

NAG Library Function Document

nag_zppequ (f07gtc)

1 Purpose

nag_zppequ (f07gtc) computes a diagonal scaling matrix S intended to equilibrate a complex n by n Hermitian positive definite matrix A , stored in packed format, and reduce its condition number.

2 Specification

```
#include <nag.h>
#include <nagf07.h>

void nag_zppequ (Nag_OrderType order, Nag_UploType uplo, Integer n,
                const Complex ap[], double s[], double *scond, double *amax,
                NagError *fail)
```

3 Description

nag_zppequ (f07gtc) computes a diagonal scaling matrix S chosen so that

$$s_j = 1/\sqrt{a_{jj}}.$$

This means that the matrix B given by

$$B = SAS,$$

has diagonal elements equal to unity. This in turn means that the condition number of B , $\kappa_2(B)$, is within a factor n of the matrix of smallest possible condition number over all possible choices of diagonal scalings (see Corollary 7.6 of Higham (2002)).

4 References

Higham N J (2002) *Accuracy and Stability of Numerical Algorithms* (2nd Edition) SIAM, Philadelphia

5 Arguments

1: **order** – Nag_OrderType *Input*

On entry: the **order** argument specifies the two-dimensional storage scheme being used, i.e., row-major ordering or column-major ordering. C language defined storage is specified by **order** = Nag_RowMajor. See Section 3.2.1.3 in the Essential Introduction for a more detailed explanation of the use of this argument.

Constraint: **order** = Nag_RowMajor or Nag_ColMajor.

2: **uplo** – Nag_UploType *Input*

On entry: indicates whether the upper or lower triangular part of A is stored in the array **ap**, as follows:

uplo = Nag_Upper
The upper triangle of A is stored.

uplo = Nag_Lower
The lower triangle of A is stored.

Constraint: **uplo** = Nag_Upper or Nag_Lower.

- 3: **n** – Integer *Input*
On entry: n , the order of the matrix A .
Constraint: $n \geq 0$.
- 4: **ap**[*dim*] – const Complex *Input*
Note: the dimension, *dim*, of the array **ap** must be at least $\max(1, n \times (n + 1)/2)$.
On entry: the n by n Hermitian matrix A , packed by rows or columns.
The storage of elements A_{ij} depends on the **order** and **uplo** arguments as follows:
if **order** = Nag_ColMajor and **uplo** = Nag_Upper,
 A_{ij} is stored in **ap**[($j - 1$) \times $j/2 + i - 1$], for $i \leq j$;
if **order** = Nag_ColMajor and **uplo** = Nag_Lower,
 A_{ij} is stored in **ap**[($2n - j$) \times ($j - 1$)/2 + $i - 1$], for $i \geq j$;
if **order** = Nag_RowMajor and **uplo** = Nag_Upper,
 A_{ij} is stored in **ap**[($2n - i$) \times ($i - 1$)/2 + $j - 1$], for $i \leq j$;
if **order** = Nag_RowMajor and **uplo** = Nag_Lower,
 A_{ij} is stored in **ap**[($i - 1$) \times $i/2 + j - 1$], for $i \geq j$.
Only the elements of **ap** corresponding to the diagonal elements A are referenced.
- 5: **s**[**n**] – double *Output*
On exit: if **fail.code** = NE_NOERROR, **s** contains the diagonal elements of the scaling matrix S .
- 6: **scond** – double * *Output*
On exit: if **fail.code** = NE_NOERROR, **scond** contains the ratio of the smallest value of **s** to the largest value of **s**. If **scond** ≥ 0.1 and **amax** is neither too large nor too small, it is not worth scaling by S .
- 7: **amax** – double * *Output*
On exit: $\max |a_{ij}|$. If **amax** is very close to overflow or underflow, the matrix A should be scaled.
- 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

Dynamic memory allocation failed.
See Section 3.2.1.2 in the Essential Introduction for further information.

NE_BAD_PARAM

On entry, argument $\langle value \rangle$ had an illegal value.

NE_INT

On entry, **n** = $\langle value \rangle$.
Constraint: $n \geq 0$.

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_MAT_NOT_POS_DEF

The $\langle value \rangle$ th diagonal element of A is not positive (and hence A cannot be positive definite).

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.

7 Accuracy

The computed scale factors will be close to the exact scale factors.

8 Parallelism and Performance

Not applicable.

