NAG Library Function Document

nag_matop_complex_gen_matrix_cond_sqrt (f01kdc)

1 Purpose

nag_matop_complex_gen_matrix_cond_sqrt (f01kdc) computes an estimate of the relative condition number, $\kappa_{A^{1/2}}$, and a bound on the relative residual, in the Frobenius norm, for the square root of a complex $n$ by $n$ matrix $A$. The principal square root, $A^{1/2}$, of $A$ is also returned.

2 Specification

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

void nag_matop_complex_gen_matrix_cond_sqrt (Integer n, Complex a[],
                                           Integer pda, double *alpha, double *condsa, NagError *fail)
```

3 Description

For a matrix with no eigenvalues on the closed negative real line, the principal matrix square root, $A^{1/2}$, of $A$ is the unique square root with eigenvalues in the right half-plane.

The Fréchet derivative of a matrix function $A^{1/2}$ in the direction of the matrix $E$ is the linear function mapping $E$ to $L(A, E)$ such that

$\left( A + E \right)^{1/2} = A^{1/2} - L(A, E) = o(\|A\|)$. 

The absolute condition number is given by the norm of the Fréchet derivative which is defined by

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

The Fréchet derivative is linear in $E$ and can therefore be written as

$$\text{vec}(L(A, E)) = K(A)\text{vec}(E),$$

where the vec operator stacks the columns of a matrix into one vector, so that $K(A)$ is $n^2 \times n^2$.

nag_matop_complex_gen_matrix_cond_sqrt (f01kdc) uses Algorithm 3.20 from Higham (2008) to compute an estimate $\gamma$ such that $\gamma \leq \|K(X)\|_F$. The quantity of $\gamma$ provides a good approximation to $\|L(A)\|_F$. The relative condition number, $\kappa_{A^{1/2}}$, is then computed via

$$\kappa_{A^{1/2}} = \frac{\|L(A)\|_F \|A\|_F}{\|A^{1/2}\|_F}. $$

$\kappa_{A^{1/2}}$ is returned in the argument `condsa`.

$A^{1/2}$ is computed using the algorithm described in Higham (1987). This is a version of the algorithm of Björck and Hammarling (1983). In addition, a blocking scheme described in Deadman et al. (2013) is used.

The computed quantity $\alpha$ is a measure of the stability of the relative residual (see Section 7). It is computed via

$$\alpha = \frac{\|A^{1/2}\|_F^2}{\|A\|_F}. $$
References


Arguments

1:   n – Integer

   Input

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

   Constraint: n ≥ 0.

2:   a[dim] – Complex

   Input/Output

   Note: the dimension, dim, of the array a must be at least pda × n.

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

   On entry: the n by n matrix A.

   On exit: the n by n principal matrix square root A^{1/2}. Alternatively, if fail.code = NE_EIGENVALUES, contains an n by n non-principal square root of A.

3:   pda – Integer

   Input

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

   Constraint: pda ≥ n.

4:   alpha – double *

   Output

   On exit: an estimate of the stability of the relative residual for the computed principal (if fail.code = NE_NOERROR) or non-principal (if fail.code = NE_EIGENVALUES) matrix square root, α.

5:   condsa – double *

   Output

   On exit: an estimate of the relative condition number, in the Frobenius norm, of the principal (if fail.code = NE_NOERROR) or non-principal (if fail.code = NE_EIGENVALUES) matrix square root at A, κ_{A^{1/2}}.

6:   fail – NagError *

   Input/Output

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

Error Indicators and Warnings

NE_ALG_FAIL

An error occurred when computing the condition number. The matrix square root was still returned but you should use nag_matop_complex_gen_matrix_sqrt (f01fnc) to check if it is the principal matrix square root.

An error occurred when computing the matrix square root. Consequently, alpha and condsa could not be computed. It is likely that the function was called incorrectly.
NE_ALLOC_FAIL
Dynamic memory allocation failed.
See Section 3.2.1.2 in the Essential Introduction for further information.

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

NE_EIGENVALUES
A has a negative or semisimple vanishing eigenvalue. A non-principal square root was returned.

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 unexpected error has been triggered by this function. Please contact NAG.
See Section 3.6.6 in the Essential Introduction for further information.

NE_NO_LICENCE
Your licence key may have expired or may not have been installed correctly.
See Section 3.6.5 in the Essential Introduction for further information.

NE_SINGULAR
A has a defective vanishing eigenvalue. The square root and condition number cannot be found in
this case.

7 Accuracy
If the computed square root is \( \hat{X} \), then the relative residual
\[
\frac{\| A - \hat{X}^2 \|_F}{\| A \|_F},
\]
is bounded approximately by \( n \alpha \varepsilon \), where \( \varepsilon \) is machine precision. The relative error in \( \hat{X} \) is bounded
