NAG Library Routine Document

F08GPF (ZHPEVX)

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

F08GPF (ZHPEVX) computes selected eigenvalues and, optionally, eigenvectors of a complex n by n Hermitian matrix A in packed storage. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

2 Specification

```
      SUBROUTINE F08GPF(JOBZ, RANGE, UPLO, N, AP, VL, VU, IL, IU, ABSTOL, M,
     1                  W, Z, LDZ, WORK, RWORK, IWORK, JFAIL, INFO)
      INTEGER           N, IL, IU, M, LDZ, IWORK(5*N), JFAIL(*), INFO
      double precision  VL, VU, ABSTOL, W(N), RWORK(7*N)
      complex*16        AP(*), Z(LDZ,*), WORK(2*N)
      CHARACTER*1       JOBZ, RANGE, UPLO
```

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

3 Description

The Hermitian matrix A is first reduced to real tridiagonal form, using unitary similarity transformations. The required eigenvalues and eigenvectors are then computed from the tridiagonal matrix; the method used depends upon whether all, or selected, eigenvalues and eigenvectors are required.

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

Demmel J W and Kahan W (1990) Accurate singular values of bidiagonal matrices *SIAM J. Sci. Statist. Comput.* **11** 873–912

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: RANGE – CHARACTER*1 *Input*

On entry: if RANGE = 'A', all eigenvalues will be found.

If RANGE = 'V', all eigenvalues in the half-open interval $(\mathrm{VL}, \mathrm{VU}]$ will be found.

If RANGE = 'I', the ILth to IUth eigenvalues will be found.

Constraint: RANGE = 'A', 'V' or 'I'.

3: 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'.

4: N – INTEGER *Input*

On entry: the dimension of the array W as declared in the (sub)program from which F08GPF (ZHPEVX) is called. n, the order of the matrix A.

Constraint: $\mathrm{N} \geq 0$.

5: 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.

6: VL – ***double precision*** *Input*
7: VU – ***double precision*** *Input*

On entry: if RANGE = 'V', the lower and upper bounds of the interval to be searched for eigenvalues.

If RANGE = 'A' or 'I', VL and VU are not referenced.

Constraint: if RANGE = 'V', $\mathrm{VL} < \mathrm{VU}$.

8: IL – INTEGER *Input*
9: IU – INTEGER *Input*

On entry: if RANGE = 'I', the indices (in ascending order) of the smallest and largest eigenvalues to be returned.

If RANGE = 'A' or 'V', IL and IU are not referenced.

Constraints:

> if RANGE = 'I' and $\mathrm{N} = 0$, $\mathrm{IL} = 1$ and $\mathrm{IU} = 0$;
> if RANGE = 'I' and $\mathrm{N} > 0$, $1 \leq \mathrm{IL} \leq \mathrm{IU} \leq \mathrm{N}$.

10: ABSTOL – ***double precision*** *Input*

On entry: the absolute error tolerance for the eigenvalues. An approximate eigenvalue is accepted as converged when it is determined to lie in an interval $[a,b]$ of width less than or equal to

$$\mathrm{ABSTOL} + \epsilon \max(|a|, |b|),$$

where ϵ is the ***machine precision***. If ABSTOL is less than or equal to zero, then $\epsilon \|T\|_1$ will be used in its place, where T is the tridiagonal matrix obtained by reducing A to tridiagonal form. Eigenvalues will be computed most accurately when ABSTOL is set to twice the underflow threshold $2 \times$ X02AMF( ), not zero. If this routine returns with $\mathrm{INFO} > 0$, indicating that some eigenvectors did not converge, try setting ABSTOL to $2 \times$ X02AMF( ). See Demmel and Kahan (1990).

11: M – INTEGER *Output*

On exit: the total number of eigenvalues found. $0 \le \mathrm{M} \le \mathrm{N}$.

If RANGE = 'A', M = N.

If RANGE = 'I', M = IU − IL + 1.

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

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

13: Z(LDZ,∗) – ***complex*16*** array *Output*

Note: the second dimension of the array Z must be at least max(1, M) if JOBZ = 'V', and at least 1 otherwise.

On exit: if JOBZ = 'V', then if INFO = 0, the first M columns of Z contain the orthonormal eigenvectors of the matrix A corresponding to the selected eigenvalues, with the ith column of Z holding the eigenvector associated with W(i).

If an eigenvector fails to converge, then that column of Z contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in JFAIL.

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

Note: you must ensure that at least max(1, M) columns are supplied in the array Z; if RANGE = 'V', the exact value of M is not known in advance and an upper bound of at least N must be used.

14: LDZ – INTEGER *Input*

On entry: the first dimension of the array Z as declared in the (sub)program from which F08GPF (ZHPEVX) is called.

