

nag_hermitian_eigensystem (f02axc)

1. Purpose

nag_hermitian_eigensystem (f02axc) calculates all the eigenvalues and eigenvectors of a complex Hermitian matrix.

2. Specification

```
#include <nag.h>
#include <nagf02.h>

void nag_hermitian_eigensystem(Integer n, Complex a[], Integer tda,
                               double r[], Complex v[], Integer tdv, NagError *fail)
```

3. Description

The complex Hermitian matrix A is first reduced to a real tridiagonal matrix by $n - 2$ unitary transformations and a subsequent diagonal transformation. The eigenvalues and eigenvectors are then derived using the QL algorithm, an adaptation of the QR algorithm.

4. Parameters

n

Input: n , the order of the matrix A .
Constraint: $n \geq 1$.

a[n][tda]

Input: the elements of the lower triangle of the n by n complex Hermitian matrix A . Elements of the array above the diagonal need not be set. See also Section 6.

tda

Input: the last dimension of the array **a** as declared in the function from which **nag_hermitian_eigensystem** is called.
Constraint: **tda** $\geq$ **n**.

r[n]

Output: the eigenvalues in ascending order.

v[n][tdv]

Output: the eigenvectors, stored by columns. The i th column corresponds to the i th eigenvector. The eigenvectors are normalised so that the sum of the squares of the moduli of the elements is equal to 1 and the element of largest modulus is real. See also Section 6.

tdv

Input: the last dimension of the array **v** as declared in the function from which **nag_hermitian_eigensystem** is called.
Constraint: **tdv** $\geq$ **n**.

fail

The NAG error parameter, see the Essential Introduction to the NAG C Library.

5. Error Indications and Warnings

NE_INT_ARG_LT

On entry, **n** must not be less than 1: **n** = $\langle value \rangle$.

NE_2_INT_ARG_LT

On entry **tda** = $\langle value \rangle$ while **n** = $\langle value \rangle$. These parameters must satisfy **tda** $\geq$ **n**.
On entry **tdv** = $\langle value \rangle$ while **n** = $\langle value \rangle$. These parameters must satisfy **tdv** $\geq$ **n**.

NE_ALLOC_FAIL

Memory allocation failed.

NE_DIAG_IMAG_NON_ZERO

Matrix diagonal element $a[\langle value \rangle][\langle value \rangle]$ has non-zero imaginary part.

NE_TOO_MANY_ITERATIONS

More than $\langle value \rangle$ iterations are required to isolate all the eigenvalues.

6. Further Comments

The time taken by the function is approximately proportional to n^3 .

The function may be called with the same actual array supplied for **a** and **v**, in which case the eigenvectors will overwrite the original matrix *A*.

6.1. Accuracy

The eigenvectors are always accurately orthogonal but the accuracy of the individual eigenvalues and eigenvectors is dependent on their inherent sensitivity to small changes in the original matrix. For a detailed error analysis see Wilkinson and Reinsch (1971) page 235.

6.2. References

Wilkinson J H and Reinsch C (1971) *Handbook for Automatic Computation (Vol. II, Linear Algebra)* Springer-Verlag pp 227-240.

7. See Also

None

8. Example

To calculate the eigenvalues and eigenvectors of the complex Hermitian matrix:

$$\begin{pmatrix} 0.50 & 0.00 & 1.84 + 1.38i & 2.08 - 1.56i \\ 0.00 & 0.50 & 1.12 + 0.84i & -0.56 + 0.42i \\ 1.84 - 1.38i & 1.12 - 0.84i & 0.50 & 0.00 \\ 2.08 + 1.56i & -0.56 - 0.42i & 0.00 & 0.50 \end{pmatrix}.$$

8.1. Program Text

```
/* nag_hermitian_eigensystem(f02axc) Example Program
 *
 * Copyright 1991 Numerical Algorithms Group.
 *
 * Mark 2, 1991.
 */

#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nagf02.h>

#define NMAX 4
#define TDA NMAX
#define TDV NMAX

main()
{
    Integer i, j, n;
    Complex a[NMAX][TDA], v[NMAX][TDV];
    double r[NMAX];

    Vprintf("f02axc Example Program Results\n");
    Vscanf("%*[^\\n]"); /* Skip heading in data file */
    Vscanf("%ld", &n);
    if (n>=1 || n<=NMAX)
    {
        for (i=0; i<n; i++)
            for (j=0; j<n; j++)
                Vscanf(" ( %lf , %lf ) ", &a[i][j].re,&a[i][j].im);
```

```

    f02axc(n, (Complex *)a, (Integer)TDA, r, (Complex *)v,
           (Integer)TDV, NAGERR_DEFAULT);
    Vprintf("Eigenvalues\n");
    for (i=0; i<n; i++)
        Vprintf("%9.4f", r[i]);
    Vprintf("\nEigenvectors\n");
    for (i=0; i<n; i++)
        for (j=0; j<n; j++)
            Vprintf("(%7.3f %7.3f )%s", v[i][j].re, v[i][j].im,
                    (j%4==3 || j==n-1) ? "\n" : " ");
    exit(EXIT_SUCCESS);
}
else
{
    Vfprintf(stderr, "n is out of range: n = %4ld,\n", n);
    exit(EXIT_FAILURE);
}
}

```

8.2. Program Data

f02axc Example Program Data

```

4
(0.50, 0.00) ( 0.00, 0.00) (1.84, 1.38 ) ( 2.08,-1.56 )
(0.00, 0.00) ( 0.50, 0.00) (1.12, 0.84 ) (-0.56, 0.42 )
(1.84,-1.38) ( 1.12,-0.84) (0.50, 0.00 ) ( 0.00, 0.00 )
(2.08, 1.56) (-0.56,-0.42) (0.00, 0.00 ) ( 0.50, 0.00 )

```

8.3. Program Results

f02axc Example Program Results

Eigenvalues

```

-3.0000 -1.0000  2.0000  4.0000

```

Eigenvectors

```

( 0.700  0.000 ) ( -0.100  0.000 ) ( -0.100  0.000 ) ( 0.700  0.000 )
( 0.100  0.000 ) ( 0.700  0.000 ) ( 0.700  0.000 ) ( 0.100  0.000 )
( -0.400  0.300 ) ( -0.400  0.300 ) ( 0.400 -0.300 ) ( 0.400 -0.300 )
( -0.400 -0.300 ) ( 0.400  0.300 ) ( -0.400 -0.300 ) ( 0.400  0.300 )

```
