NAG Toolbox

nag_matop_complex_gen_matrix_frcht_exp (f01kh)

1 Purpose

nag_matop_complex_gen_matrix_frcht_exp (f01kh) computes the Fréchet derivative $L(A, E)$ of the matrix exponential of a complex n by n matrix A applied to the complex n by n matrix E. The matrix exponential e^A is also returned.

2 Syntax

```
[a, e, ifail] = nag_matop_complex_gen_matrix_frcht_exp(a, e, 'n', n)
[a, e, ifail] = f01kh(a, e, '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.

nag_matop_complex_gen_matrix_frcht_exp (f01kh) uses the algorithms of Al–Mohy and Higham (2009a) and Al–Mohy and Higham (2009b) to compute e^A and $L(A, E)$. The matrix exponential e^A is computed using a Padé approximant and the scaling and squaring method. The Padé approximant is then differentiated in order to obtain the Fréchet derivative $L(A, E)$.

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.

2: **e**$(lde, :)$ – COMPLEX (KIND=nag_wp) array

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

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

The n by n matrix E

5.2 Optional Input Parameters

1: **n** – INTEGER

Default: the first dimension of the arrays **a**, **e**. (An error is raised if these dimensions are not equal.)

n, the order of the matrix A.

Constraint: **n** ≥ 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: **e**$(lde,:)$ – COMPLEX (KIND=nag_wp) array

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

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

The Fréchet derivative $L(A, E)$

3: **ifail** – INTEGER

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

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail $= 1$

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

ifail $= 2$

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

ifail $= 3$

An unexpected internal error has occurred. Please contact NAG.

ifail $= -1$

Constraint: **n** ≥ 0.

ifail $= -3$

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

ifail $= -5$

Constraint: $lde \geq$ **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

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), Al–Mohy and Higham (2009a) and Al–Mohy and Higham (2009b) for details and further discussion.

8 Further Comments

The cost of the algorithm is $O(n^3)$ and the complex allocatable memory required is approximately $9n^2$; see Al–Mohy and Higham (2009a) and Al–Mohy and Higham (2009b).

If the matrix exponential alone is required, without the Fréchet derivative, then nag_matop_complex_gen_matrix_exp (f01fc) should be used.

If the condition number of the matrix exponential is required then nag_matop_complex_gen_matrix_cond_exp (f01kg) 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 finds the matrix exponential e^A and the Fréchet derivative $L(A, E)$, where

$$A = \begin{pmatrix} 1+i & 2+i & 2+i & 2+i \\ 3+2i & 1 & 1 & 2+i \\ 3+2i & 2+i & 1 & 2+i \\ 3+2i & 3+2i & 3+2i & 1+i \end{pmatrix} \quad \text{and} \quad E = \begin{pmatrix} 1 & 2+i & 2 & 4+i \\ 3+2i & 0 & 1 & 0+i \\ 0+2i & 0+i & 1 & 0 \\ 1+i & 2+2i & 0+3i & 1 \end{pmatrix}.$$

9.1 Program Text

```
function f01kh_example

fprintf('f01kh example results\n\n');

% Exponential of matrix A and Frechet derivative of exp(A)E.

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];

e =  [1,    2+ i, 2,    4+i;
      3+2i, 0,    1,    0+i;
      0+2i, 0+ i, 1,    0;
      1+ i, 2+2i, 0+3i, 1];

[expa, lae, ifail] = f01kh(a,e);

[ifail] = x04da('General', ' ', expa, 'exp(A):');
disp(' ');
[ifail] = x04da('General', ' ', lae, 'L_exp(A,E):');
```

9.2 Program Results

```
    f01kh example results

 exp(A):
             1          2          3          4
 1   -157.9003  -194.6526  -186.5627  -155.7669
     -754.3717  -555.0507  -475.4533  -520.1876

 2   -206.8899  -225.4985  -212.4414  -186.5627
     -694.7443  -505.3938  -431.0611  -475.4533

 3   -208.7476  -238.4962  -225.4985  -194.6526
     -808.2090  -590.8045  -505.3938  -555.0507

 4   -133.3958  -208.7476  -206.8899  -157.9003
    -1085.5496  -808.2090  -694.7443  -754.3717

 L_exp(A,E):
             1          2          3          4
 1   1571.5852   778.4238   500.2085   740.7485
    -4640.2429 -3719.8308 -3246.0234 -3424.1963

 2   1472.7846   731.6608   473.2569   692.0895
    -4273.5048 -3432.5961 -2990.9285 -3148.4635

 3   1996.4848  1107.9174   782.1266  1031.5808
    -4568.8881 -3714.9923 -3249.1926 -3400.8557

 4   3327.1347  2015.2763  1514.3130  1873.9421
    -5829.0773 -4810.2591 -4234.6812 -4404.0163
```