NAG Library Function Document

nag_matop_real_gen_matrix_cond_std (f01jac)

1 Purpose

nag_matop_real_gen_matrix_cond_std (f01jac) computes an estimate of the absolute condition number of a matrix function f at a real n by n matrix A in the 1-norm, where f is either the exponential, logarithm, sine, cosine, hyperbolic sine (sinh) or hyperbolic cosine (cosh). The evaluation of the matrix function, $f(A)$, is also returned.

2 Specification

```
#include <nag.h>
#include <nagf01.h>
```

```
void nag_matop_real_gen_matrix_cond_std (Nag_MatFunType fun, Integer n,
     double a[], Integer pda, double *conda, double *norma, double *normfa,
     NagError *fail)
```

3 Description

The absolute condition number of f at A, $\mathrm{cond}_{\mathrm{abs}}(f,A)$ is given by the norm of the Fréchet derivative of f, $L(A)$, which is defined by

$$\|L(X)\| := \max_{E\neq 0}\frac{\|L(X,E)\|}{\|E\|},$$

where $L(X,E)$ is the Fréchet derivative in the direction E. $L(X,E)$ is linear in E and can therefore be written as

$$\mathrm{vec}(L(X,E)) = K(X)\mathrm{vec}(E),$$

where the vec operator stacks the columns of a matrix into one vector, so that $K(X)$ is $n^2 \times n^2$. nag_matop_real_gen_matrix_cond_std (f01jac) computes an estimate γ such that $\gamma \leq \|K(X)\|_1$, where $\|K(X)\|_1 \in \left[n^{-1}\|L(X)\|_1, n\|L(X)\|_1\right]$. The relative condition number can then be computed via

$$\mathrm{cond}_{\mathrm{rel}}(f,A) = \frac{\mathrm{cond}_{\mathrm{abs}}(f,A)\|A\|_1}{\|f(A)\|_1}.$$

The algorithm used to find γ is detailed in Section 3.4 of Higham (2008).

4 References

Higham N J (2008) *Functions of Matrices: Theory and Computation* SIAM, Philadelphia, PA, USA

5 Arguments

1: **fun** – Nag_MatFunType *Input*

On entry: indicates which matrix function will be used.

fun = Nag_Exp
The matrix exponential, e^A, will be used.

fun = Nag_Sin
The matrix sine, $\sin(A)$, will be used.

fun = Nag_Cos
The matrix cosine, $\cos(A)$, will be used.

fun = Nag_Sinh
The hyperbolic matrix sine, $\sinh(A)$, will be used.

fun = Nag_Cosh
The hyperbolic matrix cosine, $\cosh(A)$, will be used.

fun = Nag_Loga
The matrix logarithm, $\log(A)$, will be used.

Constraint: **fun** = Nag_Exp, Nag_Sin, Nag_Cos, Nag_Sinh, Nag_Cosh or Nag_Loga.

2: **n** – Integer *Input*

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

Constraint: **n** ≥ 0.

3: **a**[dim] – double *Input/Output*

Note: the dimension, *dim*, of the array **a** must be at least **pda** $\times$ **n**.

The (i,j)th element of the matrix A is stored in **a**$[(j-1) \times$ **pda** $+ i - 1]$.

On entry: the n by n matrix A.

On exit: the n by n matrix, $f(A)$.

4: **pda** – Integer *Input*

On entry: the stride separating matrix row elements in the array **a**.

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

5: **conda** – double * *Output*

On exit: an estimate of the absolute condition number of f at A.

6: **norma** – double * *Output*

On exit: the 1-norm of A.

7: **normfa** – double * *Output*

On exit: the 1-norm of $f(A)$.

8: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 3.6 in the Essential Introduction).

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Allocation of memory failed.

NE_BAD_PARAM

On entry, argument ⟨*value*⟩ had an illegal value.

NE_INT

On entry, **n** = ⟨*value*⟩.
Constraint: **n** ≥ 0.

NE_INT_2

On entry, **pda** = ⟨*value*⟩ and **n** = ⟨*value*⟩.
Constraint: **pda** ≥ **n**.

NE_INTERNAL_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

An internal error occurred when estimating the norm of the Fréchet derivative of f at A. Please contact NAG.

An internal error occurred when evaluating the matrix function $f(A)$. You can investigate further by calling nag_real_gen_matrix_exp (f01ecc), nag_matop_real_gen_matrix_log (f01ejc) or nag_matop_real_gen_matrix_fun_std (f01ekc) with the matrix A.

7 Accuracy

nag_matop_real_gen_matrix_cond_std (f01jac) uses the norm estimation function nag_linsys_real_gen_norm_rcomm (f04ydc) to estimate a quantity γ, where $\gamma \leq \|K(X)\|_1$ and $\|K(X)\|_1 \in \left[n^{-1}\|L(X)\|_1, n\|L(X)\|_1\right]$. For further details on the accuracy of norm estimation, see the documentation for nag_linsys_real_gen_norm_rcomm (f04ydc).

8 Parallelism and Performance

nag_matop_real_gen_matrix_cond_std (f01jac) is threaded by NAG for parallel execution in multi-threaded implementations of the NAG Library.

nag_matop_real_gen_matrix_cond_std (f01jac) 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.

