NAG Toolbox

nag_matop_complex_gen_matrix_frcht_pow (f01kf)

1 Purpose

nag_matop_complex_gen_matrix_frcht_pow (f01kf) computes the Fréchet derivative $L(A,E)$ of the pth power (where p is real) of the complex n by n matrix A applied to the complex n by n matrix E. The principal matrix power A^p is also returned.

2 Syntax

```
[a, e, ifail] = nag_matop_complex_gen_matrix_frcht_pow(a, e, p, 'n', n)
[a, e, ifail] = f01kf(a, e, p, 'n', n)
```

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 $\{z : -\pi < \mathrm{Im}(z) < \pi\}$). If A is nonsingular but has negative real eigenvalues, the principal logarithm is not defined, but a non-principal pth power can be defined by using a non-principal logarithm.

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

$$(A+E)^p - A^p - L(A,E) = o(\|E\|).$$

The derivative describes the first-order effect of perturbations in A on the matrix power A^p.

nag_matop_complex_gen_matrix_frcht_pow (f01kf) uses the algorithms of Higham and Lin (2011) and Higham and Lin (2013) to compute A^p and $L(A,E)$. 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 using a Schur decomposition, a Padé approximant and the scaling and squaring method. The Padé approximant is differentiated in order to obtain the Fréchet derivative of A^q and $L(A,E)$ is then computed using a combination of the chain rule and the product rule for Fréchet derivatives.

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 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.

3: **p** – REAL (KIND=nag_wp)

The required power of A.

5.2 Optional Input Parameters

1: **n** – INTEGER

Default: the first dimension of the arrays **a**, **e** and the second dimension of the array **a**. (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 principal matrix pth power, A^p. Alternatively if **ifail** $= 1$, a non-principal pth power is returned.

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 $= 1$

A has eigenvalues on the negative real line. The principal pth power is not defined in this case, so a non-principal power was returned.

ifail $= 2$

A is singular so the pth power cannot be computed.

ifail $= 3$

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

ifail $= 4$

An unexpected internal error occurred. This failure should not occur and suggests that the function has been called incorrectly.

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 Schur decomposition is diagonal and the computation of the fractional part of the matrix power 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. See Higham and Lin (2011) and Higham and Lin (2013) for details and further discussion.

If the condition number of the matrix power is required then nag_matop_complex_gen_matrix_cond_pow (f01ke) should be used.

8 Further Comments

The complex allocatable memory required by the algorithm is approximately $6 \times n^2$.

The cost of the algorithm is $O(n^3)$ floating-point operations; see Higham and Lin (2011) and Higham and Lin (2013).

If the matrix pth power alone is required, without the Fréchet derivative, then nag_matop_complex_gen_matrix_pow (f01fq) should be used. If the condition number of the matrix power is required then nag_matop_complex_gen_matrix_cond_pow (f01ke) should be used. The real analogue of this function is nag_matop_real_gen_matrix_frcht_pow (f01jf).

9 Example

This example finds A^p and the Fréchet derivative of the matrix power $L(A, E)$, where $p = 0.2$,

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

9.1 Program Text

```
function f01kf_example

fprintf('f01kf example results\n\n');

% Principal power p of matrix A and Frechet derivative of A^pE.

a = [ 2   3    2    1+3i;
      2+i 1    1    2+ i;
      0+i 2+2i 0+2i 0+4i;
      3   0+ i 3    1];

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

p = 0.2;

[pa, lpae, ifail] = f01kf(a,e,p);

disp('A^p:');
disp(pa);

disp('L_p(A,E):');
disp(lpae);
```

9.2 Program Results

```
f01kf example results

A^p:
   1.2029 - 0.0424i   0.0810 + 0.0428i   0.2374 - 0.1718i  -0.0520 + 0.0976i
   0.1311 - 0.0378i   1.1054 + 0.1091i  -0.0757 + 0.0066i   0.2308 + 0.1373i
  -0.0305 - 0.1948i   0.4878 + 0.2846i   1.0822 + 0.2620i  -0.1050 + 0.3131i
   0.3401 + 0.1792i  -0.3005 - 0.0857i   0.1838 - 0.0261i   1.2347 - 0.1571i

L_p(A,E):
   0.0980 - 0.0926i  -0.0980 + 0.2759i   0.0410 - 0.2629i   0.0136 + 0.1853i
  -0.0644 + 0.3359i  -0.2093 - 0.3976i   0.4315 + 0.0395i   0.1337 - 0.0976i
   0.1912 + 0.0032i   0.2279 + 0.3308i  -0.0963 + 0.1146i  -0.0925 - 0.3254i
  -0.0907 + 0.1255i  -0.0153 - 0.4022i   0.1299 + 0.0694i   0.2238 + 0.1179i
```