F08JSF (CSTEQR/ZSTEQR) – 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

F08JSF (CSTEQR/ZSTEQR) computes all the eigenvalues, and optionally all the eigenvectors, of a complex Hermitian matrix which has been reduced to tridiagonal form.

2 Specification

```
SUBROUTINE F08JSF(COMPZ, N, D, E, Z, LDZ, WORK, INFO)
ENTRY      csteqr(COMPZ, N, D, E, Z, LDZ, WORK, INFO)
INTEGER           N, LDZ, INFO
real              D(*), E(*), WORK(*)
complex           Z(LDZ,*)
CHARACTER*1       COMPZ
```

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

$$Tz_i = \lambda_i z_i \text{ for } i = 1, 2, \ldots, n.$$

The routine stores the real orthogonal matrix Z in a ***complex*** array, so that it may also be used to compute all the eigenvalues and eigenvectors of a complex Hermitian matrix A which has been reduced to tridiagonal form T:

$$\begin{aligned} A &= QTQ^H, \text{ where } Q \text{ is unitary,} \\ &= (QZ)\Lambda(QZ)^H. \end{aligned}$$

In this case, the matrix Q must be formed explicitly and passed to F08JSF, which must be called with COMPZ = 'V'. The routines which must be called to perform the reduction to tridiagonal form and form Q are:

full matrix	F08FSF (CHETRD/ZHETRD) + F08FTF (CUNGTR/ZUNGTR)
full matrix, packed storage	F08GSF (CHPTRD/ZHPTRD) + F08GTF (CUPGTR/ZUPGTR)
band matrix	F08HSF (CHBTRD/ZHBTRD) with VECT = 'V'.

F08JSF uses the implicitly shifted QR algorithm, switching between the QR and QL variants in order to handle graded matrices effectively (see Greenbaum and Dongarra [2]). The eigenvectors are normalized so that $\| z_i \|_2 = 1$, but are determined only to within a complex factor of absolute value 1.

If only the eigenvalues of T are required, it is more efficient to call F08JFF (SSTERF/DSTERF) instead. If T is positive-definite, small eigenvalues can be computed more accurately by F08JUF (CPTEQR/ZPTEQR).

4 References

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

[2] Greenbaum A and Dongarra J J (1980) Experiments with QR/QL methods for the symmetric triangular eigenproblem *LAPACK Working Note No. 17 (Technical Report CS–89–92)* University of Tennessee, Knoxville

[3] Parlett B N (1980) *The Symmetric Eigenvalue Problem* Prentice–Hall

5 Parameters

1: COMPZ — CHARACTER*1 *Input*

On entry: indicates whether the eigenvectors are to be computed as follows:

if COMPZ = 'N', then only the eigenvalues are computed (and the array Z is not referenced);
if COMPZ = 'I', then the eigenvalues and eigenvectors of T are computed (and the array Z is initialized by the routine);
if COMPZ = 'V', then the eigenvalues and eigenvectors of A are computed (and the array Z must contain the matrix Q on entry).

Constraint: COMPZ = 'N', 'V' or 'I'.

2: N — INTEGER *Input*

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

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 diagonal elements of the tridiagonal matrix T.

On exit: the n eigenvalues in ascending order, unless INFO > 0 (in which case see Section 6).

4: E($*$) — ***real*** array *Input/Output*

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

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

On exit: the array is overwritten.

5: Z(LDZ,$*$) — ***complex*** array *Input/Output*

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

On entry: if COMPZ = 'V', Z must contain the unitary matrix Q from the reduction to tridiagonal form. If COMPZ = 'I', Z need not be set.

On exit: if COMPZ = 'I' or 'V', the n required orthonormal eigenvectors stored by columns; the ith column corresponds to the ith eigenvalue, where $i = 1, 2, \ldots, n$, unless INFO > 0.

Z is not referenced if COMPZ = 'N'.

6: LDZ — INTEGER *Input*

On entry: the first dimension of the array Z as declared in the (sub)program from which F08JSF (CSTEQR/ZSTEQR) is called.

Constraints:

LDZ $\geq$ 1 if COMPZ = 'N',
LDZ $\geq$ max(1,N) if COMPZ = 'V' or 'I'.

7: WORK(∗) — ***real*** array *Workspace*

Note: the dimension of the array WORK must be at least max(1,2*(N−1)) if COMPZ = 'V' or 'I', and at least 1 if COMPZ = 'N'.

WORK is not referenced if COMPZ = 'N'.

8: 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

The algorithm has failed to find all the eigenvalues after a total of 30 × N iterations. In this case, D and E contain on exit the diagonal and off-diagonal elements, respectively, of a tridiagonal matrix orthogonally similar to T. If INFO = i, then i off-diagonal elements have not converged 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

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

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:

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

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

8 Further Comments

The total number of real floating-point operations is typically about $24n^2$ if COMPZ = 'N' and about $14n^3$ if COMPZ = 'V' or 'I', but depends on how rapidly the algorithm converges. When COMPZ = 'N', the operations are all performed in scalar mode; the additional operations to compute the eigenvectors when COMPZ = 'V' or 'I' can be vectorized and on some machines may be performed much faster.

The real analogue of this routine is F08JEF (SSTEQR/DSTEQR).

9 Example

See the examples for F08FTF (CUNGTR/ZUNGTR), F08GTF (CUPGTR/ZUPGTR) or F08HSF (CHBTRD/ZHBTRD), which illustrate the use of this routine to compute the eigenvalues and eigenvectors of a full or band Hermitian matrix.