

# NAG Library Function Document

## nag\_zheevx (f08fpc)

### 1 Purpose

nag\_zheevx (f08fpc) computes selected eigenvalues and, optionally, eigenvectors of a complex  $n$  by  $n$  Hermitian 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

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

void nag_zheevx (Nag_OrderType order, Nag_JobType job, Nag_RangeType range,
                Nag_UploType uplo, Integer n, Complex a[], Integer pda, double vl,
                double vu, Integer il, Integer iu, double abstol, Integer *m,
                double w[], Complex z[], Integer pdz, Integer jfail[], NagError *fail)
```

### 3 Description

The Hermitian matrix  $A$  is first reduced to real tridiagonal form, using unitary similarity transformations. The required eigenvalues and eigenvectors are then computed from the tridiagonal matrix; the method used depends upon whether all, or selected, eigenvalues and eigenvectors are required.

### 4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia <http://www.netlib.org/lapack/lug>

Demmel J W and Kahan W (1990) Accurate singular values of bidiagonal matrices *SIAM J. Sci. Statist. Comput.* **11** 873–912

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

### 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 2.3.1.3 in How to Use the NAG Library and its Documentation 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: **range** – Nag\_RangeType *Input*  
*On entry:* if **range** = Nag\_AllValues, all eigenvalues will be found.  
If **range** = Nag\_Interval, all eigenvalues in the half-open interval (**vl**, **vu**] will be found.  
If **range** = Nag\_Indices, the **ilth** to **iuth** eigenvalues will be found.  
*Constraint:* **range** = Nag\_AllValues, Nag\_Interval or Nag\_Indices.
- 4: **uplo** – Nag\_UploType *Input*  
*On entry:* if **uplo** = Nag\_Upper, the upper triangular part of  $A$  is stored.  
If **uplo** = Nag\_Lower, the lower triangular part of  $A$  is stored.  
*Constraint:* **uplo** = Nag\_Upper or Nag\_Lower.
- 5: **n** – Integer *Input*  
*On entry:*  $n$ , the order of the matrix  $A$ .  
*Constraint:*  $n \geq 0$ .
- 6: **a**[*dim*] – Complex *Input/Output*  
**Note:** the dimension, *dim*, of the array **a** must be at least  $\max(1, \mathbf{pda} \times \mathbf{n})$ .  
*On entry:* the  $n$  by  $n$  Hermitian matrix  $A$ .  
If **order** = Nag\_ColMajor,  $A_{ij}$  is stored in **a**[( $j - 1$ )  $\times$  **pda** +  $i - 1$ ].  
If **order** = Nag\_RowMajor,  $A_{ij}$  is stored in **a**[( $i - 1$ )  $\times$  **pda** +  $j - 1$ ].  
If **uplo** = Nag\_Upper, the upper triangular part of  $A$  must be stored and the elements of the array below the diagonal are not referenced.  
If **uplo** = Nag\_Lower, the lower triangular part of  $A$  must be stored and the elements of the array above the diagonal are not referenced.  
*On exit:* the lower triangle (if **uplo** = Nag\_Lower) or the upper triangle (if **uplo** = Nag\_Upper) of **a**, including the diagonal, is overwritten.
- 7: **pda** – Integer *Input*  
*On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **a**.  
*Constraint:* **pda**  $\geq$   $\max(1, \mathbf{n})$ .
- 8: **vl** – double *Input*  
9: **vu** – double *Input*  
*On entry:* if **range** = Nag\_Interval, the lower and upper bounds of the interval to be searched for eigenvalues.  
If **range** = Nag\_AllValues or Nag\_Indices, **vl** and **vu** are not referenced.  
*Constraint:* if **range** = Nag\_Interval, **vl** < **vu**.

- 10: **il** – Integer *Input*  
 11: **iu** – Integer *Input*

*On entry:* if **range** = Nag\_Indices, the indices (in ascending order) of the smallest and largest eigenvalues to be returned.

If **range** = Nag\_AllValues or Nag\_Interval, **il** and **iu** are not referenced.

*Constraints:*

- if **range** = Nag\_Indices and **n** = 0, **il** = 1 and **iu** = 0;
- if **range** = Nag\_Indices and **n** > 0,  $1 \leq \mathbf{il} \leq \mathbf{iu} \leq \mathbf{n}$ .

- 12: **abstol** – double *Input*

*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

$$\mathbf{abstol} + \epsilon \max(|a|, |b|),$$

