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
REAL (KIND=nag_wp)      D(N), E(N-1)
COMPLEX (KIND=nag_wp)   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:

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

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 (KIND=nag_wp) array *Input/Output*

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

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 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 F08HSF (ZHBTRD) is called.

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

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,$*$) – COMPLEX (KIND=nag_wp) array *Input/Output*

Note: the second dimension of the array Q must be at least max$(1, \text{N})$ 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 $\geq \max(1, \mathrm{N})$;
if VECT = 'N', LDQ ≥ 1.

11: WORK(N) – COMPLEX (KIND=nag_wp) 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

```
    Program f08hsfe

!     F08HSF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: nag_wp, x04dbf, zhbtrd, zsteqr
!     .. 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 ..
      Complex (Kind=nag_wp), Allocatable :: ab(:,:), q(:,:), work(:)
      Real (Kind=nag_wp), Allocatable  :: d(:), e(:), rwork(:)
      Character (1)                    :: clabs(1), rlabs(1)
!     .. Intrinsic Procedures ..
      Intrinsic                        :: max, min
!     .. Executable Statements ..
      Write (nout,*) 'F08HSF Example Program Results'
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) n, kd
      ldab = kd + 1
      ldq = n
      Allocate (ab(ldab,n),q(ldq,n),work(n),d(n),e(n-1),rwork(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**H)*A*Q (and form Q)
!     The NAG name equivalent of zhbtrd is f08hsf
      Call zhbtrd('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 zsteqr is f08jsf
      Call zsteqr('V',n,d,e,q,ldq,rwork,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)

!       Normalize the eigenvectors
        Do i = 1, n
          q(1:n,i) = q(1:n,i)/q(1,i)
        End Do

!       ifail: behaviour on error exit
```

```
!              =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
        ifail = 0
        Call x04dbf('General',' ',n,n,q,ldq,'Bracketed','F7.4','Eigenvectors', &
          'Integer',rlabs,'Integer',clabs,80,0,ifail)

      End If

99999 Format (8X,4(F7.4,11X:))
    End Program f08hsfe
```

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  ( 1.0000, 0.0000) ( 1.0000, 0.0000) ( 1.0000, 0.0000) ( 1.0000, 0.0000)
 2  (-0.2268,-0.2805) (-2.2857,-1.6226) ( 1.0765, 0.5028) ( 0.4873, 0.7267)
 3  ( 0.8338, 0.0413) (-2.0739, 0.3334) (-0.1427,-0.3885) (-1.0790, 0.0343)
 4  ( 0.2267,-0.0415) (-1.1727,-0.1848) (-1.9460, 0.9305) ( 0.8719,-0.3587)
```