

## NAG Library Function Document

### nag\_matop\_real\_gen\_matrix\_fun\_num (f01elc)

#### 1 Purpose

nag\_matop\_real\_gen\_matrix\_fun\_num (f01elc) computes the matrix function,  $f(A)$ , of a real  $n$  by  $n$  matrix  $A$ . 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_fun_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 *imnorm, NagError *fail)
```

#### 3 Description

$f(A)$  is computed using the Schur–Parlett algorithm described in Higham (2008) and Davies and Higham (2003). The coefficients of the Taylor series used in the algorithm are evaluated using the numerical differentiation algorithm of Lyness and Moler (1967).

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

#### 4 References

Davies P I and Higham N J (2003) A Schur–Parlett algorithm for computing matrix functions. *SIAM J. Matrix Anal. Appl.* **25(2)** 464–485

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

Lyness J N and Moler C B (1967) Numerical differentiation of analytic functions *SIAM J. Numer. Anal.* **4(2)** 202–210

#### 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 **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  $f(z_i)$ ; for instance  $f(z_i)$  may not be defined. If **iflag** is returned as nonzero then `nag_matop_real_gen_matrix_fun_num (f01elc)` 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. **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_fun_num (f01elc)` you may allocate memory and initialize these pointers with various quantities for use by **f** when called from `nag_matop_real_gen_matrix_fun_num (f01elc)` (see Section 2.3.1.1 in How to Use the NAG Library and its Documentation).

5: **comm** – Nag\_Comm \*

The NAG communication argument (see Section 2.3.1.1 in How to Use the NAG Library and its Documentation).

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: **imnorm** – double \* *Output*

*On exit:* if  $A$  has complex eigenvalues, `nag_matop_real_gen_matrix_fun_num (f01elc)` will use complex arithmetic to compute  $f(A)$ . The imaginary part is discarded at the end of the computation, because it will theoretically vanish. **imnorm** contains the 1-norm of the imaginary part, which should be used to check that the routine has given a reliable answer.

If  $A$  has real eigenvalues, `nag_matop_real_gen_matrix_fun_num (f01elc)` uses real arithmetic and **imnorm** = 0.

- 8: **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  $\langle value \rangle$  had an illegal value.

### NE\_CONVERGENCE

A Taylor series failed to converge after 40 terms. Further Taylor series coefficients can no longer reliably be obtained by numerical differentiation.

### NE\_INT

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

### NE\_INT\_2

On entry,  $\mathbf{pda} = \langle value \rangle$  and  $\mathbf{n} = \langle value \rangle$ .  
 Constraint:  $\mathbf{pda} \geq \mathbf{n}$ .

### 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.

An unexpected internal error occurred when ordering the eigenvalues of  $A$ . Please contact NAG.

The function was unable to compute the Schur decomposition of  $A$ .

**Note:** this failure should not occur and suggests that the function has been called incorrectly.

There was an error whilst reordering the Schur form of  $A$ .

**Note:** this failure should not occur and suggests that the function has been called incorrectly.

### 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.

### NE\_USER\_STOP

**iflag** has been set nonzero by the user.

## 7 Accuracy

For a normal matrix  $A$  (for which  $A^T A = A A^T$ ) the Schur decomposition is diagonal and the algorithm reduces to evaluating  $f$  at the eigenvalues of  $A$  and then constructing  $f(A)$  using the Schur vectors. See Section 9.4 of Higham (2008) for further discussion of the Schur–Parlett algorithm, and Lyness and Moler (1967) for a discussion of numerical differentiation.

## 8 Parallelism and Performance

`nag_matop_real_gen_matrix_fun_num` (f01elc) 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_fun_num` (f01elc) 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 Integer allocatable memory required is  $n$ . If  $A$  has real eigenvalues then up to  $6n^2$  of double allocatable memory may be required. If  $A$  has complex eigenvalues then up to  $6n^2$  of Complex allocatable memory may be required.

The cost of the Schur–Parlett algorithm depends on the spectrum of  $A$ , but is roughly between  $28n^3$  and  $n^4/3$  floating-point operations. There is an additional cost in numerically differentiating  $f$ , in order to obtain the Taylor series coefficients. If the derivatives of  $f$  are known analytically, then `nag_matop_real_gen_matrix_fun_usd` (f01emc) can be used to evaluate  $f(A)$  more accurately. If  $A$  is real symmetric then it is recommended that `nag_matop_real_symm_matrix_fun` (f01efc) be used as it is more efficient and, in general, more accurate than `nag_matop_real_gen_matrix_fun_num` (f01elc).

For any  $z$  on the real line,  $f(z)$  must be real.  $f$  must also be complex analytic on the spectrum of  $A$ . These conditions ensure that  $f(A)$  is real for real  $A$ .

For further information on matrix functions, see Higham (2008).

If estimates of the condition number of the matrix function are required then `nag_matop_real_gen_matrix_cond_num` (f01jbc) should be used.

`nag_matop_complex_gen_matrix_fun_num` (f01flc) can be used to find the matrix function  $f(A)$  for a complex matrix  $A$ .

## 10 Example

This example finds  $\cos 2A$  where

$$A = \begin{pmatrix} 3 & 0 & 1 & 2 \\ -1 & 1 & 3 & 1 \\ 0 & 2 & 2 & 1 \\ 2 & 1 & -1 & 1 \end{pmatrix}.$$

### 10.1 Program Text

