NAG Library Function Document

nag_dstevx (f08jbc)

1 Purpose
nag_dstevx (f08jbc) computes selected eigenvalues and, optionally, eigenvectors of a real symmetric tridiagonal matrix $A$. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

2 Specification

```c
#include <nag.h>
#include <nagf08.h>

void nag_dstevx (Nag_OrderType order, Nag_JobType job, Nag_RangeType range,
                Integer n, double d[], double e[], double vl, double vu, Integer il,
                Integer iu, double abstol, Integer *m, double w[], double z[],
                Integer pdz, Integer jfail[], NagError *fail)
```

3 Description

nag_dstevx (f08jbc) computes the required eigenvalues and eigenvectors of $A$ by reducing the tridiagonal matrix to diagonal form using the QR algorithm. Bisection is used to determine selected eigenvalues.

4 References


5 Arguments

1:  **order** – Nag_OrderType  

   *Input*

   On entry: the **order** argument 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 3.2.1.3 in the Essential Introduction for a more detailed explanation of the use of this argument.

   **Constraint:** **order** = Nag_RowMajor or Nag_ColMajor.

2:  **job** – Nag_JobType  

   *Input*

   On entry: indicates whether eigenvectors are computed.

   **job** = Nag_EigVals
   Only eigenvalues are computed.

   **job** = Nag_DoBoth
   Eigenvalues and eigenvectors are computed.

   **Constraint:** **job** = Nag_EigVals or Nag_DoBoth.
3: \textbf{range} – Nag_RangeType \hspace{1cm} \textit{Input}

\textit{On entry}: if \textbf{range} = Nag_AllValues, all eigenvalues will be found.
If \textbf{range} = Nag_Interval, all eigenvalues in the half-open interval \([vl, vu]\) will be found.
If \textbf{range} = Nag_Indices, the \textit{il}th to \textit{iu}th eigenvalues will be found.
\textit{Constraint}: \textbf{range} = Nag_AllValues, Nag_Interval or Nag_Indices.

4: \textbf{n} – Integer \hspace{1cm} \textit{Input}

\textit{On entry}: \textbf{n}, the order of the matrix.
\textit{Constraint}: \textbf{n} \geq 0.

5: \textbf{d[dim]} – double \hspace{1cm} \textit{Input/Output}

\textit{Note}: the dimension, \textit{dim}, of the array \textbf{d} must be at least \(\text{max}(1, \textbf{n})\).
\textit{On entry}: the \textit{n} diagonal elements of the tridiagonal matrix \textbf{A}.
\textit{On exit}: may be multiplied by a constant factor chosen to avoid over/underflow in computing the eigenvalues.

6: \textbf{e[dim]} – double \hspace{1cm} \textit{Input/Output}

\textit{Note}: the dimension, \textit{dim}, of the array \textbf{e} must be at least \(\text{max}(1, \textbf{n} - 1)\).
\textit{On entry}: the \((n - 1)\) subdiagonal elements of the tridiagonal matrix \textbf{A}.
\textit{On exit}: may be multiplied by a constant factor chosen to avoid over/underflow in computing the eigenvalues.

7: \textbf{vl} – double \hspace{1cm} \textit{Input}
8: \textbf{vu} – double \hspace{1cm} \textit{Input}

\textit{On entry}: if \textbf{range} = Nag_Interval, the lower and upper bounds of the interval to be searched for eigenvalues.
If \textbf{range} = Nag_AllValues or Nag_Indices, \textbf{vl} and \textbf{vu} are not referenced.
\textit{Constraint}: if \textbf{range} = Nag_Interval, \textbf{vl} < \textbf{vu}.

9: \textbf{il} – Integer \hspace{1cm} \textit{Input}
10: \textbf{iu} – Integer \hspace{1cm} \textit{Input}

\textit{On entry}: if \textbf{range} = Nag_Indices, the indices (in ascending order) of the smallest and largest eigenvalues to be returned.
If \textbf{range} = Nag_AllValues or Nag_Interval, \textbf{il} and \textbf{iu} are not referenced.
\textit{Constraints}:
if \textbf{range} = Nag_Indices and \textbf{n} = 0, \textbf{il} = 1 and \textbf{iu} = 0;
if \textbf{range} = Nag_Indices and \textbf{n} > 0, 1 \leq \textbf{il} \leq \textbf{iu} \leq \textbf{n}.

11: \textbf{abstol} – double \hspace{1cm} \textit{Input}

\textit{On entry}: the absolute error tolerance for the eigenvalues. An approximate eigenvalue is accepted as converged when it is determined to lie in an interval \([a, b]\) of width less than or equal to
\[\text{abstol} + \epsilon \max(|a|, |b|),\]
where \(\epsilon\) is the \textit{machine precision}. If \textbf{abstol} is less than or equal to zero, then \(\epsilon \|A\|_1\) will be used in its place. Eigenvalues will be computed most accurately when \textbf{abstol} is set to twice the underflow threshold \(2 \times \text{nag\_real\_safe\_small\_number}(\ )\), not zero. If this function returns with \textbf{fail.code} = NE_CONVERGENCE, indicating that some eigenvectors did not converge, try setting \textbf{abstol} to \(2 \times \text{nag\_real\_safe\_small\_number}(\ )\). See Demmel and Kahan (1990).
12: \( m \) – Integer *  
On exit: the total number of eigenvalues found. \( 0 \leq m \leq n \).

