

## NAG Library Function Document

### nag\_matop\_real\_gen\_matrix\_cond\_num (f01jbc)

#### 1 Purpose

nag\_matop\_real\_gen\_matrix\_cond\_num (f01jbc) computes an estimate of the absolute condition number of a matrix function  $f$  at a real  $n$  by  $n$  matrix  $A$  in the 1-norm. Numerical differentiation is used to evaluate the derivatives of  $f$  when they are required.

#### 2 Specification

```
#include <nag.h>
#include <nagf01.h>

void nag_matop_real_gen_matrix_cond_num (Integer n, double a[], Integer pda,
    void (*f)(Integer *iflag, Integer nz, const Complex z[], Complex fz[],
        Nag_Comm *comm),
    Nag_Comm *comm, Integer *iflag, double *conda, double *norma,
    double *normfa, NagError *fail)
```

#### 3 Description

The absolute condition number of  $f$  at  $A$ ,  $\text{cond}_{\text{abs}}(f, A)$  is given by the norm of the Fréchet derivative of  $f$ ,  $L(A)$ , which is defined by

$$\|L(X)\| := \max_{E \neq 0} \frac{\|L(X, E)\|}{\|E\|},$$

where  $L(X, E)$  is the Fréchet derivative in the direction  $E$ .  $L(X, E)$  is linear in  $E$  and can therefore be written as

$$\text{vec}(L(X, E)) = K(X)\text{vec}(E),$$

where the  $\text{vec}$  operator stacks the columns of a matrix into one vector, so that  $K(X)$  is  $n^2 \times n^2$ . nag\_matop\_real\_gen\_matrix\_cond\_num (f01jbc) computes an estimate  $\gamma$  such that  $\gamma \leq \|K(X)\|_1$ , where  $\|K(X)\|_1 \in [n^{-1}\|L(X)\|_1, n\|L(X)\|_1]$ . The relative condition number can then be computed via

$$\text{cond}_{\text{rel}}(f, A) = \frac{\text{cond}_{\text{abs}}(f, A)\|A\|_1}{\|f(A)\|_1}.$$

The algorithm used to find  $\gamma$  is detailed in Section 3.4 of Higham (2008).

The function  $f$  is supplied via function **f** which evaluates  $f(z_i)$  at a number of points  $z_i$ .

#### 4 References

Higham N J (2008) *Functions of Matrices: Theory and Computation* SIAM, Philadelphia, PA, USA

#### 5 Arguments

1: **n** – Integer *Input*  
*On entry:*  $n$ , the order of the matrix  $A$ .  
*Constraint:*  $n \geq 0$ .

- 2: **a**[*dim*] – double *Input/Output*  
**Note:** the dimension, *dim*, of the array **a** must be at least  $\mathbf{pda} \times \mathbf{n}$ .  
 The (*i*, *j*)th element of the matrix *A* is stored in  $\mathbf{a}[(j-1) \times \mathbf{pda} + i - 1]$ .  
*On entry:* the *n* by *n* matrix *A*.  
*On exit:* the *n* by *n* matrix,  $f(A)$ .
- 3: **pda** – Integer *Input*  
*On entry:* the stride separating matrix row elements in the array **a**.  
**Constraint:**  $\mathbf{pda} \geq \mathbf{n}$ .
- 4: **f** – function, supplied by the user *External Function*  
 The function **f** evaluates  $f(z_i)$  at a number of points  $z_i$ .

The specification of **f** is:

```
void f (Integer *iflag, Integer nz, const Complex z[], Complex fz[],
       Nag_Comm *comm)
```

- 1: **iflag** – Integer \* *Input/Output*

*On entry:* **iflag** will be zero.

*On exit:* **iflag** should either be unchanged from its entry value of zero, or may be set nonzero to indicate that there is a problem in evaluating the function  $f(z)$ ; for instance  $f(z)$  may not be defined. If **iflag** is returned as nonzero then `nag_matop_real_gen_matrix_cond_num (f01jbc)` will terminate the computation, with **fail.code** = NE\_USER\_STOP.

- 2: **nz** – Integer *Input*

*On entry:*  $n_z$ , the number of function values required.

- 3: **z[nz]** – const Complex *Input*

*On entry:* the  $n_z$  points  $z_1, z_2, \dots, z_{n_z}$  at which the function  $f$  is to be evaluated.

- 4: **fz[nz]** – Complex *Output*

*On exit:* the  $n_z$  function values.  $\mathbf{fz}[i-1]$  should return the value  $f(z_i)$ , for  $i = 1, 2, \dots, n_z$ . If  $z_i$  lies on the real line, then so must  $f(z_i)$ .

