NAG Library Function Document

nag_dgesv (f07aac)

1 Purpose

nag_dgesv (f07aac) computes the solution to a real system of linear equations

$$AX = B,$$

where A is an n by n matrix and X and B are n by r matrices.

2 Specification

```
#include <nag.h>
#include <nagf07.h>
void nag_dgesv (Nag_OrderType order, Integer n, Integer nrhs, double a[],
     Integer pda, Integer ipiv[], double b[], Integer pdb, NagError *fail)
```

3 Description

nag_dgesv (f07aac) uses the LU decomposition with partial pivoting and row interchanges to factor A as

$$A = PLU,$$

where P is a permutation matrix, L is unit lower triangular, and U is upper triangular. The factored form of A is then used to solve the system of equations $AX = B$.

4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia http://www.netlib.org/lapack/lug

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

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 number of linear equations, i.e., the order of the matrix A.

Constraint: **n** ≥ 0.

3: **nrhs** – Integer *Input*

On entry: r, the number of right-hand sides, i.e., the number of columns of the matrix B.

Constraint: **nrhs** ≥ 0.

4: **a**[dim] – double *Input/Output*

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

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 n by n coefficient matrix A.

On exit: the factors L and U from the factorization $A = PLU$; the unit diagonal elements of L are not stored.

5: **pda** – Integer *Input*

On entry: the stride separating row or column elements (depending on the value of **order**) in the array **a**.

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

6: **ipiv**[**n**] – Integer *Output*

On exit: if no constraints are violated, the pivot indices that define the permutation matrix P; at the ith step row i of the matrix was interchanged with row **ipiv**$[i-1]$. **ipiv**$[i-1] = i$ indicates a row interchange was not required.

7: **b**[dim] – double *Input/Output*

Note: the dimension, *dim*, of the array **b** must be at least

$\max(1, \mathbf{pdb} \times \mathbf{nrhs})$ when **order** = Nag_ColMajor;
$\max(1, \mathbf{n} \times \mathbf{pdb})$ when **order** = Nag_RowMajor.

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

b[$(j-1) \times$ **pdb** $+ i - 1$] when **order** = Nag_ColMajor;
b[$(i-1) \times$ **pdb** $+ j - 1$] when **order** = Nag_RowMajor.

On entry: the n by r right-hand side matrix B.

On exit: if **fail.code** = NE_NOERROR, the n by r solution matrix X.

8: **pdb** – Integer *Input*

On entry: the stride separating row or column elements (depending on the value of **order**) in the array **b**.

Constraints:

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

9: **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 3.2.1.2 in How to Use the NAG Library and its Documentation for further information.

NE_BAD_PARAM

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

NE_INT

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

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

On entry, **pda** = ⟨*value*⟩.
Constraint: **pda** > 0.

On entry, **pdb** = ⟨*value*⟩.
Constraint: **pdb** > 0.

NE_INT_2

On entry, **pda** = ⟨*value*⟩ and **n** = ⟨*value*⟩.
Constraint: **pda** ≥ max(1, **n**).

On entry, **pdb** = ⟨*value*⟩ and **n** = ⟨*value*⟩.
Constraint: **pdb** ≥ max(1, **n**).

On entry, **pdb** = ⟨*value*⟩ and **nrhs** = ⟨*value*⟩.
Constraint: **pdb** ≥ max(1, **nrhs**).

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 How to Use the NAG Library and its Documentation 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 How to Use the NAG Library and its Documentation for further information.

NE_SINGULAR

Element ⟨*value*⟩ of the diagonal is exactly zero. The factorization has been completed, but the factor U is exactly singular, so the solution could not be computed.

7 Accuracy

The computed solution for a single right-hand side, $\hat{x}$, satisfies the equation of the form

$$(A + E)\hat{x} = b,$$

where

$$\|E\|_1 = O(\epsilon)\|A\|_1$$

and ϵ is the ***machine precision***. An approximate error bound for the computed solution is given by

$$\frac{\|\hat{x} - x\|_1}{\|x\|_1} \leq \kappa(A)\frac{\|E\|_1}{\|A\|_1}$$

where $\kappa(A) = \left\|A^{-1}\right\|_1 \|A\|_1$, the condition number of A with respect to the solution of the linear equations. See Section 4.4 of Anderson *et al.* (1999) for further details.

Following the use of nag_dgesv (f07aac), nag_dgecon (f07agc) can be used to estimate the condition number of A and nag_dgerfs (f07ahc) can be used to obtain approximate error bounds. Alternatives to

nag_dgesv (f07aac), which return condition and error estimates directly are nag_real_gen_lin_solve (f04bac) and nag_dgesvx (f07abc).

