NAG Toolbox

nag_matop_complex_gen_matrix_cond_exp (f01kg)

1 Purpose

nag_matop_complex_gen_matrix_cond_exp (f01kg) computes an estimate of the relative condition number $\kappa_{\mathrm{exp}}(A)$ of the exponential of a complex n by n matrix A, in the 1-norm. The matrix exponential e^A is also returned.

2 Syntax

```
[a, condea, ifail] = nag_matop_complex_gen_matrix_cond_exp(a, 'n', n)
[a, condea, ifail] = f01kg(a, 'n', n)
```

3 Description

The Fréchet derivative of the matrix exponential of A is the unique linear mapping $E \mapsto L(A, E)$ such that for any matrix E

$$e^{A+E} - e^A - L(A, E) = o(\|E\|).$$

The derivative describes the first-order effect of perturbations in A on the exponential e^A.

The relative condition number of the matrix exponential can be defined by

$$\kappa_{\mathrm{exp}}(A) = \frac{\|L(A)\|\|A\|}{\|\exp(A)\|},$$

where $\|L(A)\|$ is the norm of the Fréchet derivative of the matrix exponential at A.

To obtain the estimate of $\kappa_{\mathrm{exp}}(A)$, nag_matop_complex_gen_matrix_cond_exp (f01kg) first estimates $\|L(A)\|$ by computing an estimate γ of a quantity $K \in \left[n^{-1}\|L(A)\|_1, n\|L(A)\|_1\right]$, such that $\gamma \leq K$.

The algorithms used to compute $\kappa_{\mathrm{exp}}(A)$ are detailed in the Al–Mohy and Higham (2009a) and Al–Mohy and Higham (2009b).

The matrix exponential e^A is computed using a Padé approximant and the scaling and squaring method. The Padé approximant is differentiated to obtain the Fréchet derivatives $L(A, E)$ which are used to estimate the condition number.

4 References

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

Al–Mohy A H and Higham N J (2009b) Computing the Fréchet derivative of the matrix exponential, with an application to condition number estimation *SIAM J. Matrix Anal. Appl.* **30(4)** 1639–1657

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 Parameters

5.1 Compulsory Input Parameters

1: **a**$(lda,:)$ – COMPLEX (KIND=nag_wp) array

The first dimension of the array **a** must be at least **n**.

The second dimension of the array **a** must be at least **n**.

The n by n matrix A.

5.2 Optional Input Parameters

1: **n** – INTEGER

Default: the first dimension of the array **a**.

n, the order of the matrix A.

Constraint: $\mathbf{n} \geq 0$.

5.3 Output Parameters

1: **a**$(lda,:)$ – COMPLEX (KIND=nag_wp) array

The first dimension of the array **a** will be **n**.

The second dimension of the array **a** will be **n**.

The n by n matrix exponential e^A.

2: **condea** – REAL (KIND=nag_wp)

An estimate of the relative condition number of the matrix exponential $\kappa_{\mathrm{exp}}(A)$.

3: **ifail** – INTEGER

$\mathbf{ifail} = 0$ unless the function detects an error (see Section 5).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

$\mathbf{ifail} = 1$

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

$\mathbf{ifail} = 2$

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

$\mathbf{ifail} = 3$

An unexpected internal error has occurred. Please contact NAG.

$\mathbf{ifail} = -1$

Constraint: $\mathbf{n} \geq 0$.

$\mathbf{ifail} = -3$

Constraint: $lda \geq \mathbf{n}$.

ifail $= -99$

An unexpected error has been triggered by this routine. Please contact NAG.

ifail $= -399$

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

ifail $= -999$

Dynamic memory allocation failed.

7 Accuracy

nag_matop_complex_gen_matrix_cond_exp (f01kg) uses the norm estimation function nag_linsys_complex_gen_norm_rcomm (f04zd) to produce an estimate γ of a quantity $K \in \left[n^{-1}\|L(A)\|_1, n\|L(A)\|_1\right]$, such that $\gamma \leq K$. For further details on the accuracy of norm estimation, see the documentation for nag_linsys_complex_gen_norm_rcomm (f04zd).

For a normal matrix A (for which $A^{\mathrm{H}}A = AA^{\mathrm{H}}$) 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 Section 10.3 of Higham (2008) for details and further discussion.

For further discussion of the condition of the matrix exponential see Section 10.2 of Higham (2008).

8 Further Comments

nag_matop_complex_gen_matrix_cond_std (f01ka) uses a similar algorithm to nag_matop_complex_gen_matrix_cond_exp (f01kg) to compute an estimate of the *absolute* condition number (which is related to the relative condition number by a factor of $\|A\|/\|\exp(A)\|$). However, the required Fréchet derivatives are computed in a more efficient and stable manner by nag_matop_complex_gen_matrix_cond_exp (f01kg) and so its use is recommended over nag_matop_complex_gen_matrix_cond_std (f01ka).

The cost of the algorithm is $O\left(n^3\right)$ and the complex allocatable memory required is approximately $15n^2$; see Al–Mohy and Higham (2009a) and Al–Mohy and Higham (2009b) for further details.

If the matrix exponential alone is required, without an estimate of the condition number, then nag_matop_complex_gen_matrix_exp (f01fc) should be used. If the Fréchet derivative of the matrix exponential is required then nag_matop_complex_gen_matrix_frcht_exp (f01kh) should be used.

As well as the excellent book Higham (2008), the classic reference for the computation of the matrix exponential is Moler and Van Loan (2003).

9 Example

This example estimates the relative condition number of the matrix exponential e^A, where

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

9.1 Program Text

```
     function f01kg_example

fprintf('f01kg example results\n\n');

% Exponential and conditioning of matrix A
a =  [1+ i, 2+ i, 2+ i, 2+i;
       3+2i, 1,    1,    2+i;
       3+2i, 2+ i, 1,    2+i;
```

```
      3+2i, 3+2i, 3+2i, 1+i];

% Compute exp(a)
[expa, condea, ifail] = f01kg(a);

% Display results
disp('exp(A):');
disp(expa);

fprintf('Estimated condition number is: %6.2f\n', condea);
```

9.2 Program Results

```
     f01kg example results

exp(A):
   1.0e+03 *

  -0.1579 - 0.7544i  -0.1947 - 0.5551i  -0.1866 - 0.4755i  -0.1558 - 0.5202i
  -0.2069 - 0.6947i  -0.2255 - 0.5054i  -0.2124 - 0.4311i  -0.1866 - 0.4755i
  -0.2087 - 0.8082i  -0.2385 - 0.5908i  -0.2255 - 0.5054i  -0.1947 - 0.5551i
  -0.1334 - 1.0855i  -0.2087 - 0.8082i  -0.2069 - 0.6947i  -0.1579 - 0.7544i

Estimated condition number is:  15.29
```