9 Further Comments

The real analogue of this function is nag_dppequ (f07gfc).

10 Example

This example equilibrates the Hermitian positive definite matrix A given by

$$A = \begin{pmatrix} 3.23 & 1.51 - 1.92i & (1.90 + 0.84i) \times 10^5 & 0.42 + 2.50i \\ 1.51 + 1.92i & 3.58 & (-0.23 + 1.11i) \times 10^5 & -1.18 + 1.37i \\ (1.90 - 0.84i) \times 10^5 & (-0.23 - 1.11i) \times 10^5 & 4.09 \times 10^{10} & (2.33 - 0.14i) \times 10^5 \\ 0.42 - 2.50i & -1.18 - 1.37i & (2.33 + 0.14i) \times 10^5 & 4.29 \end{pmatrix}.$$

Details of the scaling factors and the scaled matrix are output.

10.1 Program Text

```
/* nag_zppequ (f07gtc) Example Program.
 *
 * Copyright 2014 Numerical Algorithms Group.
 *
 * Mark 23, 2011.
 */

#include <stdio.h>
#include <nag.h>
#include <nagx04.h>
#include <nag_stdlib.h>
#include <nagf07.h>
#include <nagx02.h>

int main(void)
{
    /* Scalars */
    double      amax, big, scond, small;
    Integer     exit_status = 0, i, j, n;

    /* Arrays */
    Complex     *ap = 0;
    double      *s = 0;
    char        nag_enum_arg[40];

    /* Nag Types */
```

```

NagError      fail;
Nag_OrderType order;
Nag_UploType  uplo;

#ifdef NAG_COLUMN_MAJOR
#define A_UPPER(I, J) ap[J*(J-1)/2 + I - 1]
#define A_LOWER(I, J) ap[(2*n-J)*(J-1)/2 + I - 1]
    order = Nag_ColMajor;
#else
#define A_LOWER(I, J) ap[I*(I-1)/2 + J - 1]
#define A_UPPER(I, J) ap[(2*n-I)*(I-1)/2 + J - 1]
    order = Nag_RowMajor;
#endif

    INIT_FAIL(fail);

    printf("nag_zppequ (f07gtc) Example Program Results\n\n");
    /* Skip heading in data file */
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif

#ifdef _WIN32
    scanf_s("%"NAG_IFMT"%*[\n]", &n);
#else
    scanf("%"NAG_IFMT"%*[\n]", &n);
#endif
    if (n < 0)
    {
        printf("Invalid n\n");
        exit_status = 1;
        goto END;
    }
#ifdef _WIN32
    scanf_s(" %39s%*[\n]", nag_enum_arg, _countof(nag_enum_arg));
#else
    scanf(" %39s%*[\n]", nag_enum_arg);
#endif
    /* nag_enum_name_to_value (x04nac).
     * Converts NAG enum member name to value
     */
    uplo = (Nag_UploType) nag_enum_name_to_value(nag_enum_arg);

    /* Allocate memory */
    if (!(ap = NAG_ALLOC(n*(n+1)/2, Complex)) ||
        !(s = NAG_ALLOC(n, double)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }
    /* Read the upper or lower triangular part of the matrix A from data file */

    if (uplo == Nag_Upper)
        for (i = 1; i <= n; ++i)
            for (j = i; j <= n; ++j)
#ifdef _WIN32
                scanf_s(" ( %lf , %lf )", &A_UPPER(i, j).re, &A_UPPER(i, j).im);
#else
                scanf(" ( %lf , %lf )", &A_UPPER(i, j).re, &A_UPPER(i, j).im);
#endif
    else if (uplo == Nag_Lower)
        for (i = 1; i <= n; ++i)
            for (j = 1; j <= i; ++j)
#ifdef _WIN32
                scanf_s(" ( %lf , %lf )", &A_LOWER(i, j).re, &A_LOWER(i, j).im);
#else
                scanf(" ( %lf , %lf )", &A_LOWER(i, j).re, &A_LOWER(i, j).im);
#endif
#endif

