

NAG C Library Function Document

nag_dsprfs (f07phc)

1 Purpose

nag_dsprfs (f07phc) returns error bounds for the solution of a real symmetric indefinite system of linear equations with multiple right-hand sides, $AX = B$ using packed storage. It improves the solution by iterative refinement, in order to reduce the backward error as much as possible.

2 Specification

```
void nag_dsprfs (Nag_OrderType order, Nag_UploType uplo, Integer n, Integer nrhs,
  const double ap[], const double afp[], const Integer ipiv[], const double b[],
  Integer pdb, double x[], Integer pdx, double ferr[], double berr[],
  NagError *fail)
```

3 Description

nag_dsprfs (f07phc) returns the backward errors and estimated bounds on the forward errors for the solution of a real symmetric indefinite system of linear equations with multiple right-hand sides $AX = B$, using packed storage. The function handles each right-hand side vector (stored as a column of the matrix B) independently, so we describe the function of nag_dsprfs (f07phc) in terms of a single right-hand side b and solution x .

Given a computed solution x , the function computes the *component-wise backward error* β . This is the size of the smallest relative perturbation in each element of A and b such that x is the exact solution of a perturbed system

$$(A + \delta A)x = b + \delta b$$

$$|\delta a_{ij}| \leq \beta |a_{ij}| \quad \text{and} \quad |\delta b_i| \leq \beta |b_i|.$$

Then the function estimates a bound for the *component-wise forward error* in the computed solution, defined by:

$$\max_i |x_i - \hat{x}_i| / \max_i |x_i|$$

where $\hat{x}$ is the true solution.

For details of the method, see the f07 Chapter Introduction.

4 References

Golub G H and Van Loan C F (1996) *Matrix Computations* (3rd Edition) Johns Hopkins University Press, Baltimore

5 Parameters

1: **order** – Nag_OrderType *Input*

On entry: the **order** parameter 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 2.2.1.4 of the Essential Introduction for a more detailed explanation of the use of this parameter.

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 and how A is to be factorized, as follows:
 if **uplo** = **Nag_Upper**, the upper triangular part of A is stored and A is factorized as $PUDU^T P^T$, where U is upper triangular;
 if **uplo** = **Nag_Lower**, the lower triangular part of A is stored and A is factorized as $PLDL^T P^T$, where L is lower triangular.
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: **nrhs** – Integer *Input*
On entry: r , the number of right-hand sides.
Constraint: **nrhs** ≥ 0 .
- 5: **ap**[dim] – const double *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 original symmetric matrix A as supplied to nag_dsptrf (f07pdc).
- 6: **afp**[dim] – const double *Input*
Note: the dimension, dim , of the array **afp** must be at least $\max(1, n \times (n + 1)/2)$.
On entry: details of the factorization of A stored in packed form, as returned by nag_dsptrf (f07pdc).
- 7: **ipiv**[dim] – const Integer *Input*
Note: the dimension, dim , of the array **ipiv** must be at least $\max(1, n)$.
On entry: details of the interchanges and the block structure of D , as returned by nag_dsptrf (f07pdc).
- 8: **b**[dim] – const double *Input*
Note: the dimension, dim , of the array **b** must be at least $\max(1, pdb \times nrhs)$ when **order** = **Nag_ColMajor** and at least $\max(1, pdb \times n)$ when **order** = **Nag_RowMajor**.
 If **order** = **Nag_ColMajor**, the (i, j) th element of the matrix B is stored in **b**[($j - 1$) $\times$ **pdb** + $i - 1$] and if **order** = **Nag_RowMajor**, the (i, j) th element of the matrix B is stored in **b**[($i - 1$) $\times$ **pdb** + $j - 1$].
On entry: the n by r right-hand side matrix B .
- 9: **pdb** – Integer *Input*
On entry: the stride separating matrix row or column elements (depending on the value of **order**) in the array **b**.
Constraints:
 if **order** = **Nag_ColMajor**, **pdb** $\geq \max(1, n)$;
 if **order** = **Nag_RowMajor**, **pdb** $\geq \max(1, nrhs)$.
- 10: **x**[dim] – double *Input/Output*
Note: the dimension, dim , of the array **x** must be at least $\max(1, pdx \times nrhs)$ when **order** = **Nag_ColMajor** and at least $\max(1, pdx \times n)$ when **order** = **Nag_RowMajor**.

If **order** = **Nag_ColMajor**, the (i, j) th element of the matrix X is stored in $\mathbf{x}[(j-1) \times \mathbf{pdx} + i - 1]$ and if **order** = **Nag_RowMajor**, the (i, j) th element of the matrix X is stored in $\mathbf{x}[(i-1) \times \mathbf{pdx} + j - 1]$.

On entry: the n by r solution matrix X , as returned by nag_dspttrs (f07pec).

On exit: the improved solution matrix X .

11: **pdx** – Integer Input

On entry: the stride separating matrix row or column elements (depending on the value of **order**) in the array $\mathbf{x}$.