In these implementations, this may make calls to the user supplied functions from within an OpenMP parallel region. Thus OpenMP directives within the user functions should be avoided, unless you are using the same OpenMP runtime library (which normally means using the same compiler) as that used to build your NAG Library implementation, as listed in the Installers' Note.

Please consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

The matrix function is computed using one of three underlying matrix function routines:

if **fun** = Nag_Exp, nag_real_gen_matrix_exp (f01ecc) is used;

if **fun** = Nag_Loga, nag_matop_real_gen_matrix_log (f01ejc) is used;

else, nag_matop_real_gen_matrix_fun_std (f01ekc) is used.

Approximately $6n^2$ of real allocatable memory is required by the routine, in addition to the memory used by these underlying matrix function routines.

If only $f(A)$ is required, without an estimate of the condition number, then it is far more efficient to use the appropriate matrix function routine listed above.

nag_matop_complex_gen_matrix_cond_std (f01kac) can be used to find the condition number of the exponential, logarithm, sine, cosine, sinh or cosh matrix functions at a complex matrix.

10 Example

This example estimates the absolute and relative condition numbers of the matrix sinh function where

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

10.1 Program Text

```
/* nag_matop_real_gen_matrix_cond_std (f01jac) Example Program.
 *
 * Copyright 2013 Numerical Algorithms Group.
 *
 * Mark 24, 2013.
 */
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf01.h>
#include <nagx02.h>
#include <nagx04.h>

#define A(I,J) a[J*lda + I]

int main(void)
{
  /* Scalars */
  Integer        exit_status = 0;
  Integer        i, j, n, lda;
  double         conda, cond_rel, eps, norma, normfa;
  /* Arrays */
  double         *a = 0;
  char           function_name[100];
  /* Nag Types */
  Nag_OrderType  order = Nag_ColMajor;
  Nag_MatFunType fun;
  NagError       fail;

  INIT_FAIL(fail);

  /* Output preamble */
  printf("nag_matop_real_gen_matrix_cond_std (f01jac) ");
  printf("Example Program Results\n\n");
  fflush(stdout);

  /* Skip heading in data file */
  scanf("%*[^\n] ");

  /* Read in the problem size and the required function */
  scanf("%ld%99s%*[^\n]", &n, function_name);

  lda = n;
  if (!(a = NAG_ALLOC((lda)*(n), double))) {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }

  /* nag_enum_name_to_value (x04nac)
   * Converts Nag enum member name to value
   */
  fun = (Nag_MatFunType) nag_enum_name_to_value(function_name);

  /* Read in the matrix A from data file */
  for (i = 0; i < n; i++)
    for (j = 0; j < n; j++) scanf("%lf", &A(i, j));
  scanf("%*[^\n] ");
```

```
  /* Print matrix A using nag_gen_real_mat_print (x04cac)
   * Print real general matrix (easy-to-use)
   */
  nag_gen_real_mat_print (order, Nag_GeneralMatrix, Nag_NonUnitDiag,
                          n, n, a, lda, "A", NULL, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_real_mat_print (x04cac)\n%s\n", fail.message);
    exit_status = 2;
    goto END;
  }

  /* Find absolute condition number estimate using
   * nag_matop_real_gen_matrix_cond_std (f01jac)
   * Condition number for the exponential, logarithm, sine, cosine,
   * sinh or cosh of a real matrix
   */
  nag_matop_real_gen_matrix_cond_std (fun, n, a, lda, &conda,
                                      &norma, &normfa, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_matop_real_gen_matrix_cond_std (f01jac)\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
  }

  /* Print absolute condition number estimate */
  printf("\nf(A) = %s(A)\n", function_name);
  printf("Estimated absolute condition number is: %7.2f\n", conda);

  /* nag_machine_precision (x02ajc) The machine precision  */
  eps = nag_machine_precision;

  /* Find relative condition number estimate */
  if ( normfa>eps) {
    cond_rel = conda * norma/normfa;
    printf("Estimated relative condition number is: %7.2f\n",cond_rel);
  } else {
    printf("The estimated norm of f(A) is effectively zero and so\n");
    printf("the relative condition number is undefined.\n");
  }

 END:
  NAG_FREE(a);
  return exit_status;
}
```

10.2 Program Data

```
nag_matop_real_gen_matrix_cond_std (f01jac) Example Program Data

4       Nag_Sinh           :Value of n and fun

2.0    1.0    3.0    1.0
3.0   -1.0    0.0    2.0
1.0    0.0    3.0    1.0
1.0    2.0    0.0    3.0  :End of matrix a
```

10.3 Program Results

```
nag_matop_real_gen_matrix_cond_std (f01jac) Example Program Results

 A
            1          2          3          4
 1      2.0000     1.0000     3.0000     1.0000
 2      3.0000    -1.0000     0.0000     2.0000
 3      1.0000     0.0000     3.0000     1.0000
 4      1.0000     2.0000     0.0000     3.0000

f(A) = Nag_Sinh(A)
```

```
Estimated absolute condition number is:  204.45
Estimated relative condition number is:    7.90
```