```

```

#ifdef _WIN32
    scanf_s("%*[^\\n]");
#else
    scanf("%*[^\\n]");
#endif

/* Print the matrix A using nag_pack_complx_mat_print_comp (x04ddc). */
fflush(stdout);
nag_pack_complx_mat_print_comp(order, uplo, Nag_NonUnitDiag, n, ap,
                               Nag_BracketForm, "%11.2e", "Matrix A",
                               Nag_IntegerLabels, 0, Nag_IntegerLabels, 0,
                               80, 0, 0, &fail);

if (fail.code != NE_NOERROR)
{
    printf("Error from nag_pack_complx_mat_print_comp (x04ddc).\n%s\n",
          fail.message);
    exit_status = 1;
    goto END;
}
printf("\n");

/* Compute diagonal scaling factors using nag_zppequ (f07gtc). */
nag_zppequ(order, uplo, n, ap, s, &scnd, &amax, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_zppequ (f07gtc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Print scnd, amax and the scale factors */
printf("scnd = %10.1e, amax = %10.1e\n", scnd, amax);
printf("\nDiagonal scaling factors\n");
for (i = 0; i < n; ++i) printf("%11.1e%s", s[i], i%6 == 5?"\n":" ");
printf("\n\n");

/* Compute values close to underflow and overflow using
 * nag_real_safe_small_number (x02amc), nag_machine_precision (x02ajc) and
 * nag_real_base (x02bhc)
 */
small = nag_real_safe_small_number / (nag_machine_precision * nag_real_base);
big = 1.0 / small;
if (scnd < 0.1 || amax < small || amax > big)
{
    /* Scale A */
    if (uplo == Nag_Upper)
        for (j = 1; j <= n; ++j)
            for (i = 1; i <= j; ++i)
                {
                    A_UPPER(i, j).re *= s[i-1] * s[j-1];
                    A_UPPER(i, j).im *= s[i-1] * s[j-1];
                }
    else
        for (j = 1; j <= n; ++j)
            for (i = j; i <= n; ++i)
                {
                    A_LOWER(i, j).re *= s[i-1] * s[j-1];
                    A_LOWER(i, j).im *= s[i-1] * s[j-1];
                }

    /* Print the scaled matrix using
     * nag_pack_complx_mat_print_comp (x04ddc).
     */
    fflush(stdout);
    nag_pack_complx_mat_print_comp(order, uplo, Nag_NonUnitDiag, n, ap,
                                    Nag_BracketForm, 0, "Scaled matrix",
                                    Nag_IntegerLabels, 0, Nag_IntegerLabels,
                                    0, 80, 0, 0, &fail);

    if (fail.code != NE_NOERROR)
        {

```

```

        printf("Error from nag_pack_complex_mat_print_comp (x04ddc).\n%s\n",
               fail.message);
        exit_status = 1;
        goto END;
    }
}
END:
    NAG_FREE(ap);
    NAG_FREE(s);

    return exit_status;
}
#undef A_UPPER
#undef A_LOWER

```

10.2 Program Data

nag_zppequ (f07gtc) Example Program Data

```

4
Nag_Upper
( 3.23, 0.00) ( 1.51,-1.92) ( 1.90e+05, 0.84e+05) ( 0.42 , 2.50 )
              ( 3.58, 0.00) (-0.23e+05, 1.11e+05) (-1.18 , 1.37 )
              ( 4.09e+10, 0.00 ) ( 2.33e+05,-0.14e+05)
              ( 4.29 , 0.00 ) : A

```

10.3 Program Results

nag_zppequ (f07gtc) Example Program Results

Matrix A

```

1 ( 3.23e+00, 0.00e+00) ( 1.51e+00, -1.92e+00)
2 ( 3.58e+00, 0.00e+00)
3
4

1 ( 1.90e+05, 8.40e+04) ( 4.20e-01, 2.50e+00)
2 ( -2.30e+04, 1.11e+05) ( -1.18e+00, 1.37e+00)
3 ( 4.09e+10, 0.00e+00) ( 2.33e+05, -1.40e+04)
4 ( 4.29e+00, 0.00e+00)

```

scond = 8.9e-06, amax = 4.1e+10

Diagonal scaling factors

```

5.6e-01 5.3e-01 4.9e-06 4.8e-01

```

Scaled matrix

```

1 ( 1.0000, 0.0000) ( 0.4441, -0.5646) ( 0.5227, 0.2311)
2 ( 1.0000, 0.0000) ( -0.0601, 0.2901)
3 ( 1.0000, 0.0000)
4

1 ( 0.1128, 0.6716)
2 ( -0.3011, 0.3496)
3 ( 0.5562, -0.0334)
4 ( 1.0000, 0.0000)

```