where  $\epsilon$  is the *machine precision*. If **abstol** is less than or equal to zero, then  $\epsilon \|T\|_1$  will be used in its place, where  $T$  is the tridiagonal matrix obtained by reducing  $A$  to tridiagonal form. Eigenvalues will be computed most accurately when **abstol** is set to twice the underflow threshold  $2 \times \text{nag\_real\_safe\_small\_number}$ , not zero. If this function returns with **fail.code** = NE\_CONVERGENCE, indicating that some eigenvectors did not converge, try setting **abstol** to  $2 \times \text{nag\_real\_safe\_small\_number}$ . See Demmel and Kahan (1990).

- 13: **m** – Integer \* *Output*

*On exit:* the total number of eigenvalues found.  $0 \leq \mathbf{m} \leq \mathbf{n}$ .

If **range** = Nag\_AllValues, **m** = **n**.

If **range** = Nag\_Indices, **m** = **iu** – **il** + 1.

- 14: **w[dim]** – double *Output*

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

*On exit:* the first **m** elements contain the selected eigenvalues in ascending order.

- 15: **z[dim]** – Complex *Output*

**Note:** the dimension, *dim*, of the array **z** must be at least

- $\max(1, \mathbf{pdz} \times \mathbf{n})$  when **job** = Nag\_DoBoth;
- 1 otherwise.

The *i*th element of the *j*th vector  $Z$  is stored in

- $\mathbf{z}[(j-1) \times \mathbf{pdz} + i - 1]$  when **order** = Nag\_ColMajor;
- $\mathbf{z}[(i-1) \times \mathbf{pdz} + j - 1]$  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  $\mathbf{w}[i - 1]$ ;

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.

- 16: **pdz** – Integer *Input*

*On entry:* the stride used in the array **z**.

*Constraints:*

if **job** = Nag\_DoBoth, **pdz**  $\geq$  max(1, **n**);  
otherwise **pdz**  $\geq$  1.

17: **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.

18: **fail** – NagError \*

*Input/Output*

The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

## 6 Error Indicators and Warnings

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

### NE\_BAD\_PARAM

On entry, argument *value* had an illegal value.

### NE\_CONVERGENCE

The algorithm failed to converge; *value* eigenvectors did not converge. Their indices are stored in array **jfail**.

### NE\_ENUM\_INT\_2

On entry, **job** = *value*, **pdz** = *value* and **n** = *value*.

Constraint: if **job** = Nag\_DoBoth, **pdz**  $\geq$  max(1, **n**);  
otherwise **pdz**  $\geq$  1.

### NE\_ENUM\_INT\_3

On entry, **range** = *value*, **il** = *value*, **iu** = *value* and **n** = *value*.

Constraint: if **range** = Nag\_Indices and **n** = 0, **il** = 1 and **iu** = 0;  
if **range** = Nag\_Indices and **n** > 0,  $1 \leq \mathbf{il} \leq \mathbf{iu} \leq \mathbf{n}$ .

### NE\_ENUM\_REAL\_2

On entry, **range** = *value*, **vl** = *value* and **vu** = *value*.

Constraint: if **range** = Nag\_Interval, **vl** < **vu**.

### NE\_INT

On entry, **n** = *value*.

Constraint: **n**  $\geq$  0.

On entry, **pda** = *value*.

Constraint: **pda** > 0.

On entry, **pdz** =  $\langle value \rangle$ .  
 Constraint: **pdz** > 0.

### NE\_INT\_2

On entry, **pda** =  $\langle value \rangle$  and **n** =  $\langle value \rangle$ .  
 Constraint: **pda**  $\geq$  max(1, **n**).

### 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 2.7.6 in How to Use the NAG Library and its Documentation for further information.

### NE\_NO\_LICENCE

Your licence key may have expired or may not have been installed correctly.  
 See Section 2.7.5 in How to Use the NAG Library and its Documentation 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\_zheevx (f08fpc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag\_zheevx (f08fpc) 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  $n^3$ .

The real analogue of this function is nag\_dsyevx (f08fbc).

## 10 Example

This example finds the eigenvalues in the half-open interval  $(-2, 2]$ , and the corresponding eigenvectors, of the Hermitian matrix

$$A = \begin{pmatrix} 1 & 2 - i & 3 - i & 4 - i \\ 2 + i & 2 & 3 - 2i & 4 - 2i \\ 3 + i & 3 + 2i & 3 & 4 - 3i \\ 4 + i & 4 + 2i & 4 + 3i & 4 \end{pmatrix}.$$

## 10.1 Program Text

