NAG Library Routine Document

F01JHF

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details.

1 Purpose

F01JHF 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 Specification

```
SUBROUTINE F01JHF (N, A, LDA, E, LDE, IFAIL)

INTEGER             N, LDA, LDE, IFAIL
REAL (KIND=nag_wp) A(LDA,*), E(LDE,*)
```

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.

F01JHF 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 Arguments

1: N – INTEGER *Input*

On entry: n, the order of the matrix A.

Constraint: $\mathrm{N} \geq 0$.

2: A(LDA, $*$) – REAL (KIND=nag_wp) array *Input/Output*

Note: the second dimension of the array A must be at least N.

On entry: the n by n matrix A.

On exit: the n by n matrix exponential e^A.

3: LDA – INTEGER *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which F01JHF is called.

Constraint: LDA $\geq$ N.

4: E(LDE, $*$) – REAL (KIND=nag_wp) array *Input/Output*

Note: the second dimension of the array E must be at least N.

On entry: the n by n matrix E

On exit: the Fréchet derivative $L(A, E)$

5: LDE – INTEGER *Input*

On entry: the first dimension of the array E as declared in the (sub)program from which F01JHF is called.

Constraint: LDE $\geq$ N.

6: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation for details.

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this argument, the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

On exit: IFAIL $= 0$ unless the routine detects an error or a warning has been flagged (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL $= 0$ or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL $= 1$

The linear equations to be solved for the Padé approximant are singular; it is likely that this routine 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 $= -1$

On entry, N $= \langle value \rangle$.
Constraint: N ≥ 0.

IFAIL $= -3$

On entry, LDA $= \langle value \rangle$ and N $= \langle value \rangle$.
Constraint: LDA $\geq$ N.

IFAIL $= -5$

On entry, LDE $= \langle value \rangle$ and N $= \langle value \rangle$.
Constraint: LDE $\geq$ N.

IFAIL $= -99$

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

See Section 3.9 in How to Use the NAG Library and its Documentation for further information.

IFAIL $= -399$

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

See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

IFAIL $= -999$

Dynamic memory allocation failed.

See Section 3.7 in How to Use the NAG Library and its Documentation for further information.

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 Parallelism and Performance

F01JHF is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

F01JHF makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 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 F01ECF should be used.

If the condition number of the matrix exponential is required then F01JGF 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).

10 Example

This example finds the matrix exponential e^A and the Fréchet derivative $L(A,E)$, where

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

10.1 Program Text

```
    Program f01jhfe

!     F01JHF Example Program Text

!     Mark 26 Release. NAG Copyright 2016.

!     .. Use Statements ..
      Use nag_library, Only: f01jhf, nag_wp, x04caf
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
!     .. Local Scalars ..
      Integer                          :: i, ifail, lda, lde, n
!     .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable  :: a(:,:), e(:,:)
!     .. Executable Statements ..
      Write (nout,*) 'F01JHF Example Program Results'
      Write (nout,*)
      Flush (nout)
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) n
      lda = n
      lde = n
      Allocate (a(lda,n))
      Allocate (e(lde,n))
!     Read A from data file
      Read (nin,*)(a(i,1:n),i=1,n)
!     Read E from data file
      Read (nin,*)(e(i,1:n),i=1,n)

!     ifail: behaviour on error exit
!             =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
      ifail = 0

!     Find exp( A ) and L_exp(A,E)
      Call f01jhf(n,a,lda,e,lde,ifail)

!     Print solution
      Call x04caf('General',' ',n,n,a,lda,'Exp(A)',ifail)
      Write (nout,*)
      Call x04caf('General',' ',n,n,e,lde,'L_exp(A,E)',ifail)

    End Program f01jhfe
```

10.2 Program Data

```
F01JHF Example Program Data

  4                      :Value of N

  1.0   2.0   2.0   2.0
  3.0   1.0   1.0   2.0
  3.0   2.0   1.0   2.0
  3.0   3.0   3.0   1.0  :End of matrix A

  1.0   0.0   1.0   2.0
  0.0   0.0   0.0   1.0
  4.0   2.0   1.0   2.0
  0.0   3.0   2.0   1.0  :End of matrix E
```

10.3 Program Results

```
 F01JHF Example Program 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
```