F08JCF (SSTEVD/DSTEVD) - NAG Fortran Library Routine Document

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

F08JCF (SSTEVD/DSTEVD) computes all the eigenvalues, and optionally all the eigenvectors, of a real symmetric tridiagonal matrix. If the eigenvectors are requested, then it uses a divide and conquer algorithm to compute eigenvalues and eigenvectors. However, if only eigenvalues are required, then it uses the Pal-Walker-Kahan variant of the QL or QR algorithm.

2 Specification

```
SUBROUTINE FO8JCF(JOB, N, D, E, Z, LDZ, WORK, LWORK, IWORK, 1 LIWORK, INFO)

ENTRY sstevd(JOB, N, D, E, Z, LDZ, WORK, LWORK, IWORK, 1 LIWORK, INFO)

INTEGER N, LDZ, LWORK, IWORK(*), LIWORK, INFO real D(*), E(*), Z(LDZ,*), WORK(*)

CHARACTER*1 JOB
```

The ENTRY statement enables the routine to be called by its LAPACK name.

3 Description

This routine computes all the eigenvalues, and optionally all the eigenvectors, of a real symmetric tridiagonal matrix T. In other words, it can compute the spectral factorization of T as

$$T = Z\Lambda Z^T$$
,

where Λ is a diagonal matrix whose diagonal elements are the eigenvalues λ_i , and Z is the orthogonal matrix whose columns are the eigenvectors z_i . Thus

$$Tz_i = \lambda_i z_i$$
 for $i = 1, 2, \dots, n$.

4 References

[1] Golub G H and Van Loan C F (1996) Matrix Computations Johns Hopkins University Press (3rd Edition), Baltimore

5 Parameters

1: JOB — CHARACTER*1

Input

On entry: indicates whether eigenvectors are computed as follows:

if JOB = 'N', then only eigenvalues are computed;

if JOB = 'V', then eigenvalues and eigenvectors are computed.

Constraint: JOB = 'N' or 'V'.

2: N — INTEGER

Input

On entry: n, the order of the matrix A.

Constraint: $N \geq 0$.

3: D(*) - real 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 T.

On exit: the eigenvalues of the matrix T in ascending order.

4: E(*) — real array

Input/Output

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

On entry: the n-1 off-diagonal elements of the tridiagonal matrix T. The nth element of this array is used as workspace.

On exit: the array is overwritten with intermediate results.

5: Z(LDZ, *) - real array

Output

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

On exit: if JOB = V', then this is overwritten by the orthogonal matrix Z which contains the eigenvectors of T.

If JOB = 'N', then Z is not referenced.

6: LDZ — INTEGER

Input

On entry: the leading dimension of the array Z as declared in the (sub)program from which F08JCF (SSTEVD/DSTEVD) is called.

Constraints:

$$LDZ \ge max(1,N)$$
 if $JOB = 'V'$; $LDZ > 1$ if $JOB = 'N'$.

7: WORK(*) - real array

Work space

Note: the dimension of the array WORK must be at least LWORK.

On exit: if LWORK > 0, then WORK(1) contains the required minimal size of LWORK.

8: LWORK — INTEGER

Input

On entry: the dimension of the array WORK as declared in the (sub)program from which F08JCF (SSTEVD/DSTEVD) is called.

Constraints:

```
if JOB = 'N' or N \leq 1, then LWORK \geq 1; if JOB = 'V' and N > 1, then LWORK \geq 2 \times N<sup>2</sup> + (3+2k) \times N + 1 where k is the smallest integer which satisfies 2^k \geq N.
```

9: IWORK(*) — INTEGER array

Work space

Note: the dimension of the array IWORK must be at least LIWORK.

On exit: if LIWORK > 0, then IWORK(1) contains the required minimal size of LIWORK.

10: LIWORK — INTEGER

Input

On entry: the dimension of the array IWORK as declared in the (sub)program from which F08JCF (SSTEVD/DSTEVD) is called.

