.50 + 0.00i \end{pmatrix}.$$

Here A is Hermitian and is treated as a band matrix. The program first calls F08HSF (ZHBTRD) to reduce A to tridiagonal form T, and to form the unitary matrix Q; the results are then passed to F08JSF (ZSTEQR) which computes the eigenvalues and eigenvectors of A.

9.1 Program Text

```
*     F08HSF 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 ..
      COMPLEX *16      AB(LDAB,NMAX), Q(LDQ,NMAX), WORK(NMAX)
      DOUBLE PRECISION D(NMAX), E(NMAX-1), RWORK(2*NMAX-2)
      CHARACTER        CLABS(1), RLABS(1)
*     .. External Subroutines ..
      EXTERNAL         X04DBF, ZHBTRD, ZSTEQR
*     .. Intrinsic Functions ..
      INTRINSIC        MAX, MIN
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F08HSF 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,I-KD),I)
   40       CONTINUE
         END IF
*
*        Reduce A to tridiagonal form T = (Q**H)*A*Q (and form Q)
*
         CALL ZHBTRD('V',UPLO,N,KD,AB,LDAB,D,E,Q,LDQ,WORK,INFO)
*
*        Calculate all the eigenvalues and eigenvectors of A
*
         CALL ZSTEQR('V',N,D,E,Q,LDQ,RWORK,INFO)
*
         WRITE (NOUT,*)
         IF (INFO.GT.0) 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 X04DBF('General',' ',N,N,Q,LDQ,'Bracketed','F7.4',
     +                  'Eigenvectors','Integer',RLABS,'Integer',CLABS,
     +                  80,0,IFAIL)
*
         END IF
      END IF
*
99999 FORMAT (8X,4(F7.4,11X,:))
      END
```

9.2 Program Data

```
F08HSF Example Program Data
  4  2                                                         :Values of N and KD
  'L'                                                          :Value of UPLO
 (-3.13, 0.00)
 ( 1.94, 2.10) (-1.91, 0.00)
 (-3.40,-0.25) (-0.82, 0.89) (-2.87, 0.00)
               (-0.67,-0.34) (-2.10, 0.16) ( 0.50, 0.00)   :End of matrix A
```

9.3 Program Results

```
 F08HSF Example Program Results

 Eigenvalues
       -7.0042          -4.0038           0.5968           3.0012

 Eigenvectors
                  1                 2                 3                 4
 1  ( 0.7293, 0.0000) (-0.2128, 0.1511) (-0.3354,-0.1604) (-0.5114,-0.0163)
 2  (-0.1654,-0.2046) ( 0.7316, 0.0000) (-0.2804,-0.3413) (-0.2374,-0.3796)
 3  ( 0.6081, 0.0301) ( 0.3910,-0.3843) (-0.0144, 0.1532) ( 0.5523, 0.0000)
 4  ( 0.1653,-0.0303) ( 0.2775,-0.1378) ( 0.8019, 0.0000) (-0.4517, 0.1693)
```