If range = Nag_AllValues, \( m = n \).
If range = Nag_Indices, \( m = iu - il + 1 \).

13: \( w[n] \) – double  
On exit: the first \( m \) elements contain the selected eigenvalues in ascending order.

14: \( z[dim] \) – double  
Note: the dimension, \( dim \), of the array \( z \) must be at least \( \max(1, pdz \times n) \) when job = Nag_DoBoth;
1 otherwise.

The \( (i,j) \)th element of the matrix \( Z \) is stored in
\[
z[(j - 1) \times pdz + i - 1] \quad \text{when order = Nag_ColMajor;}
z[(i - 1) \times pdz + j - 1] \quad \text{when order = Nag_RowMajor.}
\]

On exit: if job = Nag_DoBoth, then

if fail.code = NE_NOERROR, the first \( m \) columns of \( Z \) contain the orthonormal eigenvectors of the matrix \( A \) corresponding to the selected eigenvalues, with the \( i \)th column of \( Z \) holding the eigenvector associated with \( w[i - 1] \);

if an eigenvector fails to converge (fail.code = NE_CONVERGENCE), then that column of \( Z \) contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in jfail.

If job = Nag_EigVals, \( z \) is not referenced.

15: \( pdz \) – Integer  
Input

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

Constraints:

if job = Nag_DoBoth, \( pdz \geq \max(1, n) \);
otherwise \( pdz \geq 1 \).

16: \( jfail[dim] \) – Integer  
Output

Note: the dimension, \( dim \), of the array \( jfail \) must be at least \( \max(1, n) \).

On exit: if job = Nag_DoBoth, then

if fail.code = NE_NOERROR, the first \( m \) elements of \( jfail \) are zero;
if fail.code = NE_CONVERGENCE, \( jfail \) contains the indices of the eigenvectors that failed to converge.

If job = Nag_EigVals, \( jfail \) is not referenced.

17: \( fail \) – NagError *  
Input/Output

The NAG error argument (see Section 3.6 in the Essential Introduction).
6 Error Indicators and Warnings

**NE_ALLOC_FAIL**
Dynamic memory allocation failed.
See Section 3.2.1.2 in the Essential Introduction for further information.

**NE_BAD_PARAM**
On entry, argument \( \text{value} \) had an illegal value.

**NE_CONVERGENCE**
The algorithm failed to converge; \( \text{value} \) eigenvectors did not converge. Their indices are stored in array \( \text{jfail} \).

**NE_ENUM_INT_2**
On entry, \( \text{job} = \langle \text{value} \rangle \), \( \text{pdz} = \langle \text{value} \rangle \) and \( n = \langle \text{value} \rangle \).
Constraint: if \( \text{job} = \text{Nag_DoBoth} \), \( \text{pdz} \geq \max(1,n) \);
otherwise \( \text{pdz} \geq 1 \).

**NE_ENUM_INT_3**
On entry, \( \text{range} = \langle \text{value} \rangle \), \( il = \langle \text{value} \rangle \), \( iu = \langle \text{value} \rangle \) and \( n = \langle \text{value} \rangle \).
Constraint: if \( \text{range} = \text{Nag_Indices} \) and \( n = 0 \), \( il = 1 \) and \( iu = 0 \);
if \( \text{range} = \text{Nag_Indices} \) and \( n > 0 \), \( 1 \leq il \leq iu \leq n \).

**NE_ENUM_REAL_2**
On entry, \( \text{range} = \langle \text{value} \rangle \), \( vl = \langle \text{value} \rangle \) and \( vu = \langle \text{value} \rangle \).
Constraint: if \( \text{range} = \text{Nag_Interval} \), \( \text{vl} < \text{vu} \).

**NE_INT**
On entry, \( n = \langle \text{value} \rangle \).
Constraint: \( n \geq 0 \).

On entry, \( \text{pdz} = \langle \text{value} \rangle \).
Constraint: \( \text{pdz} > 0 \).

**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 contact NAG for assistance.
An unexpected error has been triggered by this function. Please contact NAG.
See Section 3.6.6 in the Essential Introduction for further information.

**NE_NO_LICENCE**
Your licence key may have expired or may not have been installed correctly.
See Section 3.6.5 in the Essential Introduction for further information.

7 Accuracy
The computed eigenvalues and eigenvectors are exact for a nearby matrix \( (A + E) \), where
\[
||E||_2 = O(\epsilon) ||A||_2,
\]
and \( \epsilon \) is the machine precision. See Section 4.7 of Anderson et al. (1999) for further details.
8 Parallelism and Performance

nag_dstevx (f08jbc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_dstevx (f08jbc) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this function. Please also consult the Users’ Note for your implementation for any additional implementation-specific information.