- 5: **comm** – Nag\_Comm \*  
 Pointer to structure of type Nag\_Comm; the following members are relevant to **f**.

**user** – double \*

**iuser** – Integer \*

**p** – Pointer

The type Pointer will be `void *`. Before calling `nag_matop_real_gen_matrix_cond_num (f01jbc)` you may allocate memory and initialize these pointers with various quantities for use by **f** when called from `nag_matop_real_gen_matrix_cond_num (f01jbc)` (see Section 3.2.1.1 in the Essential Introduction).

- 5: **comm** – Nag\_Comm \*  
 The NAG communication argument (see Section 3.2.1.1 in the Essential Introduction).

- 6: **iflag** – Integer \* *Output*  
*On exit:* **iflag** = 0, unless **iflag** has been set nonzero inside **f**, in which case **iflag** will be the value set and **fail** will be set to **fail.code** = NE\_USER\_STOP.
- 7: **conda** – double \* *Output*  
*On exit:* an estimate of the absolute condition number of  $f$  at  $A$ .
- 8: **norma** – double \* *Output*  
*On exit:* the 1-norm of  $A$ .
- 9: **normfa** – double \* *Output*  
*On exit:* the 1-norm of  $f(A)$ .
- 10: **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  $\langle value \rangle$  had an illegal value.

### NE\_INT

On entry, **n** =  $\langle value \rangle$ .  
Constraint: **n**  $\geq$  0.

### NE\_INT\_2

On entry, **pda** =  $\langle value \rangle$  and **n** =  $\langle value \rangle$ .  
Constraint: **pda**  $\geq$  **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 internal error occurred when estimating the norm of the Fréchet derivative of  $f$  at  $A$ . Please contact NAG.

An internal error occurred when evaluating the matrix function  $f(A)$ . You can investigate further by calling `nag_matop_real_gen_matrix_fun_num` (f01elc) with the matrix  $A$  and the function  $f$ .

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.

### NE\_USER\_STOP

**iflag** has been set nonzero by the user-supplied function.

## 7 Accuracy

nag\_matop\_real\_gen\_matrix\_cond\_num (f01jbc) uses the norm estimation function nag\_linsys\_real\_gen\_norm\_rcomm (f04ydc) to estimate a quantity  $\gamma$ , where  $\gamma \leq \|K(X)\|_1$  and  $\|K(X)\|_1 \in [n^{-1}\|L(X)\|_1, n\|L(X)\|_1]$ . For further details on the accuracy of norm estimation, see the documentation for nag\_linsys\_real\_gen\_norm\_rcomm (f04ydc).

## 8 Parallelism and Performance

nag\_matop\_real\_gen\_matrix\_cond\_num (f01jbc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library. In these implementations, this function may make calls to the user-supplied functions from within an OpenMP parallel region. Thus OpenMP pragmas within the user functions can only be used if you are compiling the user-supplied function and linking the executable in accordance with the instructions in the Users' Note for your implementation. You must also ensure that you use the NAG communication argument **comm** in a thread safe manner, which is best achieved by only using it to supply read-only data to the user functions.

nag\_matop\_real\_gen\_matrix\_cond\_num (f01jbc) 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 matrix function is computed using the underlying matrix function routine nag\_matop\_real\_gen\_matrix\_fun\_num (f01elc). Approximately  $6n^2$  of real allocatable memory is required by the routine, in addition to the memory used by the underlying matrix function routine.

If only  $f(A)$  is required, without an estimate of the condition number, then it is far more efficient to use the underlying matrix function routine.

The complex analogue of this function is nag\_matop\_complex\_gen\_matrix\_cond\_num (f01kbc).

## 10 Example

This example estimates the absolute and relative condition numbers of the matrix function  $\cos 2A$  where

$$A = \begin{pmatrix} -1 & -1 & -2 & 1 \\ 0 & 1 & -1 & 0 \\ -1 & -2 & 1 & -1 \\ 0 & -1 & 0 & -1 \end{pmatrix}.$$

