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, LDZ, WORK, IWORK, JFAIL, INFO)

INTEGER            N, IL, IU, M, LDZ, IWORK(5*N), JFAIL(*), INFO
REAL (KIND=nag_wp) 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, 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: indicates whether eigenvectors are computed.

JOBZ = 'N'
Only eigenvalues are computed.

JOBZ = 'V'
Eigenvalues and eigenvectors are computed.

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($*$) – REAL (KIND=nag_wp) 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($*$) – REAL (KIND=nag_wp) 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 – REAL (KIND=nag_wp) *Input*
7: VU – REAL (KIND=nag_wp) *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 – REAL (KIND=nag_wp) *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) – REAL (KIND=nag_wp) array *Output*

On exit: the first M elements contain the selected eigenvalues in ascending order.

13: Z(LDZ, ∗) – REAL (KIND=nag_wp) 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 (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, 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 ≥ max(1, N);
otherwise LDZ ≥ 1.

15: WORK(5 × N) – REAL (KIND=nag_wp) array *Workspace*

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

17: 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 = 'N', 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

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

The algorithm failed to converge; $\langle value \rangle$ eigenvectors did not converge. Their indices are stored in array JFAIL.

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 Parallelism and Performance

F08JBF (DSTEVX) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

F08JBF (DSTEVX) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 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.

10 Example

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

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

10.1 Program Text

```
    Program f08jbfe

!     F08JBF Example Program Text

!     Mark 25 Release. NAG Copyright 2014.

!     .. Use Statements ..
      Use nag_library, Only: dstevx, nag_wp, x02amf, x04caf
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: abstol, vl, vu
      Integer                          :: ifail, il, info, iu, ldz, m, n
!     .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable  :: d(:), e(:), w(:), work(:), z(:,:)
      Integer, Allocatable             :: iwork(:), jfail(:)
!     .. Executable Statements ..
      Write (nout,*) 'F08JBF Example Program Results'
```

```
      Write (nout,*)
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) n
      ldz = n
      m = n
      Allocate (d(n),e(n),w(n),work(5*n),z(ldz,m),iwork(5*n),jfail(n))

!     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(1:n)
      Read (nin,*) e(1:n-1)

!     Set the absolute error tolerance for eigenvalues.  With ABSTOL
!     set to zero, the default value would be used instead

      abstol = 2.0E0_nag_wp*x02amf()

!     Solve the symmetric eigenvalue problem
!     The NAG name equivalent of dstevx is f08jbf
      Call dstevx('Vectors','Values in range',n,d,e,vl,vu,il,iu,abstol,m,w,z, &
        ldz,work,iwork,jfail,info)

      If (info>=0) Then

!       Print solution

        Write (nout,99999) 'Number of eigenvalues found =', m
        Write (nout,*)
        Write (nout,*) 'Eigenvalues'
        Write (nout,99998) w(1:m)
        Flush (nout)

!       ifail: behaviour on error exit
!              =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
        ifail = 0
        Call x04caf('General',' ',n,m,z,ldz,'Selected eigenvectors',ifail)

        If (info>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(1:m)
        End If
      Else
        Write (nout,99999) 'Failure in DSTEVX. INFO =', info
      End If

99999 Format (1X,A,I5)
99998 Format (3X,(8F8.4))
99997 Format (3X,(8I8))
    End Program f08jbfe
```

10.2 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
```

10.3 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
```