NAG Fortran Library Routine Document

F08JAF (DSTEV)

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

F08JAF (DSTEV) computes all eigenvalues and, optionally, eigenvectors of a real symmetric n by n tridiagonal matrix A.

2 Specification

```
SUBROUTINE F08JAF (JOBZ, N, D, E, Z, LDZ, WORK, INFO)
INTEGER             N, LDZ, INFO
double precision    D(*), E(*), Z(LDZ,*), WORK(*)
CHARACTER*1         JOBZ
```

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

3 Description

F08JAF (DSTEV) computes all eigenvalues, and optionally the eigenvectors of A using a combination of the QR and QL algorithms, with an implicit shift.

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 URL: http://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: N – INTEGER *Input*

On entry: n, the order of the matrix.

Constraint: N ≥ 0.

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

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

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

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

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

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

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

On exit: the contents of E are destroyed.

5: Z(LDZ,∗) – ***double precision*** 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 $\mathrm{D}(i)$.

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

6: LDZ – INTEGER *Input*

On entry: the first dimension of the array Z as declared in the (sub)program from which F08JAF (DSTEV) is called.

Constraints:

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

7: WORK(∗) – ***double precision*** array *Workspace*

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

On exit: if JOBZ = 'N', WORK is not referenced.

8: 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 $= -i$, the ith argument had an illegal value.

INFO > 0

If INFO $= i$, the algorithm failed to converge; i off-diagonal elements of E 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

The total number of floating point operations is proportional to n^2 if JOBZ = 'N' and is proportional to n^3 if JOBZ = 'V'.

9 Example

To find all the eigenvalues and eigenvectors of the symmetric tridiagonal matrix

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

together with approximate error bounds for the computed eigenvalues and eigenvectors.

9.1 Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     F08JAF Example Program Text
*     Mark 21 Release. NAG Copyright 2004.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX
      PARAMETER        (NMAX=20)
      INTEGER          LDZ
      PARAMETER        (LDZ=NMAX)
*     .. Local Scalars ..
      DOUBLE PRECISION EERRBD, EPS
      INTEGER          I, IFAIL, INFO, N
*     .. Local Arrays ..
      DOUBLE PRECISION D(NMAX), E(NMAX-1), RCONDZ(NMAX), WORK(2*NMAX-2),
     +                 Z(LDZ,NMAX), ZERRBD(NMAX)
*     .. External Functions ..
      DOUBLE PRECISION X02AJF
      EXTERNAL         X02AJF
*     .. External Subroutines ..
      EXTERNAL         DDISNA, DSTEV, X04CAF
*     .. Intrinsic Functions ..
      INTRINSIC        ABS, MAX
*     .. Executable Statements ..
      WRITE (NOUT,*) 'F08JAF Example Program Results'
      WRITE (NOUT,*)
*     Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N
      IF (N.LE.NMAX) THEN
*
*        Read the diagonal and off-diagonal elements of the matrix A
*        from data file
*
         READ (NIN,*) (D(I),I=1,N)
         READ (NIN,*) (E(I),I=1,N-1)
*
*        Solve the symmetric tridiagonal eigenvalue problem
*
         CALL DSTEV('Vectors',N,D,E,Z,LDZ,WORK,INFO)
*
         IF (INFO.EQ.0) THEN
*
*           Print solution
*
            WRITE (NOUT,*) 'Eigenvalues'
            WRITE (NOUT,99999) (D(I),I=1,N)
*
            IFAIL = 0
            CALL X04CAF('General',' ',N,N,Z,LDZ,'Eigenvectors',IFAIL)
*
*           Get the machine precision, EPS and compute the approximate
*           error bound for the computed eigenvalues.  Note that for
*           the 2-norm, max( abs(D(i)) ) = norm(A), and since the
```

```
*           eigenvalues are returned in ascending order
*           max( abs(D(i)) ) = max( abs(D(1)), abs(D(n)))
*
            EPS = X02AJF()
            EERRBD = EPS*MAX(ABS(D(1)),ABS(D(N)))
*
*           Call DDISNA (F08FLF) to estimate reciprocal condition
*           numbers for the eigenvectors
*
            CALL DDISNA('Eigenvectors',N,N,D,RCONDZ,INFO)
*
*           Compute the error estimates for the eigenvectors
*
            DO 20 I = 1, N
               ZERRBD(I) = EERRBD/RCONDZ(I)
   20       CONTINUE
*
*           Print the approximate error bounds for the eigenvalues
*           and vectors
*
            WRITE (NOUT,*)
            WRITE (NOUT,*) 'Error estimate for the eigenvalues'
            WRITE (NOUT,99998) EERRBD
            WRITE (NOUT,*)
            WRITE (NOUT,*) 'Error estimates for the eigenvectors'
            WRITE (NOUT,99998) (ZERRBD(I),I=1,N)
         ELSE
            WRITE (NOUT,99997) 'Failure in DSTEV. INFO =', INFO
         END IF
      ELSE
         WRITE (NOUT,*) 'NMAX too small'
      END IF
      STOP
*
99999 FORMAT (3X,(8F8.4))
99998 FORMAT (4X,1P,6E11.1)
99997 FORMAT (1X,A,I4)
      END
```

9.2 Program Data

```
F08JAF Example Program Data

  4                         :Value of N

  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

```
 F08JAF Example Program Results

 Eigenvalues
     0.6476  3.5470  8.6578 17.1477
 Eigenvectors
          1       2       3       4
 1   0.9396  0.3388  0.0494  0.0034
 2  -0.3311  0.8628  0.3781  0.0545
 3   0.0853 -0.3648  0.8558  0.3568
 4  -0.0167  0.0879 -0.3497  0.9326

 Error estimate for the eigenvalues
        1.9E-15

 Error estimates for the eigenvectors
        6.6E-16    6.6E-16    3.7E-16    2.2E-16
```