# NAG C Library Function Document nag zstein (f08jxc)

# 1 Purpose

nag\_zstein (f08jxc) 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

void nag\_zstein (Nag\_OrderType order, Integer n, const double d[], const double e[], Integer m, const double w[], const Integer iblock[], const Integer isplit[], Complex z[], Integer pdz, Integer ifailv[], NagError \*fail)

# 3 Description

nag\_zstein (f08jxc) 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 nag\_dstebz (f08jjc) with  $\mathbf{order} = \mathbf{Nag\_ByBlock}$ , but may also be used when the eigenvalues have been computed by other f08 or f02 functions.

The eigenvectors of T are real, but are stored by this function 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 nag zunmtr (f08fuc) or nag zupmtr (f08guc).

nag dstebz (f08jjc) determines whether the matrix T splits into block diagonal form:

and passes details of the block structure to this function in the arrays **iblock** and **isplit**. This function 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: **order** – Nag\_OrderType

Input

On entry: the **order** parameter specifies the two-dimensional storage scheme being used, i.e., row-major ordering or column-major ordering. C language defined storage is specified by **order** = **Nag\_RowMajor**. See Section 2.2.1.4 of the Essential Introduction for a more detailed explanation of the use of this parameter.

 $Constraint: order = Nag\_RowMajor or Nag\_ColMajor.$ 

[NP3645/7] f08jxc.1

2:  $\mathbf{n}$  - Integer Input

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

Constraint:  $\mathbf{n} \geq 0$ .

3:  $\mathbf{d}[dim]$  – const double

Input

**Note:** the dimension, dim, of the array **d** must be at least max $(1, \mathbf{n})$ .

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

4:  $\mathbf{e}[dim]$  – const double

Input

**Note:** the dimension, dim, of the array **e** must be at least  $max(1, \mathbf{n} - 1)$ .

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

5:  $\mathbf{m}$  - Integer Input

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

Constraint:  $0 \le \mathbf{m} \le \mathbf{n}$ .

6:  $\mathbf{w}[dim]$  – const double

Input

**Note:** the dimension, dim, of the array w must be at least max $(1, \mathbf{n})$ .

On entry: the eigenvalues of the tridiagonal matrix T stored in  $\mathbf{w}[0]$  to  $\mathbf{w}[m]$ , as returned by nag\_dstebz (f08jjc) with  $\mathbf{rank} = \mathbf{Nag\_ByBlock}$ . 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],  $w[i] \le w[i+1]$  for i = 0, 1, ..., m-2.

7: **iblock**[dim] – const Integer

Input

**Note:** the dimension, dim, of the array **iblock** must be at least  $max(1, \mathbf{n})$ .

On entry: the first m elements must contain the sub-matrix indices associated with the specified eigenvalues, as returned by nag\_dstebz (f08jjc) with **order** = **Nag\_ByBlock**. If the eigenvalues were not computed by nag\_dstebz (f08jjc) with **order** = **Nag\_ByBlock**, set **iblock**[i-1] to 1 for  $i=1,2,\ldots,m$ .

Constraint:  $iblock[i] \le iblock[i+1]$  for i = 0, 1, ..., m-2.

8: isplit[dim] - const Integer

Input

**Note:** the dimension, dim, of the array **isplit** must be at least max $(1, \mathbf{n})$ .

On entry: the points at which T breaks up into sub-matrices, as returned by nag\_dstebz (f08jjc) with  $\mathbf{rank} = \mathbf{Nag\_ByBlock}$ . If the eigenvalues were not computed by nag\_dstebz (f08jjc) with  $\mathbf{rank} = \mathbf{Nag\_ByBlock}$ , set  $\mathbf{isplit}[0]$  to  $\mathbf{n}$ .

9:  $\mathbf{z}[dim]$  – Complex

Output

**Note:** the dimension, dim, of the array  $\mathbf{z}$  must be at least  $\max(1, \mathbf{pdz} \times \mathbf{m})$  when  $\mathbf{order} = \mathbf{Nag\_ColMajor}$  and at least  $\max(1, \mathbf{pdz} \times \mathbf{n})$  when  $\mathbf{order} = \mathbf{Nag\_RowMajor}$ .

If **order** = **Nag\_ColMajor**, the (i, j)th element of the matrix Z is stored in  $\mathbf{z}[(j-1) \times \mathbf{pdz} + i - 1]$  and if **order** = **Nag\_RowMajor**, the (i, j)th element of the matrix Z is stored in  $\mathbf{z}[(i-1) \times \mathbf{pdz} + j - 1]$ .

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

10: **pdz** – Integer Input

On entry: the stride separating matrix row or column elements (depending on the value of **order**) in the array z.

f08jxc.2 [NP3645/7]

Constraints:

```
if order = Nag_ColMajor, pdz \geq \max(1, \mathbf{n}); if order = Nag_RowMajor, pdz \geq \max(1, \mathbf{m}).
```

## 11: **ifailv**[dim] – Integer

Output

**Note:** the dimension, dim, of the array **ifailv** must be at least max $(1, \mathbf{m})$ .

On exit: if fail = 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.

#### 12: **fail** – NagError \*

Output

The NAG error parameter (see the Essential Introduction).

# 6 Error Indicators and Warnings

## NE\_INT

```
On entry, \mathbf{n} = \langle value \rangle.
Constraint: \mathbf{n} \geq 0.
On entry, \mathbf{pdz} = \langle value \rangle.
Constraint: \mathbf{pdz} > 0.
```

# NE\_INT\_2

```
On entry, \mathbf{m} = \langle value \rangle, \mathbf{n} = \langle value \rangle.
Constraint: 0 \le \mathbf{m} \le \mathbf{n}.
On entry, \mathbf{pdz} = \langle value \rangle, \mathbf{n} = \langle value \rangle.
Constraint: \mathbf{pdz} \ge \max(1, \mathbf{n}).
On entry, \mathbf{pdz} = \langle value \rangle, \mathbf{m} = \langle value \rangle.
Constraint: \mathbf{pdz} \ge \max(1, \mathbf{m}).
```

## NE\_INT\_ARRAY

```
On entry, \mathbf{iblock}[i]\mathbf{w}[i]\mathbf{iblock}[i] = \langle value \rangle.
Constraint: if \mathbf{iblock}[i] = \mathbf{iblock}[i+1], \mathbf{w}[i] \leq \mathbf{w}[i+1] for i = 0, \dots, \mathbf{m} - 2.
On entry, \mathbf{iblock}[i]\mathbf{w}[i]\mathbf{iblock}[i] = \langle value \rangle.
Constraint: \mathbf{iblock}[i] \leq \mathbf{iblock}[i+1] for i = 0, \dots, \mathbf{m} - 2.
```

#### **NE CONVERGENCE**

 $\langle value \rangle$  eigenvectors (as indicated by argument **ifailv**) each failed to converge in 5 iterations. The current iterate after 5 iterations is stored in the corresponding column of **z**.

#### NE\_ALLOC\_FAIL

Memory allocation failed.

## NE\_BAD\_PARAM

On entry, parameter  $\langle value \rangle$  had an illegal value.

## NE\_INTERNAL\_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please consult NAG for assistance.

[NP3645/7] f08jxc.3

# 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  $\epsilon$  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 function may not be orthogonal to so high a degree of accuracy as those computed by nag\_zsteqr (f08jsc).

# **8** Further Comments

The real analogue of this function is nag dstein (f08jkc).

# 9 Example

See Section 9 of the document for nag\_zunmtr (f08fuc).

f08jxc.4 (last) [NP3645/7]