```

/* nag_zheevx (f08fpc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <naga02.h>
#include <nagf08.h>
#include <nagx04.h>

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

#ifdef NAG_COLUMN_MAJOR
#define A(I, J) a[(J - 1) * pda + I - 1]
#define Z(I, J) z[(J - 1) * pdz + I - 1]
    order = Nag_ColMajor;
#else
#define A(I, J) a[(I - 1) * pda + J - 1]
#define Z(I, J) z[(I - 1) * pdz + J - 1]
    order = Nag_RowMajor;
#endif

    INIT_FAIL(fail);

    printf("nag_zheevx (f08fpc) Example Program Results\n\n");

    /* Skip heading in data file */
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "%*[\n]", &n);
#else
    scanf("%" NAG_IFMT "%*[\n]", &n);
#endif

    m = n;

    /* Allocate memory */
    if (!(a = NAG_ALLOC(n * n, Complex)) ||
        !(z = NAG_ALLOC(n * m, Complex)) ||
        !(w = NAG_ALLOC(n, double)) || !(index = NAG_ALLOC(n, Integer)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }

    pda = n;
#ifdef NAG_COLUMN_MAJOR

```

```

    pdz = n;
#else
    pdz = m;
#endif

    /* Read the lower and upper bounds of the interval to be searched,
     * and read the upper triangular part of the matrix A from data file.
     */
#ifdef _WIN32
    scanf_s("%lf%lf%*[\n]", &vl, &vu);
#else
    scanf("%lf%lf%*[\n]", &vl, &vu);
#endif
    for (i = 1; i <= n; ++i)
        for (j = i; j <= n; ++j)
#ifdef _WIN32
            scanf_s(" ( %lf , %lf )", &A(i, j).re, &A(i, j).im);
#else
            scanf(" ( %lf , %lf )", &A(i, j).re, &A(i, j).im);
#endif
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif

    /* Set the absolute error tolerance for eigenvalues.
     * With abstol set to zero, the default value is used instead.
     */
    abstol = 0.0;

    /* nag_zheevx (f08fpc).
     * Solve the Hermitian eigenvalue problem.
     */
    nag_zheevx(order, Nag_DoBoth, Nag_Interval, Nag_Upper, n, a, pda, vl,
               vu, il, iu, abstol, &m, w, z, pdz, index, &fail);
    if (fail.code != NE_NOERROR && fail.code != NE_CONVERGENCE) {
        printf("Error from nag_zheevx (f08fpc).\n%s\n", fail.message);
        exit_status = 1;
        goto END;
    }

    /* nag_complex_divide (a02cdc).
     * Normalize the eigenvectors.
     */
    for (j = 1; j <= m; j++)
        for (i = n; i >= 1; i--)
            Z(i, j) = nag_complex_divide(Z(i, j), Z(1, j));

    /* Print solution */
    printf("Number of eigenvalues found =%5" NAG_IFMT "\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_complx_mat_print (x04dac).
     * Print selected eigenvectors.
     */
    INIT_FAIL(fail_print);
    fflush(stdout);
    nag_gen_complx_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_complx_mat_print (x04dac).\n%s\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" NAG_IFMT "%s", index[j], (j + 1) % 8 == 0 ? "\n" : " ");
}

END:
NAG_FREE(a);
NAG_FREE(z);
NAG_FREE(w);
NAG_FREE(index);

return exit_status;
}

#undef A
#undef Z

```

## 10.2 Program Data

```

nag_zheevx (f08fpc) Example Program Data
4                                     :Value of n
-2.0      2.0                       :Values of vl and vu
(1.0, 0.0) (2.0, -1.0) (3.0, -1.0) (4.0, -1.0)
           (2.0, 0.0) (3.0, -2.0) (4.0, -2.0)
           (3.0, 0.0) (4.0, -3.0)
           (4.0, 0.0) :End of matrix A

```

## 10.3 Program Results

nag\_zheevx (f08fpc) Example Program Results

Number of eigenvalues found = 2

Eigenvalues  
-0.6886 1.1412

Selected eigenvectors

|   | 1       | 2       |
|---|---------|---------|
| 1 | 1.0000  | 1.0000  |
|   | 0.0000  | -0.0000 |
| 2 | -0.7703 | 0.0516  |
|   | -0.1746 | 1.2795  |
| 3 | 0.4559  | -1.1962 |
|   | 0.4892  | -0.2954 |
| 4 | -0.3464 | 0.7876  |
|   | -0.4448 | -0.5075 |

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