

## NAG Library Function Document

### nag\_matop\_real\_gen\_matrix\_pow (f01eqc)

#### 1 Purpose

nag\_matop\_real\_gen\_matrix\_pow (f01eqc) computes the principal real power  $A^p$ , for arbitrary  $p$ , of a real  $n$  by  $n$  matrix  $A$ .

#### 2 Specification

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

void nag_matop_real_gen_matrix_pow (Integer n, double a[], Integer pda,
    double p, NagError *fail)
```

#### 3 Description

For a matrix  $A$  with no eigenvalues on the closed negative real line,  $A^p$  ( $p \in \mathbb{R}$ ) can be defined as

$$A^p = \exp(p \log(A))$$

where  $\log(A)$  is the principal logarithm of  $A$  (the unique logarithm whose spectrum lies in the strip  $\{z : -\pi < \text{Im}(z) < \pi\}$ ).

$A^p$  is computed using the real version of the Schur–Padé algorithm described in Higham and Lin (2011) and Higham and Lin (2013).

The real number  $p$  is expressed as  $p = q + r$  where  $q \in (-1, 1)$  and  $r \in \mathbb{Z}$ . Then  $A^p = A^q A^r$ . The integer power  $A^r$  is found using a combination of binary powering and, if necessary, matrix inversion. The fractional power  $A^q$  is computed, entirely in real arithmetic, using a real Schur decomposition and a Padé approximant.

#### 4 References

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

Higham N J and Lin L (2011) A Schur–Padé algorithm for fractional powers of a matrix *SIAM J. Matrix Anal. Appl.* **32(3)** 1056–1078

Higham N J and Lin L (2013) An improved Schur–Padé algorithm for fractional powers of a matrix and their Fréchet derivatives *MIMS Eprint 2013.1* Manchester Institute for Mathematical Sciences, School of Mathematics, University of Manchester <http://eprints.ma.man.ac.uk/>

#### 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  $p$ th power,  $A^p$ .

- 3: **pda** – Integer *Input*  
*On entry:* the stride separating matrix row elements in the array **a**.  
*Constraint:* **pda**  $\geq$  **n**.
- 4: **p** – double *Input*  
*On entry:* the required power of *A*.
- 5: **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 unexpected error has been triggered by this function. Please contact NAG.  
See Section 3.6.6 in the Essential Introduction for further information.

### NE\_NEGATIVE\_EIGVAL

*A* has eigenvalues on the negative real line. The principal *p*th power is not defined.  
nag\_matop\_complex\_gen\_matrix\_pow (f01fqc) can be used to find a complex, non-principal *p*th power.

### 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\_SINGULAR

*A* is singular so the *p*th power cannot be computed.

### NW\_SOME\_PRECISION\_LOSS

$A^p$  has been computed using an IEEE double precision Padé approximant, although the arithmetic precision is higher than IEEE double precision.

## 7 Accuracy

For positive integer  $p$ , the algorithm reduces to a sequence of matrix multiplications. For negative integer  $p$ , the algorithm consists of a combination of matrix inversion and matrix multiplications.

For a normal matrix  $A$  (for which  $A^T A = A A^T$ ) and non-integer  $p$ , the Schur decomposition is diagonal and the algorithm reduces to evaluating powers of the eigenvalues of  $A$  and then constructing  $A^p$  using the Schur vectors. This should give a very accurate result. In general however, no error bounds are available for the algorithm.

## 8 Parallelism and Performance

`nag_matop_real_gen_matrix_pow` (f01eqc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

`nag_matop_real_gen_matrix_pow` (f01eqc) 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 cost of the algorithm is  $O(n^3)$ . The exact cost depends on the matrix  $A$  but if  $p \in (-1, 1)$  then the cost is independent of  $p$ .  $O(4 \times n^2)$  of real allocatable memory is required by the function.

If estimates of the condition number of  $A^p$  are required then `nag_matop_real_gen_matrix_cond_pow` (f01jec) should be used.

## 10 Example

This example finds  $A^p$  where  $p = 0.2$  and

$$A = \begin{pmatrix} 3 & 3 & 2 & 1 \\ 3 & 1 & 0 & 2 \\ 1 & 1 & 4 & 3 \\ 3 & 0 & 3 & 1 \end{pmatrix}.$$

### 10.1 Program Text

```

/* nag_matop_real_gen_matrix_pow (f01eqc) Example Program.
 *
 * Copyright 2014 Numerical Algorithms Group.
 *
 * Mark 24, 2013.
 */
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf01.h>
#include <nagx04.h>

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

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

```

```

/* Nag Types */
Nag_OrderType order = Nag_ColMajor;
NagError      fail;

INIT_FAIL(fail);

/* Output preamble */
printf("nag_matop_real_gen_matrix_pow (f01eqc) ");
printf("Example Program Results\n\n");
fflush(stdout);

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

/* Read in the problem size and the required power */
#ifdef _WIN32
scanf_s("%NAG_IFMT", &n);
#else
scanf("%NAG_IFMT", &n);
#endif
#ifdef _WIN32
scanf_s("%lf", &p);
#else
scanf("%lf", &p);
#endif
#ifdef _WIN32
scanf_s("%*[\n]");
#else
scanf("%*[\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++) {
    for (j = 0; j < n; j++) {
#ifdef _WIN32
scanf_s("%lf", &A(i, j));
#else
scanf("%lf", &A(i, j));
#endif
    }
}
#ifdef _WIN32
scanf_s("%*[\n] ");
#else
scanf("%*[\n] ");
#endif

/* Find matrix pth power using
 * nag_matop_real_gen_matrix_pow (f01eqc)
 * General power of a real matrix
 */
nag_matop_real_gen_matrix_pow (n, a, pda, p, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_matop_real_gen_matrix_pow (f01eqc)\n%s\n",
        fail.message);
    exit_status = 1;
    goto END;
}

/* Print matrix A^p 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^p", 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;
}

END:
NAG_FREE(a);
return exit_status;
}

```

## 10.2 Program Data

nag\_matop\_real\_gen\_matrix\_pow (f01eqc) Example Program Data

```

4      0.2          : Values of n and p

3.0    3.0    2.0    1.0
3.0    1.0    0.0    2.0
1.0    1.0    4.0    3.0
3.0    0.0    3.0    1.0 : End of matrix a

```

## 10.3 Program Results

nag\_matop\_real\_gen\_matrix\_pow (f01eqc) Example Program Results

A^p	1	2	3	4
1	1.2446	0.2375	0.2172	-0.1359
2	0.0925	1.1239	-0.1453	0.3731
3	-0.0769	0.1972	1.3131	0.1837
4	0.3985	-0.2902	0.1085	1.1560

---