Constraints:

```
if JOB = 'N' or N \leq 1, then LIWORK \geq 1; if JOB = 'V' and N > 1, then LIWORK \geq 5 \times N + 2.
```

11: 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, the *i*th parameter had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0

If INFO = i, then the algorithm failed to converge; i indicates the number of elements of an intermediate tridiagonal form which did not converge to zero.

7 Accuracy

The computed eigenvalues and eigenvectors are exact for a nearby matrix T + E, where

$$||E||_2 = O(\epsilon)||T||_2$$

and ϵ is the *machine precision*.

If λ_i is an exact eigenvalue and $\tilde{\lambda}_i$ is the corresponding computed value, then

$$|\tilde{\lambda}_i - \lambda_i| \le c(n)\epsilon ||T||_2$$

where c(n) is a modestly increasing function of n.

If z_i is the corresponding exact eigenvector, and \tilde{z}_i is the corresponding computed eigenvector, then the angle $\theta(\tilde{z}_i, z_i)$ between them is bounded as follows:

$$\theta(\tilde{z}_i, z_i) \leq \frac{c(n)\epsilon \|T\|_2}{\min\limits_{i \neq j} |\lambda_i - \lambda_j|}.$$

Thus the accuracy of a computed eigenvector depends on the gap between its eigenvalue and all the other eigenvalues.

8 Further Comments

There is no complex analogue of this routine.

9 Example

To compute all the eigenvalues and eigenvectors of the symmetric tridiagonal matrix T, where

$$T = \begin{pmatrix} 1.0 & 1.0 & 0.0 & 0.0 \\ 1.0 & 4.0 & 1.0 & 0.0 \\ 0.0 & 1.0 & 9.0 & 1.0 \\ 0.0 & 0.0 & 1.0 & 16.0 \end{pmatrix}.$$

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.

```
FO8JCF Example Program Text.
Mark 19 Release. NAG Copyright 1999.
.. Parameters ..
             NIN, NOUT
INTEGER
PARAMETER
                (NIN=5,NOUT=6)
INTEGER
              NMAX, LDZ
PARAMETER
               (NMAX=8,LDZ=NMAX)
INTEGER
               LWORK, LIWORK
PARAMETER
               (LWORK=4*NMAX*NMAX,LIWORK=5*NMAX+2)
.. Local Scalars ..
         I, IFAIL, INFO, N
INTEGER
CHARACTER
                JOB
.. Local Arrays ..
real
                D(NMAX), E(NMAX), WORK(LWORK), Z(LDZ,NMAX)
INTEGER
                IWORK(LIWORK)
.. External Subroutines ..
                sstevd, XO4CAF
EXTERNAL
.. Executable Statements ..
WRITE (NOUT,*) 'FO8JCF Example Program Results'
Skip heading in data file
READ (NIN,*)
READ (NIN,*) N
IF (N.LE.NMAX) THEN
   Read T from data file
   READ (NIN,*) (D(I), I=1,N)
   READ (NIN,*) (E(I), I=1, N-1)
   READ (NIN,*) JOB
   Calculate all the eigenvalues and eigenvectors of T
   CALL sstevd(JOB,N,D,E,Z,LDZ,WORK,LWORK,IWORK,LIWORK,INFO)
   WRITE (NOUT, *)
   IF (INFO.GT.O) THEN
      WRITE (NOUT,*) 'Failure to converge.'
      Print eigenvalues and eigenvectors
      WRITE (NOUT,*) 'Eigenvalues'
      WRITE (NOUT,99999) (D(I),I=1,N)
      WRITE (NOUT,*)
      IFAIL = 0
      CALL X04CAF('General',' ',N,N,Z,LDZ,'Eigenvectors',IFAIL)
   END IF
END IF
STOP
```

```
99999 FORMAT (3X,(8F8.4))
END
```

9.2 Program Data

FO8JCF Example Program Data

4 :Value of N
1.0 4.0 9.0 16.0
1.0 2.0 3.0 :End of T
'V' :Value of JOB

9.3 Program Results

F08JCF 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