Constraints:

if **order** = **Nag_ColMajor**, $\mathbf{pdx} \geq \max(1, \mathbf{n})$;
if **order** = **Nag_RowMajor**, $\mathbf{pdx} \geq \max(1, \mathbf{nrhs})$.

12: **ferr**[dim] – double Output

Note: the dimension, dim , of the array **ferr** must be at least $\max(1, \mathbf{nrhs})$.

On exit: **ferr**[$j-1$] contains an estimated error bound for the j th solution vector, that is, the j th column of X , for $j = 1, 2, \dots, r$.

13: **berr**[dim] – double Output

Note: the dimension, dim , of the array **berr** must be at least $\max(1, \mathbf{nrhs})$.

On exit: **berr**[$j-1$] contains the component-wise backward error bound β for the j th solution vector, that is, the j th column of X , for $j = 1, 2, \dots, r$.

14: **fail** – NagError * Output

The NAG error parameter (see the Essential Introduction).

6 Error Indicators and Warnings

NE_INT

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

Constraint: **n** ≥ 0 .

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

Constraint: **nrhs** ≥ 0 .

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

Constraint: **pdb** > 0 .

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

Constraint: **pdx** > 0 .

NE_INT_2

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

Constraint: **pdb** $\geq \max(1, \mathbf{n})$.

On entry, **pdb** = $\langle value \rangle$, **nrhs** = $\langle value \rangle$.

Constraint: **pdb** $\geq \max(1, \mathbf{nrhs})$.

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

Constraint: **pdx** $\geq \max(1, \mathbf{n})$.

On entry, **pdx** = $\langle value \rangle$, **nrhs** = $\langle value \rangle$.

Constraint: **pdx** $\geq \max(1, \mathbf{nrhs})$.

NE_ALLOC_FAIL

Memory allocation failed.

NE_BAD_PARAM

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

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 consult NAG for assistance.

7 Accuracy

The bounds returned in **ferr** are not rigorous, because they are estimated, not computed exactly; but in practice they almost always overestimate the actual error.

8 Further Comments

For each right-hand side, computation of the backward error involves a minimum of $4n^2$ floating-point operations. Each step of iterative refinement involves an additional $6n^2$ operations. At most 5 steps of iterative refinement are performed, but usually only 1 or 2 steps are required.

Estimating the forward error involves solving a number of systems of linear equations of the form $Ax = b$; the number is usually 4 or 5 and never more than 11. Each solution involves approximately $2n^2$ operations.

The complex analogues of this function are nag_zhprfs (f07pvc) for Hermitian matrices and nag_zsprfs (f07qvc) for symmetric matrices.

9 Example

To solve the system of equations $AX = B$ using iterative refinement and to compute the forward and backward error bounds, where

$$A = \begin{pmatrix} 2.07 & 3.87 & 4.20 & -1.15 \\ 3.87 & -0.21 & 1.87 & 0.63 \\ 4.20 & 1.87 & 1.15 & 2.06 \\ -1.15 & 0.63 & 2.06 & -1.81 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} -9.50 & 27.85 \\ -8.38 & 9.90 \\ -6.07 & 19.25 \\ -0.96 & 3.93 \end{pmatrix}.$$

Here A is symmetric indefinite, stored in packed form, and must first be factorized by nag_dsprtf (f07pdc).

9.1 Program Text

```
/* nag_dsprfs (f07phc) Example Program.
 *
 * Copyright 2001 Numerical Algorithms Group.
 *
 * Mark 7, 2001.
 */

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

int main(void)
{
    /* Scalars */
    Integer i, j, n, nrhs, ap_len, afp_len, pdb, pdx, ferr_len, berr_len;
    Integer exit_status=0;
    NagError fail;
```

```

Nag_UploType uplo_enum;
Nag_OrderType order;
/* Arrays */
Integer *ipiv=0;
char    uplo[2];
double  *afp=0, *ap=0, *b=0, *berr=0, *ferr=0, *x=0;

#ifdef NAG_COLUMN_MAJOR
#define A_LOWER(I,J) ap[(2*n-J)*(J-1)/2 + I - 1]
#define A_UPPER(I,J) ap[J*(J-1)/2 + I - 1]
#define B(I,J) b[(J-1)*pdb + I - 1]
#define X(I,J) x[(J-1)*pdx + 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]
#define B(I,J) b[(I-1)*pdb + J - 1]
#define X(I,J) x[(I-1)*pdx + J - 1]
    order = Nag_RowMajor;
#endif

    INIT_FAIL(fail);
    Vprintf("f07phc Example Program Results\n\n");
    /* Skip heading in data file */
    Vscanf("%*[^\\n] ");
    Vscanf("%ld%ld%*[^\\n] ", &n, &nrhs);
    ap_len = n * (n + 1)/2;
    afp_len = n * (n + 1)/2;
#ifdef NAG_COLUMN_MAJOR
    pdb = n;
    pdx = n;
#else
    pdb = nrhs;
    pdx = nrhs;
#endif

    ferr_len = nrhs;
    berr_len = nrhs;

    /* Allocate memory */
    if ( !(ipiv = NAG_ALLOC(n, Integer)) ||
        !(afp = NAG_ALLOC(ap_len, double)) ||
        !(ap = NAG_ALLOC(afp_len, double)) ||
        !(b = NAG_ALLOC(n * nrhs, double)) ||
        !(berr = NAG_ALLOC(berr_len, double)) ||
        !(ferr = NAG_ALLOC(ferr_len, double)) ||
        !(x = NAG_ALLOC(n * nrhs, double)) )
    {
        Vprintf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }

    /* Read A and B from data file, and copy A to AFP and B to X */

    Vscanf(" ' %1s '%*[^\\n] ", uplo);
    if (*(unsigned char *)uplo == 'L')
        uplo_enum = Nag_Lower;
    else if (*(unsigned char *)uplo == 'U')
        uplo_enum = Nag_Upper;
    else
    {
        Vprintf("Unrecognised character for Nag_UploType type\n");
        exit_status = -1;
        goto END;
    }
    if (uplo_enum == Nag_Upper)
    {
        for (i = 1; i <= n; ++i)
        {
            for (j = i; j <= n; ++j)

