

# NAG Library Function Document

## nag\_real\_gen\_matrix\_exp (f01ecc)

### 1 Purpose

nag\_real\_gen\_matrix\_exp (f01ecc) computes the matrix exponential,  $e^A$ , of a real  $n$  by  $n$  matrix  $A$ .

### 2 Specification

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

void nag_real_gen_matrix_exp (Nag_OrderType order, Integer n, double a[],
                             Integer pda, NagError *fail)
```

### 3 Description

$e^A$  is computed using a Padé approximant and the scaling and squaring method described in Al-Mohy and Higham (2009).

### 4 References

Al-Mohy A H and Higham N J (2009) A new scaling and squaring algorithm for the matrix exponential *SIAM J. Matrix Anal.* **31(3)** 970–989

Higham N J (2005) The scaling and squaring method for the matrix exponential revisited *SIAM J. Matrix Anal. Appl.* **26(4)** 1179–1193

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

Moler C B and Van Loan C F (2003) Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later *SIAM Rev.* **45** 3–49

### 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: **n** – Integer *Input*

*On entry:*  $n$ , the order of the matrix  $A$ .

*Constraint:*  $n \geq 0$ .

3: **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

$$\begin{aligned} &\mathbf{a}[(j-1) \times \mathbf{pda} + i - 1] \text{ when } \mathbf{order} = \text{Nag\_ColMajor}; \\ &\mathbf{a}[(i-1) \times \mathbf{pda} + j - 1] \text{ when } \mathbf{order} = \text{Nag\_RowMajor}. \end{aligned}$$

*On entry:* the  $n$  by  $n$  matrix  $A$ .

On exit: the  $n$  by  $n$  matrix exponential  $e^A$ .

4: **pda** – Integer *Input*

On entry: the stride separating row or column elements (depending on the value of **order**) in the array **a**.

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

5: **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 3.2.1.2 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\_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 How to Use the NAG Library and its Documentation for further information.

An unexpected internal error has occurred. Please contact NAG.

### NE\_NO\_LICENCE

Your licence key may have expired or may not have been installed correctly.

See Section 3.6.5 in How to Use the NAG Library and its Documentation for further information.

### NE\_SINGULAR

The linear equations to be solved are nearly singular and the Padé approximant probably has no correct figures; it is likely that this function has been called incorrectly.

The linear equations to be solved for the Padé approximant are singular; it is likely that this function has been called incorrectly.

### NW\_SOME\_PRECISION\_LOSS

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

## 7 Accuracy

For a normal matrix  $A$  (for which  $A^T A = A A^T$ ) the computed matrix,  $e^A$ , is guaranteed to be close to the exact matrix, that is, the method is forward stable. No such guarantee can be given for non-normal matrices. See Al–Mohy and Higham (2009) and Section 10.3 of Higham (2008) for details and further discussion.

If estimates of the condition number of the matrix exponential are required then `nag_matop_real_gen_matrix_cond_exp` (f01jgc) should be used.

## 8 Parallelism and Performance

`nag_real_gen_matrix_exp` (f01ecc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

`nag_real_gen_matrix_exp` (f01ecc) 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  $n$ , and the double allocatable memory required is approximately  $6 \times n^2$ .

The cost of the algorithm is  $O(n^3)$ ; see Section 5 of Al–Mohy and Higham (2009). The real allocatable memory required is approximately  $6 \times n^2$ .

If the Fréchet derivative of the matrix exponential is required then `nag_matop_real_gen_matrix_frcht_exp` (f01jhc) should be used.

As well as the excellent book cited above, the classic reference for the computation of the matrix exponential is Moler and Van Loan (2003).

## 10 Example

This example finds the matrix exponential of the matrix

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

### 10.1 Program Text

```

/* nag_real_gen_matrix_exp (f01ecc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */
/* Pre-processor includes */
#include <stdio.h>
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf01.h>
#include <nagx04.h>

int main(void)
{

```

```

/*Integer scalar and array declarations */
Integer exit_status = 0;
Integer i, j, n;
Integer pda;
NagError fail;
/*Double scalar and array declarations */
double *a = 0;
Nag_OrderType order;

INIT_FAIL(fail);

printf("%s\n", "nag_real_gen_matrix_exp (f01ecc) Example Program Results");
printf("\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
#ifdef NAG_COLUMN_MAJOR
pda = n;
#define A(I, J) a[(J-1)*pda + I-1]
order = Nag_ColMajor;
#else
pda = n;
#define A(I, J) a[(I-1)*pda + J-1]
order = Nag_RowMajor;
#endif
if (!(a = NAG_ALLOC(pda * n, double)))
{
printf("Allocation failure\n");
exit_status = -1;
goto END;
}
/* Read A from data file */
for (i = 1; i <= n; i++) {
for (j = 1; 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 exp( A ) */
/*
* nag_real_gen_matrix_exp (f01ecc)
* Real matrix exponential
*/
nag_real_gen_matrix_exp(order, n, a, pda, &fail);
if (fail.code != NE_NOERROR) {
printf("Error from nag_real_gen_matrix_exp (f01ecc).\n%s\n",
fail.message);
exit_status = 1;
goto END;
}
/* Print solution */
/*
* nag_gen_real_mat_print (x04cac)
* Print real general matrix (easy-to-use)
*/
fflush(stdout);
nag_gen_real_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, n,
a, pda, "Exp(A)", 0, &fail);
if (fail.code != NE_NOERROR) {
printf("Error from nag_gen_real_mat_print (x04cac).\n%s\n", fail.message);
exit_status = 1;
}
}

```

```

END:
  NAG_FREE(a);

  return exit_status;
}

```

## 10.2 Program Data

nag\_real\_gen\_matrix\_exp (f01ecc) Example Program Data

```

4                               :Value of n

1.0  2.0  2.0  2.0
3.0  1.0  1.0  2.0
3.0  2.0  1.0  2.0
3.0  3.0  3.0  1.0 :End of matrix A

```

## 10.3 Program Results

nag\_real\_gen\_matrix\_exp (f01ecc) Example Program Results

```

Exp(A)
      1          2          3          4
1    740.7038   610.8500   542.2743   549.1753
2    731.2510   603.5524   535.0884   542.2743
3    823.7630   679.4257   603.5524   610.8500
4    998.4355   823.7630   731.2510   740.7038

```

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