Constraints:

if JOBZ = 'V', LDZ ≥ max(1, N);
otherwise LDZ ≥ 1.

15: WORK(2 × N) – ***complex*16*** array *Workspace*

16: RWORK(7 × N) – ***double precision*** array *Workspace*

17: IWORK(5 × N) – INTEGER array *Workspace*

18: JFAIL(∗) – INTEGER array *Output*

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

On exit: if JOBZ = 'V', then if INFO = 0, the first M elements of JFAIL are zero.

If INFO > 0, JFAIL contains the indices of the eigenvectors that failed to converge.

If JOBZ = 'E', JFAIL is not referenced.

19: 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 $= i$, then i eigenvectors failed to converge. Their indices are stored in array JFAIL. Please see ABSTOL.

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

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

The real analogue of this routine is F08GBF (DSPEVX).

9 Example

This example finds the eigenvalues in the half-open interval $(-2, 2]$, and the corresponding eigenvectors, of the Hermitian matrix

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

9.1 Program Text

```
*     F08GPF Example Program Text
*     Mark 21 Release. NAG Copyright 2004.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, MMAX
      PARAMETER        (NMAX=10,MMAX=5)
      INTEGER          LDZ
      PARAMETER        (LDZ=NMAX)
      CHARACTER        UPLO
      PARAMETER        (UPLO='U')
      DOUBLE PRECISION ZERO
      PARAMETER        (ZERO=0.0D+0)
*     .. Local Scalars ..
      DOUBLE PRECISION ABSTOL, VL, VU
      INTEGER          I, IFAIL, IL, INFO, IU, J, M, N
*     .. Local Arrays ..
      COMPLEX *16      AP((NMAX*(NMAX+1))/2), WORK(2*NMAX), Z(LDZ,MMAX)
      DOUBLE PRECISION RWORK(7*NMAX), W(NMAX)
      INTEGER          IWORK(5*NMAX), JFAIL(NMAX)
*     .. External Subroutines ..
      EXTERNAL         X04DAF, ZHPEVX
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F08GPF Example Program Results'
      WRITE (NOUT,*)
*     Skip heading in data file
```

```
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
*
*        Read the lower and upper bounds of the interval to be searched,
*        and read the upper or lower triangular part of the matrix A
*        from data file
*
         READ (NIN,*) VL, VU
         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
*
*        Set the absolute error tolerance for eigenvalues.  With ABSTOL
*        set to zero, the default value is used instead
*
         ABSTOL = ZERO
*
*        Solve the Hermitian eigenvalue problem
*
         CALL ZHPEVX('Vectors','Values in range',UPLO,N,AP,VL,VU,IL,IU,
     +               ABSTOL,M,W,Z,LDZ,WORK,RWORK,IWORK,JFAIL,INFO)
*
         IF (INFO.GE.0 .AND. M.LE.MMAX) THEN
*
*           Print solution
*
            WRITE (NOUT,99999) 'Number of eigenvalues found =', M
            WRITE (NOUT,*)
            WRITE (NOUT,*) 'Eigenvalues'
            WRITE (NOUT,99998) (W(J),J=1,M)
*
            IFAIL = 0
            CALL X04DAF('General',' ',N,M,Z,LDZ,'Selected eigenvectors',
     +                  IFAIL)
            IF (INFO.GT.0) THEN
               WRITE (NOUT,99999)
     +           'INFO eigenvectors failed to converge, INFO =', INFO
               WRITE (NOUT,*)
     +           'Indices of eigenvectors that did not converge'
               WRITE (NOUT,99997) (JFAIL(J),J=1,M)
            END IF
         ELSE IF (M.GT.MMAX) THEN
            WRITE (NOUT,99996) 'M greater than MMAX, M =', M,
     +        ', MMAX =', MMAX
         ELSE
            WRITE (NOUT,99999) 'Failure in ZHPEVX. INFO =', INFO
         END IF
      ELSE
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'NMAX too small'
      END IF
*
99999 FORMAT (1X,A,I5)
99998 FORMAT (3X,(8F8.4))
99997 FORMAT (3X,(8I8))
99996 FORMAT (1X,A,I5,A,I5)
      END
```

9.2 Program Data

```
F08GPF Example Program Data

  4                                                 :Value of N
 -2.0         2.0                                   :Values of VL and VU

 (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

```
 F08GPF Example Program Results

 Number of eigenvalues found =    2

 Eigenvalues
    -0.6886  1.1412
 Selected eigenvectors
          1       2
 1  -0.3975 -0.3746
     0.5105 -0.2414

 2   0.3953  0.2895
    -0.3238 -0.4917

 3  -0.4309  0.3768
     0.0383  0.3994

 4   0.3648 -0.4175
     0.0000  0.0000
```