8 Parallelism and Performance

nag_dgesv (f07aac) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_dgesv (f07aac) 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' Notefor your implementation for any additional implementation-specific information.

9 Further Comments

The total number of floating-point operations is approximately $\frac{2}{3}n^3 + 2n^2r$, where r is the number of right-hand sides.

The complex analogue of this function is nag_zgesv (f07anc).

10 Example

This example solves the equations

$$Ax = b,$$

where A is the general matrix

$$A = \begin{pmatrix} 1.80 & 2.88 & 2.05 & -0.89 \\ 5.25 & -2.95 & -0.95 & -3.80 \\ 1.58 & -2.69 & -2.90 & -1.04 \\ -1.11 & -0.66 & -0.59 & 0.80 \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 9.52 \\ 24.35 \\ 0.77 \\ -6.22 \end{pmatrix}.$$

Details of the LU factorization of A are also output.

10.1 Program Text

```
/* nag_dgesv (f07aac) 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>

int main(void)
{
  /* Scalars */
  Integer exit_status = 0, i, j, n, nrhs, pda, pdb;

  /* Arrays */
  double *a = 0, *b = 0;
  Integer *ipiv = 0;

  /* Nag Types */
```

```
  NagError fail;
  Nag_OrderType order;

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

  INIT_FAIL(fail);

  printf("nag_dgesv (f07aac) 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 " %" NAG_IFMT "%*[^\n]", &n, &nrhs);
#else
  scanf("%" NAG_IFMT " %" NAG_IFMT "%*[^\n]", &n, &nrhs);
#endif
  if (n < 0 || nrhs < 0) {
    printf("Invalid n or nrhs\n");
    exit_status = 1;
    return exit_status;
  }

  pda = n;
#ifdef NAG_COLUMN_MAJOR
  pdb = n;
#else
  pdb = nrhs;
#endif

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

  /* Read A and B from data file */
  for (i = 1; i <= n; ++i)
#ifdef _WIN32
    for (j = 1; j <= n; ++j)
      scanf_s("%lf", &A(i, j));
#else
    for (j = 1; j <= n; ++j)
      scanf("%lf", &A(i, j));
#endif
#ifdef _WIN32
  scanf_s("%*[^\n]");
#else
  scanf("%*[^\n]");
#endif

  for (i = 1; i <= n; ++i)
#ifdef _WIN32
    for (j = 1; j <= nrhs; ++j)
      scanf_s("%lf", &B(i, j));
#else
```

```
    for (j = 1; j <= nrhs; ++j)
      scanf("%lf", &B(i, j));
#endif
#ifdef _WIN32
  scanf_s("%*[^\n]");
#else
  scanf("%*[^\n]");
#endif

  /* Solve the equations Ax = b for x using
   * nag_dgesv (f07aac)
   */
  nag_dgesv(order, n, nrhs, a, pda, ipiv, b, pdb, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_dgesv (f07aac).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  /* Print solution */
  printf("Solution\n");
  for (i = 1; i <= n; ++i)
    for (j = 1; j <= nrhs; ++j)
      printf("%11.4f%s", B(i, j), j % 7 == 0 || j == nrhs ? "\n" : " ");

  /* Print details of factorization using
   * nag_gen_real_mat_print (x04cac)
   */
  printf("\n");
  fflush(stdout);
  nag_gen_real_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, n, a,
                         pda, "Details of factorization", 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;
  }

  /* Print pivot indices */
  printf("\nPivot indices\n");
  for (i = 1; i <= n; ++i)
    printf("%11" NAG_IFMT "%s", ipiv[i - 1], i % 7 == 0
           || i == n ? "\n" : " ");
END:
  NAG_FREE(a);
  NAG_FREE(b);
  NAG_FREE(ipiv);
  return exit_status;
}

#undef A
#undef B
```

10.2 Program Data

```
nag_dgesv (f07aac) Example Program Data

  4      1                   :Value of n, nrhs

  1.80   2.88   2.05  -0.89
  5.25  -2.95  -0.95  -3.80
  1.58  -2.69  -2.90  -1.04
 -1.11  -0.66  -0.59   0.80   :End of matrix A

  9.52  24.35   0.77  -6.22   :End of vector b
```

10.3 Program Results

```
nag_dgesv (f07aac) Example Program Results

Solution
     1.0000
    -1.0000
     3.0000
    -5.0000

 Details of factorization
            1          2          3          4
 1      5.2500    -2.9500    -0.9500    -3.8000
 2      0.3429     3.8914     2.3757     0.4129
 3      0.3010    -0.4631    -1.5139     0.2948
 4     -0.2114    -0.3299     0.0047     0.1314

Pivot indices
          2          2          3          4
```