NAG Toolbox

nag_matop_real_gen_matrix_cond_pow (f01je)

1 Purpose

nag_matop_real_gen_matrix_cond_pow (f01je) computes an estimate of the relative condition number κ_{A^p} of the pth power (where p is real) of a real n by n matrix A, in the 1-norm. The principal matrix power A^p is also returned.

2 Syntax

```
[a, condpa, ifail] = nag_matop_real_gen_matrix_cond_pow(a, p, 'n', n)
[a, condpa, ifail] = f01je(a, 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 $\{z : -\pi < \mathrm{Im}(z) < \pi\}$).

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.

The relative condition number of the matrix pth power can be defined by

$$\kappa_{A^p} = \frac{\|L(A)\|\|A\|}{\|A^p\|},$$

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

nag_matop_real_gen_matrix_cond_pow (f01je) uses the algorithms of Higham and Lin (2011) and Higham and Lin (2013) to compute κ_{A^p} and A^p. 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.

To obtain an estimate of κ_{A^p}, nag_matop_real_gen_matrix_cond_pow (f01je) 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 $\gamma \leq K$. This requires multiple Fréchet derivatives to be computed. Fréchet derivatives of A^q are obtained by differentiating the Padé approximant. Fréchet derivatives of A^p are 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,:) – 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: **p** – REAL (KIND=nag_wp)

The required power of A.

5.2 Optional Input Parameters

1: **n** – INTEGER

Default: the first dimension of the array **a** 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: $\mathbf{n} \geq 0$.

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 principal matrix pth power, A^p.

2: **condpa** – REAL (KIND=nag_wp)

If $\mathbf{ifail} = 0$ or 3, an estimate of the relative condition number of the matrix pth power, κ_{A^p}. Alternatively, if $\mathbf{ifail} = 4$, the absolute condition number of the matrix pth power.

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:

$\mathbf{ifail} = 1$

A has eigenvalues on the negative real line. The principal pth power is not defined in this case; nag_matop_complex_gen_matrix_cond_pow (f01ke) can be used to find a complex, non-principal pth power.

$\mathbf{ifail} = 2$

A is singular so the pth power cannot be computed.

$\mathbf{ifail} = 3$

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

ifail $= 4$

The relative condition number is infinite. The absolute condition number was returned instead.

ifail $= 5$

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 $= -99$

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_real_gen_matrix_cond_pow (f01je) uses the norm estimation function nag_linsys_real_gen_norm_rcomm (f04yd) 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_real_gen_norm_rcomm (f04yd).

For a normal matrix A (for which $A^{\mathrm{T}}A = AA^{\mathrm{T}}$), 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.

8 Further Comments

The amount of real allocatable memory required by the algorithm is typically of the order $10 \times n^2$.

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

If the matrix pth power alone is required, without an estimate of the condition number, then nag_matop_real_gen_matrix_pow (f01eq) should be used. If the Fréchet derivative of the matrix power is required then nag_matop_real_gen_matrix_frcht_pow (f01jf) should be used. If A has negative real eigenvalues then nag_matop_complex_gen_matrix_cond_pow (f01ke) can be used to return a complex, non-principal pth power and its condition number.

9 Example

This example estimates the relative condition number of the matrix power A^p, where $p = 0.2$ and

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

9.1 Program Text

```
function f01je_example

fprintf('f01je example results\n\n');

% Principal power p of matrix A and relative condition number.

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

p = 0.2;

[pa, condpa, ifail] = f01je(a,p);

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

fprintf('\nEstimated relative condition number is : %6.2f\n', condpa);
```

9.2 Program Results

```
f01je example results

A^p:
    1.2368    0.1977    0.1749   -0.0314
   -0.0543    1.1643   -0.0947    0.3145
    0.0537    0.3514    1.3254    0.0214
    0.3339   -0.2125    0.1880    1.0581

Estimated relative condition number is :   2.75
```