NAG Library Routine Document

F08GNF (ZHPEV)

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

F08GNF (ZHPEV) computes all the eigenvalues and, optionally, all the eigenvectors of a complex n by n Hermitian matrix A in packed storage.

2 Specification

```
SUBROUTINE F08GNF(JOBZ, UPLO, N, AP, W, Z, LDZ, WORK, RWORK, INFO)
INTEGER             N, LDZ, INFO
double precision    W(N), RWORK(3*N-2)
complex*16          AP(*), Z(LDZ,*), WORK(2*N-1)
CHARACTER*1         JOBZ, UPLO
```

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

3 Description

The Hermitian matrix A is first reduced to real tridiagonal form, using unitary similarity transformations, and then the QR algorithm is applied to the tridiagonal matrix to compute the eigenvalues and (optionally) the eigenvectors.

4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphiahttp://www.netlib.org/lapack/lug

Golub G H and Van Loan C F (1996) *Matrix Computations* (3rd Edition) Johns Hopkins University Press, Baltimore

5 Parameters

1: JOBZ – CHARACTER*1 *Input*

On entry: if JOBZ = 'N', compute eigenvalues only.

If JOBZ = 'V', compute eigenvalues and eigenvectors.

Constraint: JOBZ = 'N' or 'V'.

2: UPLO – CHARACTER*1 *Input*

On entry: if UPLO = 'U', the upper triangular part of A is stored.

If UPLO = 'L', the lower triangular part of A is stored.

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

3: N – INTEGER *Input*

On entry: the dimension of the array W as declared in the (sub)program from which F08GNF (ZHPEV) is called. n, the order of the matrix A.

Constraint: N $\geq$ 0.

4: AP($*$) – ***complex*16*** array *Input/Output*

Note: the dimension of the array AP must be at least $\max(1, \mathrm{N} \times (\mathrm{N}+1)/2)$.

On entry: the n by n Hermitian matrix A, packed by columns.

More precisely,

if UPLO = 'U', the upper triangle of A must be stored with element A_{ij} in $\mathrm{AP}(i + j(j-1)/2)$ for $i \leq j$;

if UPLO = 'L', the lower triangle of A must be stored with element A_{ij} in $\mathrm{AP}(i + (2n-j)(j-1)/2)$ for $i \geq j$.

On exit: AP is overwritten by the values generated during the reduction to tridiagonal form. The elements of the diagonal and the off-diagonal of the tridiagonal matrix overwrite the corresponding elements of A.

5: W(N) – ***double precision*** array *Output*

On exit: if INFO = 0, the eigenvalues in ascending order.

6: Z(LDZ,$*$) – ***complex*16*** array *Output*

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

On exit: if JOBZ = 'V', then if INFO = 0, Z contains the orthonormal eigenvectors of the matrix A, with the ith column of Z holding the eigenvector associated with $\mathrm{W}(i)$.

If JOBZ = 'N', Z is not referenced.

7: LDZ – INTEGER *Input*

On entry: the first dimension of the array Z as declared in the (sub)program from which F08GNF (ZHPEV) is called.

Constraints:

if JOBZ = 'V', LDZ $\geq \max(1, \mathrm{N})$;
otherwise LDZ ≥ 1.

8: WORK($2 \times \mathrm{N} - 1$) – ***complex*16*** array *Workspace*

9: RWORK($3 \times \mathrm{N} - 2$) – ***double precision*** array *Workspace*

10: 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.

INFO > 0

If INFO $= i$, the algorithm failed to converge; i elements of an intermediate tridiagonal form did not converge to zero.

7 Accuracy

The computed eigenvalues and eigenvectors are exact for a nearby matrix $(A + E)$, where

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

and ϵ is the ***machine precision***. See Section 4.7 of Anderson *et al.* (1999) for further details.

8 Further Comments

Each eigenvector is normalized so that the element of largest absolute value is real and positive.

The total number of floating-point operations is proportional to n^3.