### 10.1 Program Text

```
/* nag_matop_real_gen_matrix_cond_num (f01jbc) Example Program.
 *
 * Copyright 2014 Numerical Algorithms Group.
 *
 * Mark 24, 2013.
 */
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf01.h>
#include <nagx02.h>
#include <nagx04.h>

#ifdef __cplusplus
extern "C" {
#endif
```

```

    static void NAG_CALL f(Integer *iflag, Integer nz, const Complex z[],
                          Complex fz[], Nag_Comm *comm);
#ifdef __cplusplus
}
#endif

#define A(I,J) a[J*pda + I]

int main(void)
{
    /* Scalars */
    Integer      exit_status = 0;
    Integer      i, iflag, j, n, pda;
    double       conda, cond_rel, eps, norma, normfa;
    /* Arrays */
    static double ruser[1] = {-1.0};
    double       *a = 0;
    /* Nag Types */
    Nag_OrderType order = Nag_ColMajor;
    Nag_Comm     comm;
    NagError     fail;

    INIT_FAIL(fail);

    /* Output preamble */
    printf("nag_matop_real_gen_matrix_cond_num (f01jbc) ");
    printf("Example Program Results\n\n");

    /* For communication with user-supplied functions: */
    comm.user = ruser;

    fflush(stdout);

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

    /* Read in the problem size */
#ifdef _WIN32
    scanf_s("%"NAG_IFMT"%*[\n]", &n);
#else
    scanf("%"NAG_IFMT"%*[\n]", &n);
#endif

    pda = n;
    if (!(a = NAG_ALLOC((pda)*(n), double))) {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }

    /* Read in the matrix A from data file */
    for (i = 0; i < n; i++)
#ifdef _WIN32
        for (j = 0; j < n; j++) scanf_s("%lf", &A(i, j));
#else
        for (j = 0; j < n; j++) scanf("%lf", &A(i, j));
#endif
    #ifdef _WIN32
        scanf_s("%*[\n] ");
    #else
        scanf("%*[\n] ");
    #endif

    /* Print matrix A using nag_gen_real_mat_print (x04cac)
     * Print real general matrix (easy-to-use)
     */
}

```

```

nag_gen_real_mat_print (order, Nag_GeneralMatrix, Nag_NonUnitDiag,
                        n, n, a, pda, "A", NULL, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_real_mat_print (x04cac)\n%s\n", fail.message);
    exit_status = 2;
    goto END;
}

/* Find absolute condition number estimate of f(A) for a real matrix A using
 * nag_matop_real_gen_matrix_cond_num (f01jbc)
 * which uses numerical differentiation.
 */
nag_matop_real_gen_matrix_cond_num (n, a, pda, f, &comm, &iflag,
                                    &conda, &norma, &normfa, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_matop_real_gen_matrix_cond_num (f01jbc)\n%s\n",
          fail.message);
    exit_status = 1;
    goto END;
}

/* Print absolute condition number estimate */
printf("\nf(A) = cos(2A)\n");
printf("Estimated absolute condition number is: %7.2f\n",conda);

/* nag_machine_precision (x02ajc) The machine precision */
eps = nag_machine_precision;

/* Find relative condition number estimate */
if ( normfa>eps) {
    cond_rel = conda * norma/normfa;
    printf("Estimated relative condition number is: %7.2f\n",cond_rel);
}
else {
    printf("The estimated norm of f(A) is effectively zero");
    printf("and so the relative condition number is undefined.\n");
}

END:
NAG_FREE(a);
return exit_status;
}

static void NAG_CALL f(Integer *iflag, Integer nz, const Complex z[],
                      Complex fz[], Nag_Comm *comm)
{
    /* Scalars */
    Integer j;
#pragma omp master
    if (comm->user[0] == -1.0)
    {
        printf("(User-supplied callback f, first invocation.)\n");
        comm->user[0] = 0.0;
    }
    for (j = 0; j < nz; j++) {
        /*Complex representation of cos 2z */
        fz[j].re = cos(2.0*z[j].re)*cosh(2.0*z[j].im);
        fz[j].im = -sin(2.0*z[j].re)*sinh(2.0*z[j].im);
    }
    /* Set iflag nonzero to terminate execution for any reason. */
    *iflag = 0;
}

```

## 10.2 Program Data

nag\_matop\_real\_gen\_matrix\_cond\_num (f01jbc) Example Program Data

```
4                               :Value of n
-1.0  -1.0  -2.0   1.0
 0.0   1.0  -1.0   0.0
-1.0  -2.0   1.0  -1.0
 0.0  -1.0   0.0  -1.0 :End of matrix a
```

## 10.3 Program Results

nag\_matop\_real\_gen\_matrix\_cond\_num (f01jbc) Example Program Results

```
A
      1      2      3      4
1  -1.0000  -1.0000  -2.0000  1.0000
2   0.0000   1.0000  -1.0000  0.0000
3  -1.0000  -2.0000   1.0000  -1.0000
4   0.0000  -1.0000   0.0000  -1.0000
(User-supplied callback f, first invocation.)
```

```
f(A) = cos(2A)
Estimated absolute condition number is:   4.10
Estimated relative condition number is:  14.48
```

---