NAG Library Routine Document

F08JSF (ZSTEQR)

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 (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)

INTEGER                 N, LDZ, INFO
REAL (KIND=nag_wp)      D(*), E(*), WORK(*)
COMPLEX (KIND=nag_wp)   Z(LDZ,*)
CHARACTER(1)            COMPZ
```

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

3 Description

F08JSF (ZSTEQR) 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

$$T = Z\Lambda Z^{\mathrm{T}},$$

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

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

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:

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

In this case, the matrix Q must be formed explicitly and passed to F08JSF (ZSTEQR), 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 (ZHETRD) and F08FTF (ZUNGTR)
full matrix, packed storage	F08GSF (ZHPTRD) and F08GTF (ZUPGTR)
band matrix	F08HSF (ZHBTRD) with VECT = 'V'.

F08JSF (ZSTEQR) uses the implicitly shifted QR algorithm, switching between the QR and QL variants in order to handle graded matrices effectively (see Greenbaum and Dongarra (1980)). 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 (DSTERF) instead. If T is positive definite, small eigenvalues can be computed more accurately by F08JUF (ZPTEQR).

4 References

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

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

Parlett B N (1998) *The Symmetric Eigenvalue Problem* SIAM, Philadelphia

5 Parameters

1: COMPZ – CHARACTER(1) *Input*

On entry: indicates whether the eigenvectors are to be computed.

COMPZ = 'N'
Only the eigenvalues are computed (and the array Z is not referenced).

COMPZ = 'I'
The eigenvalues and eigenvectors of T are computed (and the array Z is initialized by the routine).

COMPZ = 'V'
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: $\mathrm{N} \geq 0$.

3: D($*$) – REAL (KIND=nag_wp) array *Input/Output*

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.

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

4: E($*$) – REAL (KIND=nag_wp) array *Input/Output*

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.

On exit: E is overwritten.

5: Z(LDZ,$*$) – COMPLEX (KIND=nag_wp) array *Input/Output*

Note: the second dimension of the array Z must be at least $\max(1, \mathrm{N})$ 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 as columns of Z; the ith column corresponds to the ith eigenvalue, where $i = 1, 2, \ldots, n$, unless INFO > 0.

If COMPZ = '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 F08JSF (ZSTEQR) is called.

Constraints:

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

7: WORK($*$) – REAL (KIND=nag_wp) array *Workspace*

Note: the dimension of the array WORK must be at least $\max(1, 2 \times (\mathrm{N} - 1))$ if COMPZ $=$ 'V' or 'I' and at least 1 if COMPZ $=$ 'N'.

If COMPZ $=$ '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 $= -i$, argument i 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 $30 \times \mathrm{N}$ iterations. In this case, D and E contain on exit the diagonal and off-diagonal elements, respectively, of a tridiagonal matrix 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

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

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:

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

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 (DSTEQR).

9 Example

See Section 9 in F08FTF (ZUNGTR), F08GTF (ZUPGTR) or F08HSF (ZHBTRD), which illustrate the use of this routine to compute the eigenvalues and eigenvectors of a full or band Hermitian matrix.