```

```

        Vscanf("%lf", &A_UPPER(i,j));
    }
    Vscanf("%*[^\\n] ");
}
else
{
    for (i = 1; i <= n; ++i)
    {
        for (j = 1; j <= i; ++j)
            Vscanf("%lf", &A_LOWER(i,j));
    }
    Vscanf("%*[^\\n] ");
}
for (i = 1; i <= n; ++i)
{
    for (j = 1; j <= nrhs; ++j)
        Vscanf("%lf", &B(i,j));
}
Vscanf("%*[^\\n] ");

for (i = 1; i <= n * (n + 1) / 2; ++i)
    afp[i - 1] = ap[i - 1];
for (i = 1; i <= n; ++i)
{
    for (j = 1; j <= nrhs; ++j)
        X(i,j) = B(i,j);
}
/* Factorize A in the array AFP */
f07pdc(order, uplo_enum, n, afp, ipiv, &fail);
if (fail.code != NE_NOERROR)
{
    Vprintf("Error from f07pdc.%s\\n", fail.message);
    exit_status = 1;
    goto END;
}
/* Compute solution in the array X */
f07pec(order, uplo_enum, n, nrhs, afp, ipiv, x, pdx, &fail);
if (fail.code != NE_NOERROR)
{
    Vprintf("Error from f07pec.%s\\n", fail.message);
    exit_status = 1;
    goto END;
}
/* Improve solution, and compute backward errors and */
/* estimated bounds on the forward errors */
f07phc(order, uplo_enum, n, nrhs, ap, afp, ipiv, b, pdb,
        x, pdx, ferr, berr, &fail);
if (fail.code != NE_NOERROR)
{
    Vprintf("Error from f07phc.%s\\n", fail.message);
    exit_status = 1;
    goto END;
}
/* Print solution */
x04cac(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, nrhs, x, pdx,
        "Solution(s)", 0, &fail);
if (fail.code != NE_NOERROR)
{
    Vprintf("Error from x04cac.%s\\n", fail.message);
    exit_status = 1;
    goto END;
}
Vprintf("\\nBackward errors (machine-dependent)\\n");
for (j = 1; j <= nrhs; ++j)
    Vprintf("%11.1e%s", berr[j-1], j%7==0 ? "\\n":" ");
Vprintf("\\nEstimated forward error bounds (machine-dependent)\\n");
for (j = 1; j <= nrhs; ++j)
    Vprintf("%11.1e%s", ferr[j-1], j%7==0 ? "\\n":" ");
Vprintf("\\n");
END:
if (ipiv) NAG_FREE(ipiv);

```

```

    if (afp) NAG_FREE(afp);
    if (ap) NAG_FREE(ap);
    if (b) NAG_FREE(b);
    if (berr) NAG_FREE(berr);
    if (ferr) NAG_FREE(ferr);
    if (x) NAG_FREE(x);
    return exit_status;
}

```

9.2 Program Data

f07phc Example Program Data

```

4 2          :Values of N and NRHS
'L'         :Value of UPLO
2.07
3.87 -0.21
4.20  1.87  1.15
-1.15  0.63  2.06 -1.81 :End of matrix A
-9.50 27.85
-8.38  9.90
-6.07 19.25
-0.96  3.93          :End of matrix B

```

9.3 Program Results

f07phc Example Program Results

```

Solution(s)
          1          2
1    -4.0000    1.0000
2    -1.0000    4.0000
3     2.0000    3.0000
4     5.0000    2.0000

```

Backward errors (machine-dependent)

```

4.1e-17    5.5e-17

```

Estimated forward error bounds (machine-dependent)

```

2.3e-14    3.3e-14

```
