NAG Library Routine Document

F08JBF (DSTEVX)

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

F08JBF (DSTEVX) computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix A. 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 F08JBF(JOBZ, RANGE, N, D, E, VL, VU, IL, IU, ABSTOL, M, W, Z,
     1                  LDZ, WORK, IWORK, JFAIL, INFO)
      INTEGER           N, IL, IU, M, LDZ, IWORK(5*N), JFAIL(*), INFO
      double precision  D(*), E(*), VL, VU, ABSTOL, W(N), Z(LDZ,*), WORK(5*N)
      CHARACTER*1       JOBZ, RANGE
```

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

3 Description

F08JBF (DSTEVX) computes the required eigenvalues and eigenvectors of A by reducing the tridiagonal matrix to diagonal form using the QR algorithm. Bisection is used to determine selected eigenvalues.

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: N – INTEGER *Input*

On entry: n, the order of the matrix.

Constraint: $N \geq 0$.

4: D(*) – ***double precision*** array *Input/Output*

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

On entry: the n diagonal elements of the tridiagonal matrix A.

On exit: may be multiplied by a constant factor chosen to avoid over/underflow in computing the eigenvalues.

5: E(*) – ***double precision*** array *Input/Output*

Note: the dimension of the array E must be at least $\max(1, N - 1)$.

On entry: the $(n - 1)$ subdiagonal elements of the tridiagonal matrix A.

On exit: may be multiplied by a constant factor chosen to avoid over/underflow in computing the eigenvalues.

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', VL < 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 $N = 0$, $IL = 1$ and $IU = 0$;
if RANGE = 'I' 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

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

where ϵ is the ***machine precision***. If ABSTOL is less than or equal to zero, then $\epsilon \|A\|_1$ will be used in its place. 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 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. $0 \leq M \leq N$.

If RANGE = 'A', $M = N$.

If RANGE = 'I', $M = IU - IL + 1$.

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

On exit: the first M elements contain 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 $\max(1, \mathrm{M})$.

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 $\mathrm{W}(i)$.

If an eigenvector fails to converge (INFO > 0), 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 $\max(1, \mathrm{M})$ 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 F08JBF (DSTEVX) is called.

Constraints:

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

15: WORK($5 \times \mathrm{N}$) – ***double precision*** array *Workspace*

16: IWORK($5 \times \mathrm{N}$) – INTEGER array *Workspace*

17: JFAIL($*$) – INTEGER array *Output*

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

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.

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^2 if JOBZ = 'N' and is proportional to n^3 if JOBZ = 'V' and RANGE = 'A', otherwise the number of floating-point operations will depend upon the number of computed eigenvectors.

9 Example

This example finds the eigenvalues in the half-open interval $(0, 5]$, and the corresponding eigenvectors, of the symmetric tridiagonal matrix

$$A = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 4 & 2 & 0 \\ 0 & 2 & 9 & 3 \\ 0 & 0 & 3 & 16 \end{pmatrix}.$$

9.1 Program Text

```
*     F08JBF Example Program Text
*     Mark 21 Release.  NAG Copyright 2004.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, MMAX
      PARAMETER        (NMAX=20,MMAX=10)
      INTEGER          LDZ
      PARAMETER        (LDZ=NMAX)
*     .. Local Scalars ..
      DOUBLE PRECISION ABSTOL, VL, VU
      INTEGER          I, IFAIL, IL, INFO, IU, J, M, N
*     .. Local Arrays ..
      DOUBLE PRECISION D(NMAX), E(NMAX), W(NMAX), WORK(5*NMAX),
     +                 Z(LDZ,MMAX)
      INTEGER          IWORK(5*NMAX), JFAIL(NMAX)
*     .. External Functions ..
      DOUBLE PRECISION X02AMF
      EXTERNAL         X02AMF
*     .. External Subroutines ..
      EXTERNAL         DSTEVX, X04CAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F08JBF 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 diagonal and off-diagonal elements of the matrix
*        A from data file
*
         READ (NIN,*) VL, VU
         READ (NIN,*) (D(I),I=1,N)
         READ (NIN,*) (E(I),I=1,N-1)
*
*        Set the absolute error tolerance for eigenvalues.  With ABSTOL
*        set to zero, the default value would be used instead
*
         ABSTOL = 2*X02AMF()
```

```
*
*        Solve the symmetric eigenvalue problem
*
         CALL DSTEVX('Vectors','Values in range',N,D,E,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 DSTEVX. 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

```
F08JBF Example Program Data

  4                    :Value of N

  0.0  5.0             :Values of VL and VU

  1.0  4.0  9.0  16.0  :End of diagonal elements
  1.0  2.0  3.0        :End of off-diagonal elements
```

9.3 Program Results

```
 F08JBF Example Program Results

 Number of eigenvalues found =    2

 Eigenvalues
     0.6476  3.5470
 Selected eigenvectors
          1       2
 1   0.9396  0.3388
 2  -0.3311  0.8628
 3   0.0853 -0.3648
 4  -0.0167  0.0879
```