9 Further Comments

The total number of floating-point operations is proportional to \( n^2 \) if \( \text{job} = \text{Nag_EigVals} \) and is proportional to \( n^3 \) if \( \text{job} = \text{Nag_DoBoth} \) and \( \text{range} = \text{Nag_AllValues} \), otherwise the number of floating-point operations will depend upon the number of computed eigenvectors.

10 Example

This example finds the eigenvalues in the half-open interval \( (0, 5] \), and the corresponding eigenvectors, of the symmetric tridiagonal matrix

\[
A = \begin{pmatrix}
1 & 1 & 0 & 0 \\
1 & 4 & 2 & 0 \\
0 & 2 & 9 & 3 \\
0 & 0 & 3 & 16
\end{pmatrix}.
\]

10.1 Program Text

```c
/* nag_dstevx (f08jbc) Example Program. */
/* Copyright 2014 Numerical Algorithms Group. */
/* Mark 23, 2011. */
#
#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf08.h>
#include <nagx02.h>
#include <nagx04.h>

int main(void)
{
    /* Scalars */
    double abstol, vl, vu;
    Integer exit_status = 0, i, il = 0, iu = 0, j, m, n, pdz;
    /* Arrays */
    double *d = 0, *e = 0, *w = 0, *z = 0;
    Integer *index = 0;
    /* Nag Types */
    Nag_OrderType order;
    NagError fail, fail_print;

    #ifdef NAG_COLUMN_MAJOR
    order = Nag_ColMajor;
    #else
    order = Nag_RowMajor;
    #endif

    INIT_FAIL(fail);
    printf("nag_dstevx (f08jbc) Example Program Results\n\n");
```
/* Skip heading in data file */
#endif
if (!(d = NAG_ALLOC(n, double)) ||
    !(e = NAG_ALLOC(n, double)) ||
    !(w = NAG_ALLOC(n, double)) ||
    !(z = NAG_ALLOC(pdz * n, double)) ||
    !(index = NAG_ALLOC(n, Integer)))
{
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
}

/* Read the lower and upper bounds of the interval to be searched,
* and read the diagonal and off-diagonal elements of the matrix
* A from data file. */
#endif
for (i = 0; i < n; ++i)
    if (!(d = NAG_ALLOC(n, double)) ||
        !(e = NAG_ALLOC(n, double)) ||
        !(w = NAG_ALLOC(n, double)) ||
        !(z = NAG_ALLOC(pdz * n, double)) ||
        !(index = NAG_ALLOC(n, Integer)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }

/* nag_real_safe_small_number (X02AMC).
* Set the absolute error tolerance for eigenvalues. With abstol
* set to zero, the default value would be used instead. */
abstol = nag_real_safe_small_number * 2;

/* nag_dstevx (f08jbc).
* Solve the symmetric eigenvalue problem. */
if (fail.code != NE_NOERROR && fail.code != NE_CONVERGENCE)
{  printf("Error from nag_dstevx (f08jbc).\n", fail.message);
  exit_status = 1;
  goto END;
}

/* Print solution */
printf("Number of eigenvalues found =%5\n", m);
printf("\nEigenvalues\n");
for (j = 0; j < m; ++j)
  printf("%8.4f%s", w[j], (j+1)%8 == 0?"\n": "");
printf("\n\n");

/* nag_gen_real_mat_print (x04cac).
* Print selected eigenvectors.
*/
INIT_FAIL(fail_print);
fflush(stdout);
nag_gen_real_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, m, z,
pdz, "Selected eigenvectors", 0, &fail_print);
if (fail_print.code != NE_NOERROR)
{
  printf("Error from nag_gen_real_mat_print (x04cac).\n", fail_print.message);
  exit_status = 1;
  goto END;
}
if (fail.code == NE_CONVERGENCE)
{
  printf("eigenvectors failed to converge\n");
  printf("Indices of eigenvectors that did not converge\n");
  for (j = 0; j < m; ++j)
    printf("%8\n", index[j], (j+1)%8 == 0?"\n": "");
  printf("\n");
}

END:
NAG_FREE(d);
NAG_FREE(e);
NAG_FREE(w);
NAG_FREE(z);
NAG_FREE(index);
return exit_status;
}

10.2 Program Data

nag_dstevx (f08jbc) Example Program Data

<table>
<thead>
<tr>
<th>Value of n</th>
<th>Values of vl and vu</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>4.0 5.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>End of diagonal elements</th>
<th>End of off-diagonal elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0 2.0 3.0</td>
<td>1.0 4.0 9.0 16.0</td>
</tr>
</tbody>
</table>

10.3 Program Results

nag_dstevx (f08jbc) Example Program Results

Number of eigenvalues found = 2

Eigenvalues
0.6476 3.5470

Selected eigenvectors
<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.9396</td>
<td>0.3388</td>
</tr>
<tr>
<td>2</td>
<td>-0.3311</td>
<td>0.8628</td>
</tr>
<tr>
<td>3</td>
<td>0.0853</td>
<td>-0.3648</td>
</tr>
<tr>
<td>4</td>
<td>-0.0167</td>
<td>0.0879</td>
</tr>
</tbody>
</table>