NAG Fortran Library Routine Document

F08JXF (CSTEIN/ZSTEIN)

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

F08JXF (CSTEIN/ZSTEIN) computes the eigenvectors of a real symmetric tridiagonal matrix corresponding to specified eigenvalues, by inverse iteration, storing the eigenvectors in a ***complex*** array.

2 Specification

```
 SUBROUTINE F08JXF(N, D, E, M, W, IBLOCK, ISPLIT, Z, LDZ, WORK, IWORK,
1                  IFAILV, INFO)
 ENTRY      cstein (N, D, E, M, W, IBLOCK, ISPLIT, Z, LDZ, WORK, IWORK,
1                  IFAILV, INFO)
 INTEGER           N, M, IBLOCK(*), ISPLIT(*), LDZ, IWORK(*), IFAILV(*),
1                  INFO
 real              D(*), E(*), W(*), WORK(*)
 complex           Z(LDZ,*)
```

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

3 Description

This routine computes the eigenvectors of a real symmetric tridiagonal matrix T corresponding to specified eigenvalues, by inverse iteration (see Jessup and Ipsen (1992)). It is designed to be used in particular after the specified eigenvalues have been computed by F08JJF (SSTEBZ/DSTEBZ) with ORDER = 'B', but may also be used when the eigenvalues have been computed by other F08 or F02 routines.

The eigenvectors of T are real, but are stored by this routine in a ***complex*** array. If T has been formed by reduction of a full complex Hermitian matrix A to tridiagonal form, then eigenvectors of T may be transformed to (complex) eigenvectors of A, by a call to F08FUF (CUNMTR/ZUNMTR) or F08GUF (CUPMTR/ZUPMTR).

F08JJF determines whether the matrix T splits into block diagonal form:

$$T = \begin{pmatrix} T_1 & & & & \\ & T_2 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & T_p \end{pmatrix}$$

and passes details of the block structure to this routine in the arrays IBLOCK and ISPLIT. This routine can then take advantage of the block structure by performing inverse iteration on each block T_i separately, which is more efficient than using the whole matrix.

4 References

Golub G H and van Loan C F (1996) *Matrix Computations* (3rd Edition) Johns Hopkins University Press, Baltimore

Jessup E and Ipsen I C F (1992) Improving the accuracy of inverse iteration *SIAM J. Sci. Statist. Comput.* **13** 550–572

5 Parameters

1: N – INTEGER *Input*

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

Constraint: N ≥ 0.

2: D(∗) – ***real*** array *Input*

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

On entry: the diagonal elements of the tridiagonal matrix T.

3: E(∗) – ***real*** array *Input*

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

On entry: the off-diagonal elements of the tridiagonal matrix T.

4: M – INTEGER *Input*

On entry: m, the number of eigenvectors to be returned.

Constraint: $0 \leq \mathrm{M} \leq \mathrm{N}$.

5: W(∗) – ***real*** array *Input*

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

On entry: the eigenvalues of the tridiagonal matrix T stored in W(1) to W(m), as returned by F08JJF (SSTEBZ/DSTEBZ) with ORDER = 'B'. Eigenvalues associated with the first sub-matrix must be supplied first, in non-decreasing order; then those associated with the second sub-matrix, again in non-decreasing order; and so on.

Constraint: if IBLOCK(i) = IBLOCK($i+1$), W(i) $\leq$ W($i+1$) for $i = 1, 2, \ldots, m-1$.

6: IBLOCK(∗) – INTEGER array *Input*

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

On entry: the first m elements must contain the sub-matrix indices associated with the specified eigenvalues, as returned by F08JJF (SSTEBZ/DSTEBZ) with ORDER = 'B'. If the eigenvalues were not computed by F08JJF with ORDER = 'B', set IBLOCK(i) to 1 for $i = 1, 2, \ldots, m$.

Constraint: IBLOCK(i) $\leq$ IBLOCK($i+1$) for $i = 1, 2, \ldots, m-1$.

7: ISPLIT(∗) – INTEGER array *Input*

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

On entry: the points at which T breaks up into sub-matrices, as returned by F08JJF (SSTEBZ/DSTEBZ) with ORDER = 'B'. If the eigenvalues were not computed by F08JJF with ORDER = 'B', set ISPLIT(1) to N.

8: Z(LDZ,*) – ***complex*** array *Output*

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

On exit: the m eigenvectors, stored by columns; the ith column corresponds to the ith specified eigenvalue, unless INFO > 0 (in which case see Section 6).

9: LDZ – INTEGER *Input*

On entry: the first dimension of the array Z as declared in the (sub)program from which F08JXF (CSTEIN/ZSTEIN) is called.

Constraint: LDZ $\geq \max(1, \mathrm{N})$.

10: WORK(∗) – ***real*** array *Workspace*

Note: the dimension of the array WORK must be at least $\max(1, 5 * \mathrm{N})$.

11: IWORK(∗) – INTEGER array *Workspace*

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

12: IFAILV(∗) – INTEGER array *Output*

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

On exit: if INFO $= i > 0$, the first i elements of IFAILV contain the indices of any eigenvectors which have failed to converge. The rest of the first M elements of IFAILV are set to 0.

13: 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 ith parameter had an illegal value. An explanatory message is output, and execution of the program is terminated.

INFO > 0

If INFO $= i$, then i eigenvectors (as indicated by the parameter IFAILV above) each failed to converge in 5 iterations. The current iterate after 5 iterations is stored in the corresponding column of Z.

7 Accuracy

Each computed eigenvector z_i is the exact eigenvector of a nearby matrix $A + E_i$, such that $\|E_i\| = O(\epsilon)\|A\|$, where ϵ is the ***machine precision***. Hence the residual is small:

$$\|Az_i - \lambda_i z_i\| = O(\epsilon)\|A\|.$$

However, a set of eigenvectors computed by this routine may not be orthogonal to so high a degree of accuracy as those computed by F08JSF (CSTEQR/ZSTEQR).

8 Further Comments

The real analogue of this routine is F08JKF (SSTEIN/DSTEIN).

9 Example

See Section 9 of the document for F08FUF (CUNMTR/ZUNMTR).