```
/* nag_matop_real_gen_matrix_fun_num (f01elc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

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

```

#include <nagf01.h>
#include <nagx02.h>
#include <nagx04.h>
#include <math.h>

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

int main(void)
{
    /* Scalars */
    Integer exit_status = 0;
    Integer i, iflag, j, n, pda;
    double imnorm;

    /* Arrays */
    static double ruser[1] = { -1.0 };
    double *a = 0;

    /* Nag Types */
    Nag_Comm comm;
    Nag_OrderType order;
    NagError fail;

    INIT_FAIL(fail);

#define A(I, J)  a[(J-1)*pda + I-1]

    order = Nag_ColMajor;

    /* Output preamble */
    printf("nag_matop_real_gen_matrix_fun_num (f01elc) ");
    printf("Example Program Results\n\n");
    fflush(stdout);

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

    /* 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 = 1; i <= n; i++)
#ifdef _WIN32
        for (j = 1; j <= n; j++)

```

```

        scanf_s("%lf", &A(i, j));
#else
    for (j = 1; j <= n; j++)
        scanf("%lf", &A(i, j));
#endif
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif
/* Find the matrix function using
 * nag_matop_real_gen_matrix_fun_num (f01elc)
 * Function of a real matrix
 */
nag_matop_real_gen_matrix_fun_num(n, a, pda, f, &comm, &iflag, &imnorm,
                                  &fail);

if (fail.code != NE_NOERROR) {
    printf("Error from nag_matop_real_gen_matrix_fun_num (f01elc)\n%s\n",
          fail.message);
    exit_status = 1;
    goto END;
}

if (fabs(imnorm) > pow(nag_machine_precision, 0.8)) {
    printf("\nWARNING: the error estimate returned in imnorm is larger than"
          " expected;\n");
    printf("        the matrix solution printed below is suspect:\n");
    printf("        imnorm = %13.4e.\n\n", imnorm);
}

/* Print solution using
 * nag_gen_real_mat_print (x04dac)
 * Print real general matrix (easy-to-use)
 */
nag_gen_real_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, n, a,
                       pda, "f(A) = cos(2A)", NULL, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_real_mat_print (x04dac)\n%s\n", fail.message);
    exit_status = 2;
    goto END;
}

END:
    NAG_FREE(a);
    return exit_status;
}

static void NAG_CALL f(Integer *iflag, Integer n, 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");
        fflush(stdout);
        comm->user[0] = 0.0;
    }
    for (j = 0; j < n; 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_fun_num (f01elc) Example Program Data
4                                     :Value of n
3.0    0.0    1.0    2.0
-1.0   1.0   3.0   1.0
0.0    2.0   2.0   1.0
2.0    1.0  -1.0   1.0 :End of matrix a
```

## 10.3 Program Results

```
nag_matop_real_gen_matrix_fun_num (f01elc) Example Program Results
```

```
(User-supplied callback f, first invocation.)
f(A) = cos(2A)
      1          2          3          4
1   -0.1704   -1.1597   -0.1878   -0.7307
2   -0.3950   -0.4410    0.7606    0.0655
3   -0.0950   -0.0717    0.0619   -0.4351
4   -0.1034    0.6424   -1.3964    0.1042
```

---