

# NAG Library Function Document

## nag\_dpoequ (f07ffc)

### 1 Purpose

nag\_dpoequ (f07ffc) computes a diagonal scaling matrix  $S$  intended to equilibrate a real  $n$  by  $n$  symmetric positive definite matrix  $A$  and reduce its condition number.

### 2 Specification

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

void nag_dpoequ (Nag_OrderType order, Integer n, const double a[],
                 Integer pda, double s[], double *scond, double *amax, NagError *fail)
```

### 3 Description

nag\_dpoequ (f07ffc) 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 2.3.1.3 in How to Use the NAG Library and its Documentation for a more detailed explanation of the use of this argument.

*Constraint:* **order** = Nag\_RowMajor or Nag\_ColMajor.

2: **n** – Integer *Input*

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

*Constraint:* **n**  $\geq 0$ .

3: **a**[ $dim$ ] – const double *Input*

**Note:** the dimension,  $dim$ , of the array **a** must be at least  $\max(1, pda \times n)$ .

The  $(i, j)$ th element of the matrix  $A$  is stored in

**a**[ $(j - 1) \times pda + i - 1$ ] when **order** = Nag\_ColMajor;  
**a**[ $(i - 1) \times pda + j - 1$ ] when **order** = Nag\_RowMajor.

*On entry:* the matrix  $A$  whose scaling factors are to be computed. Only the diagonal elements of the array **a** are referenced.

- 4:   **pda** – Integer *Input*  
*On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **a**.  
*Constraint:* **pda**  $\geq \max(1, n)$ .
- 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**  $\geq 0.1$  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 2.7 in How to Use the NAG Library and its Documentation).

## 6 Error Indicators and Warnings

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

See Section 2.3.1.2 in How to Use the NAG Library and its Documentation 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**  $\geq 0$ .

*On entry,* **pda** =  $\langle value \rangle$ .

*Constraint:* **pda**  $> 0$ .

### NE\_INT\_2

*On entry,* **pda** =  $\langle value \rangle$  and **n** =  $\langle value \rangle$ .

*Constraint:* **pda**  $\geq \max(1, n)$ .

### 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 2.7.6 in How to Use the NAG Library and its Documentation 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 2.7.5 in How to Use the NAG Library and its Documentation for further information.

**7 Accuracy**

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

**8 Parallelism and Performance**

nag\_dpoequ (f07ffc) is not threaded in any implementation.

**9 Further Comments**

The complex analogue of this function is nag\_zpoequ (f07ftc).

**10 Example**

This example equilibrates the symmetric positive definite matrix  $A$  given by

$$A = \begin{pmatrix} 4.16 & -3.12 \times 10^5 & 0.56 & -0.10 \\ -3.12 \times 10^5 & 5.03 \times 10^{10} & -0.83 \times 10^5 & 1.18 \times 10^5 \\ 0.56 & -0.83 \times 10^5 & 0.76 & 0.34 \\ -0.10 & 1.18 \times 10^5 & 0.34 & 1.18 \end{pmatrix}.$$

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

**10.1 Program Text**

```
/* nag_dpoequ (f07ffc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#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, scnd, small;
    Integer i, j, n, pda;
    Integer exit_status = 0;
    /* Arrays */
    double *a = 0, *s = 0;

    /* Nag Types */
    NagError fail;
    Nag_OrderType order;

#ifdef NAG_COLUMN_MAJOR
```

```

#define A(I, J) a[(J-1)*pda + I - 1]
    order = Nag_ColMajor;
#else
#define A(I, J) a[(I-1)*pda + J - 1]
    order = Nag_RowMajor;
#endif

    INIT_FAIL(fail);

    printf("nag_dpoequ (f07ffc) 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;
    }

    pda = n;
    /* Allocate memory */
    if (!(a = NAG_ALLOC(n * n, double)) || !(s = NAG_ALLOC(n, double)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }

    /* Read the upper triangular part of the matrix A from data file */
    for (i = 1; i <= n; ++i)
#ifdef _WIN32
        for (j = i; j <= n; ++j)
            scanf_s("%lf", &A(i, j));
#else
        for (j = i; j <= n; ++j)
            scanf("%lf", &A(i, j));
#endif
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif

    /* Print the matrix A using nag_gen_real_mat_print (x04cac). */
    fflush(stdout);
    nag_gen_real_mat_print(order, Nag_UpperMatrix, Nag_NonUnitDiag, n, n, a,
                           pda, "Matrix A", 0, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_gen_real_mat_print (x04cac).\n%s\n", fail.message);
        exit_status = 1;
        goto END;
    }

    printf("\n");
    /* Compute diagonal scaling factors using nag_dpoequ (f07ffc). */
    nag_dpoequ(order, n, a, pda, s, &scond, &amax, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_dpoequ (f07ffc).\n%s\n", fail.message);
        exit_status = 1;
        goto END;
    }
}

```

```

/* Print scond, amax and the scale factors */
printf("scond = %10.1e, amax = %10.1e\n\n", scond, amax);
printf("Diagonal scaling factors\n");
for (i = 0; i < n; ++i)
    printf("%11.1e%s", s[i], i % 7 == 6 ? "\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 (scond < 0.1 || amax < small || amax > big) {
    /* Scale A */
    for (j = 1; j <= n; ++j)
        for (i = 1; i <= j; ++i)
            A(i, j) *= s[i - 1] * s[j - 1];

    /* Print the scaled matrix using nag_gen_real_mat_print (x04cac). */
    fflush(stdout);
    nag_gen_real_mat_print(order, Nag_UpperMatrix, Nag_NonUnitDiag, n, n, a,
                           pda, "Scaled matrix", 0, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_gen_real_mat_print (x04cac).\n%s\n",
               fail.message);
        exit_status = 1;
        goto END;
    }
}

END:
    NAG_FREE(a);
    NAG_FREE(s);

    return exit_status;
}

#undef A

```

## 10.2 Program Data

```

nag_dpoequ (f07ffc) Example Program Data
4                                     : n
4.16      -3.12e+05    0.56      -0.10
           5.03e+10   -0.83e+05    1.18e+05
                   0.76      0.34
                   1.18      : matrix A

```

## 10.3 Program Results

```

nag_dpoequ (f07ffc) Example Program Results

Matrix A
      1      2      3      4
1  4.1600e+00 -3.1200e+05  5.6000e-01 -1.0000e-01
2           5.0300e+10 -8.3000e+04  1.1800e+05
3                   7.6000e-01  3.4000e-01
4                   1.1800e+00

scond =      3.9e-06, amax =      5.0e+10

Diagonal scaling factors
      4.9e-01      4.5e-06      1.1e+00      9.2e-01

Scaled matrix

```

	1	2	3	4
1	1.0000	-0.6821	0.3149	-0.0451
2		1.0000	-0.4245	0.4843
3			1.0000	0.3590
4				1.0000

---