NAG Toolbox

nag_matop_real_gen_matrix_frcht_exp (f01jh)

1 Purpose

nag_matop_real_gen_matrix_frcht_exp (f01jh) computes the Fréchet derivative $L(A,E)$ of the matrix exponential of a real n by n matrix A applied to the real n by n matrix E. The matrix exponential e^A is also returned.

2 Syntax

```
[a, e, ifail] = nag_matop_real_gen_matrix_frcht_exp(a, e, 'n', n)
[a, e, ifail] = f01jh(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_real_gen_matrix_frcht_exp (f01jh) 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,:) – REAL (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,:) – REAL (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: $\mathbf{n} \geq 0$.

5.3 Output Parameters

1: **a**$(lda,:)$ – REAL (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**$(lde,:)$ – REAL (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: $\mathbf{n} \geq 0$.

ifail $= -3$

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

ifail $= -5$

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

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

For a normal matrix A (for which $A^{\mathrm{T}}A = AA^{\mathrm{T}}$) 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 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 real 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_real_gen_matrix_exp (f01ec) should be used.

If the condition number of the matrix exponential is required then nag_matop_real_gen_matrix_cond_exp (f01jg) 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

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

9.1 Program Text

```
     function f01jh_example

fprintf('f01jh example results\n\n');

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

a = [ 1 2 2 2;
      3 1 1 2;
      3 2 1 2;
      3 3 3 1];

e = [ 1 0 1 2;
      0 0 0 1;
      4 2 1 2;
      0 3 2 1];

[expa, lae, ifail] = f01jh(a,e);

[ifail] = x04ca('General', ' ', expa, 'exp(A):');
disp(' ');
[ifail] = x04ca('General', ' ', lae, 'L_exp(A,E):');
```

9.2 Program Results

```
     f01jh example 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

 L_exp(A,E):
             1          2          3          4
 1   3571.5724  2989.2581  2652.3449  2818.7416
 2   3202.0590  2684.2631  2381.4500  2542.7976
 3   4341.3950  3628.9329  3219.3516  3408.1831
 4   4821.2945  4035.9700  3580.0124  3804.4690
```