approximately by \( n \alpha \varepsilon \).

8 Parallelism and Performance
nag_matop_complex_gen_matrix_cond_sqrt (f01kdc) is threaded by NAG for parallel execution in
multithreaded implementations of the NAG Library.
nag_matop_complex_gen_matrix_cond_sqrt (f01kdc) 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 function. Please also consult the Users’ Note for your
implementation for any additional implementation-specific information.
9 Further Comments

Approximately $3 \times n^2$ of complex allocatable memory is required by the function.

The cost of computing the matrix square root is $85n^3/3$ floating-point operations. The cost of computing the condition number depends on how fast the algorithm converges. It typically takes over twice as long as computing the matrix square root.

If condition estimates are not required then it is more efficient to use nag_matop_complex_gen_matrix_sqrt (f01fnc) to obtain the matrix square root alone. Condition estimates for the square root of a real matrix can be obtained via nag_matop_real_gen_matrix_cond_sqrt (f01jdc).

10 Example

This example estimates the matrix square root and condition number of the matrix

$$A = \begin{pmatrix}
29 + 35i & 31 + 61i & -38 + 49i & -17 - 6i \\
52 - 59i & 58 - 29i & 97 + 39i & -32 + 15i \\
20 - 31i & 44 - i & 37 + 19i & -26 + 19i \\
-70 + 72i & -90 + 8i & -87 - 43i & 47 - 5i
\end{pmatrix}.$$ 

10.1 Program Text

/* nag_matop_complex_gen_matrix_cond_sqrt (f01kdc) Example Program. */
* Copyright 2014 Numerical Algorithms Group.
* Mark 24, 2013.
*/
#include <nag.h>
#include <nag_stdlib.h>
#include <nagf01.h>
#include <nagx04.h>
#define A(I,J) a[J*pda + I]

int main(void)
{
    /* Scalars */
    Integer exit_status = 0;
    Integer i, j, n, pda;
    double alpha, condsa;
    /* Arrays */
    Complex *a = 0;
    /* Nag Types */
    Nag_OrderType order = Nag_ColMajor;
    NagError fail;

    INIT_FAIL(fail);

    /* Output preamble */
    printf("nag_matop_complex_gen_matrix_cond_sqrt (f01kdc) ");
    printf("Example Program Results\n\n");
    fflush(stdout);

    /* Skip heading in data file */
    #ifdef _WIN32
    scanf_s("%*[\n ]");
    #else
    scanf("%*[\n ]");
    #endif

    /* Read in the problem size */
    #ifdef _WIN32
    scanf_s("%*[NAG_IFMT]" vs[\n "]", &n);
    #else
    scanf("%*[\n "]", &n);
    #endif
#else
    scanf("%"NAG_IPMT"%*\n", &n);
#endif

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

/* Read in the matrix A from data file */
for (i = 0; i < n; i++)
#ifdef _WIN32
    for (j = 0; j < n; j++) scanf_s(" ( %lf , %lf ) ", &A(i,j).re, &A(i,j).im);
#else
    for (j = 0; j < n; j++) scanf(" ( %lf , %lf ) ", &A(i,j).re, &A(i,j).im);
#endif
#ifdef _WIN32
    scanf_s("%*\n");
#else
    scanf("%*\n");
#endif

/* Find matrix square root, condition number and residual bound using
nag_matop_complex_gen_matrix_cond_sqrt (f01kdc)
Condition number for the square root of a complex matrix */
nag_matop_complex_gen_matrix_cond_sqrt (n, a, pda, &alpha, &condsa, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_matop_complex_gen_matrix_cond_sqrt (f01kdc)\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Print matrix sqrt(A) using nag_gen_complx_mat_print (x04dac)
Print complex general matrix (easy-to-use) */
nag_gen_complx_mat_print (order, Nag_GeneralMatrix, Nag_NonUnitDiag,
n, n, a, pda, "sqrt(A)", NULL, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_complx_mat_print (x04dac)\n", fail.message);
    exit_status = 2;
    goto END;
}

/* Print condition number estimates */
printf("Estimated relative condition number is: %7.2f\n",condsa);
printf("Condition number for the relative residual is: %7.2f\n",alpha);

END:
NAG_FREE(a);
return exit_status;
}

10.2 Program Data

nag_matop_complex_gen_matrix_cond_sqrt (f01kdc) Example Program Data

4 :Value of n
    ( 29.0, 35.0) ( 31.0, 61.0) (-38.0, 49.0) (-17.0, -6.0)
    ( 52.0,-59.0) ( 58.0,-29.0) ( 97.0, 39.0) (-32.0, 15.0)
    ( 20.0,-31.0) ( 44.0, -1.0) ( 37.0, 19.0) (-26.0, 19.0)
    (-70.0, 72.0) (-90.0, 8.0) (-87.0,-43.0) ( 47.0, -5.0) :End of matrix a
10.3 Program Results

nag_matop_complex_gen_matrix_cond_sqrt (f01kdc) Example Program Results

sqrt(A)  

\begin{tabular}{cccc}
  & 1 & 2 & 3 & 4 \\
1 & 2.0000e+00 & 1.0000e+00 & -2.0000e+00 & -2.0000e+00 \\
  & 3.0000e+00 & 8.0000e+00 & -7.5495e-15 & 1.0000e+00 \\
2 & 5.0000e+00 & 7.0000e+00 & 7.0000e+00 & 3.9968e-15 \\
  & -4.0000e+00 & -6.0000e+00 & 6.0000e+00 & 3.5527e-15 \\
3 & 1.0000e+00 & 2.0000e+00 & 4.0000e+00 & -2.0000e+00 \\
  & -2.0000e+00 & 1.0000e+00 & 1.0000e+00 & 2.0000e+00 \\
4 & -3.0000e+00 & -2.0000e+00 & -7.0000e+00 & 6.0000e+00 \\
  & 7.0000e+00 & 2.0000e+00 & -1.0000e+00 & 2.0000e+00 \\
\end{tabular}

Estimated relative condition number is: 21.17 
Condition number for the relative residual is: 1.86