The real analogue of this routine is F08GAF (DSPEV).

9 Example

This example finds all the eigenvalues of the Hermitian matrix

$$A = \begin{pmatrix} 1 & 2-i & 3-i & 4-i \\ 2+i & 2 & 3-2i & 4-2i \\ 3+i & 3+2i & 3 & 4-3i \\ 4+i & 4+2i & 4+3i & 4 \end{pmatrix},$$

together with approximate error bounds for the computed eigenvalues.

9.1 Program Text

```
*     F08GNF Example Program Text
*     Mark 21 Release. NAG Copyright 2004.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX
      PARAMETER        (NMAX=10)
      CHARACTER        UPLO
      PARAMETER        (UPLO='U')
*     .. Local Scalars ..
      DOUBLE PRECISION EERRBD, EPS
      INTEGER          I, INFO, J, N
*     .. Local Arrays ..
      COMPLEX *16      AP((NMAX*(NMAX+1))/2), DUMMY(1,1), WORK(2*NMAX-1)
      DOUBLE PRECISION RWORK(3*NMAX-2), W(NMAX)
*     .. External Functions ..
      DOUBLE PRECISION X02AJF
      EXTERNAL         X02AJF
*     .. External Subroutines ..
      EXTERNAL         ZHPEV
*     .. Intrinsic Functions ..
      INTRINSIC        ABS, MAX
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F08GNF Example Program Results'
      WRITE (NOUT,*)
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
*
*        Read the upper or lower triangular part of the matrix A from
*        data file
*
         IF (UPLO.EQ.'U') THEN
            READ (NIN,*) ((AP(I+(J*(J-1))/2),J=I,N),I=1,N)
         ELSE IF (UPLO.EQ.'L') THEN
            READ (NIN,*) ((AP(I+((2*N-J)*(J-1))/2),J=1,I),I=1,N)
         END IF
```

```
*
*        Solve the Hermitian eigenvalue problem
*
         CALL ZHPEV('No vectors',UPLO,N,AP,W,DUMMY,1,WORK,RWORK,INFO)
*
         IF (INFO.EQ.0) THEN
*
*           Print solution
*
            WRITE (NOUT,*) 'Eigenvalues'
            WRITE (NOUT,99999) (W(J),J=1,N)
*
*           Get the machine precision, EPS and compute the approximate
*           error bound for the computed eigenvalues.  Note that for
*           the 2-norm, max( abs(W(i)) ) = norm(A), and since the
*           eigenvalues are returned in ascending order
*           max( abs(W(i)) ) = max( abs(W(1)), abs(W(n)))
*
            EPS = X02AJF()
            EERRBD = EPS*MAX(ABS(W(1)),ABS(W(N)))
*
*           Print the approximate error bound for the eigenvalues
*
            WRITE (NOUT,*)
            WRITE (NOUT,*) 'Error estimate for the eigenvalues'
            WRITE (NOUT,99998) EERRBD
         ELSE
            WRITE (NOUT,99997) 'Failure in ZHPEV. INFO =', INFO
         END IF
      ELSE
         WRITE (NOUT,*) 'NMAX too small'
      END IF
*
99999 FORMAT (3X,(8F8.4))
99998 FORMAT (4X,1P,6E11.1)
99997 FORMAT (1X,A,I4)
      END
```

9.2 Program Data

```
F08GNF Example Program Data

  4                                                    :Value of N

 (1.0, 0.0)  (2.0, -1.0)  (3.0, -1.0)  (4.0, -1.0)
             (2.0,  0.0)  (3.0, -2.0)  (4.0, -2.0)
                          (3.0,  0.0)  (4.0, -3.0)
                                       (4.0,  0.0) :End of matrix A
```

9.3 Program Results

```
 F08GNF Example Program Results

 Eigenvalues
    -4.2443 -0.6886  1.1412 13.7916

 Error estimate for the eigenvalues
        1.5E-15
```