

NAG Library Routine Document

F08GBF (DSPEVX)

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

F08GBF (DSPEVX) computes selected eigenvalues and, optionally, eigenvectors of a real n by n symmetric 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 F08GBF(JOBZ, RANGE, UPLO, N, AP, VL, VU, IL, IU, ABSTOL, M,
1              W, Z, LDZ, WORK, IWORK, JFAIL, INFO)
      INTEGER      N, IL, IU, M, LDZ, IWORK(5*N), JFAIL(N), INFO
      double precision AP(*), VL, VU, ABSTOL, W(N), Z(LDZ,*), WORK(8*N)
      CHARACTER*1  JOBZ, RANGE, UPLO
```

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

3 Description

The symmetric matrix A is first reduced to tridiagonal form, using orthogonal 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, Philadelphia <http://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 (VL, 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 arrays W and JFAIL as declared in the (sub)program from which F08GBF (DSPEVX) is called. n , the order of the matrix A .
Constraint: $N \geq 0$.
- 5: AP(*) – **double precision** array *Input/Output*
Note: the dimension of the array AP must be at least $\max(1, N \times (N + 1)/2)$.
On entry: the n by n symmetric matrix A , packed by columns.
 More precisely,
 if UPLO = 'U', the upper triangle of A must be stored with element A_{ij} in
 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
 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 'T', VL and VU are not referenced.
Constraint: if RANGE = 'V', VL < VU.
- 8: IL – INTEGER *Input*
 9: IU – INTEGER *Input*
On entry: if RANGE = 'T', 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 = 'T' and $N = 0$, IL = 1 and IU = 0;
 if RANGE = 'T' and $N > 0$, $1 \leq IL \leq IU \leq N$.
- 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

$$\text{ABSTOL} + \epsilon \max(|a|, |b|),$$
 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 $2 \times \text{X02AMF}()$, not zero. If this routine returns with INFO > 0, indicating that some eigenvectors did not converge, try setting ABSTOL to $2 \times \text{X02AMF}()$. See Demmel and Kahan (1990).

- 11: M – INTEGER *Output*
On exit: the total number of eigenvalues found. $0 \leq M \leq N$.
 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,*) – **double precision** 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 i th 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 F08GBF (DSPEVX) is called.
Constraints:
 if JOBZ = 'V', $LDZ \geq \max(1, N)$;
 otherwise $LDZ \geq 1$.
- 15: WORK($8 \times N$) – **double precision** array *Workspace*
- 16: IWORK($5 \times N$) – INTEGER array *Workspace*
- 17: JFAIL(N) – INTEGER array *Output*
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.
- 18: 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 complex analogue of this routine is F08GPF (ZHPEVX).

9 Example

This example finds the eigenvalues in the half-open interval $(-1, 1]$, and the corresponding eigenvectors, of the symmetric matrix

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

9.1 Program Text

```
*      F08GBF 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 ..
      DOUBLE PRECISION AP((NMAX*(NMAX+1))/2), W(NMAX), WORK(8*NMAX),
+      Z(LDZ,MMAX)
      INTEGER          IWORK(5*NMAX), JFAIL(NMAX)
*      .. External Subroutines ..
      EXTERNAL        DSPEVX, X04CAF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F08GBF 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 symmetric eigenvalue problem
*
    CALL DSPEVX('Vectors','Values in range',UPLO,N,AP,VL,VU,IL,IU,
+             ABSTOL,M,W,Z,LDZ,WORK,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 X04CAF('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 DSPEVX. 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

F08GBF Example Program Data

```

      4                      :Value of N
-1.0  1.0                  :Values of VL and VU

      1.0  2.0  3.0  4.0
           2.0  3.0  4.0
                3.0  4.0
                   4.0 :End of matrix A

```

9.3 Program Results

F08GBF Example Program Results

Number of eigenvalues found = 2

Eigenvalues

```
      -0.5146 -0.2943
Selected eigenvectors
      1      2
1  -0.5144  0.2767
2   0.4851 -0.6634
3   0.5420  0.6504
4  -0.4543 -0.2457
```
