NAG Library Function Document

nag_dgtrfs (f07chc)

1 Purpose

nag_dgtrfs (f07chc) computes error bounds and refines the solution to a real system of linear equations $AX = B$ or $A^{\mathrm{T}}X = B$, where A is an n by n tridiagonal matrix and X and B are n by r matrices, using the LU factorization returned by nag_dgttrf (f07cdc) and an initial solution returned by nag_dgttrs (f07cec). Iterative refinement is used to reduce the backward error as much as possible.

2 Specification

```
#include <nag.h>
#include <nagf07.h>
void nag_dgtrfs (Nag_OrderType order, Nag_TransType trans, Integer n,
     Integer nrhs, const double dl[], const double d[], const double du[],
     const double dlf[], const double df[], const double duf[],
     const double du2[], const Integer ipiv[], const double b[], Integer pdb,
     double x[], Integer pdx, double ferr[], double berr[], NagError *fail)
```

3 Description

nag_dgtrfs (f07chc) should normally be preceded by calls to nag_dgttrf (f07cdc) and nag_dgttrs (f07cec). nag_dgttrf (f07cdc) uses Gaussian elimination with partial pivoting and row interchanges to factorize the matrix A as

$$A = PLU,$$

where P is a permutation matrix, L is unit lower triangular with at most one nonzero subdiagonal element in each column, and U is an upper triangular band matrix, with two superdiagonals. nag_dgttrs (f07cec) then utilizes the factorization to compute a solution, $\hat{X}$, to the required equations. Letting $\hat{x}$ denote a column of $\hat{X}$, nag_dgtrfs (f07chc) computes a *component-wise backward error*, β, the smallest relative perturbation in each element of A and b such that $\hat{x}$ is the exact solution of a perturbed system

$$(A + E)\hat{x} = b + f, \quad \text{with} \quad |e_{ij}| \leq \beta |a_{ij}|, \quad \text{and} \quad |f_j| \leq \beta |b_j|.$$

The function also estimates a bound for the *component-wise forward error* in the computed solution defined by $\max |x_i - \hat{x}_i| / \max |\hat{x}_i|$, where x is the corresponding column of the exact solution, X.

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

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: **trans** – Nag_TransType *Input*

On entry: specifies the equations to be solved as follows:

trans = Nag_NoTrans
Solve $AX = B$ for X.

trans = Nag_Trans or Nag_ConjTrans
Solve $A^{\mathrm{T}}X = B$ for X.

Constraint: **trans** = Nag_NoTrans, Nag_Trans or Nag_ConjTrans.

3: **n** – Integer *Input*

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

Constraint: $\mathbf{n} \geq 0$.

4: **nrhs** – Integer *Input*

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

Constraint: $\mathbf{nrhs} \geq 0$.

5: **dl**[dim] – const double *Input*

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

On entry: must contain the $(n - 1)$ subdiagonal elements of the matrix A.

6: **d**[dim] – const double *Input*

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

On entry: must contain the n diagonal elements of the matrix A.

7: **du**[dim] – const double *Input*

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

On entry: must contain the $(n - 1)$ superdiagonal elements of the matrix A.

8: **dlf**[dim] – const double *Input*

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

On entry: must contain the $(n - 1)$ multipliers that define the matrix L of the LU factorization of A.

9: **df**[dim] – const double *Input*

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

On entry: must contain the n diagonal elements of the upper triangular matrix U from the LU factorization of A.

10: **duf**[dim] – const double *Input*

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

On entry: must contain the $(n - 1)$ elements of the first superdiagonal of U.

11: **du2**[dim] – const double *Input*

Note: the dimension, *dim*, of the array **du2** must be at least $\max(1, \mathbf{n} - 2)$.

On entry: must contain the $(n - 2)$ elements of the second superdiagonal of U.

12: **ipiv**[dim] – const Integer *Input*

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

On entry: must contain the n pivot indices that define the permutation matrix P. At the ith step, row i of the matrix was interchanged with row **ipiv**$[i-1]$, and **ipiv**$[i-1]$ must always be either i or $(i+1)$, **ipiv**$[i-1] = i$ indicating that a row interchange was not performed.

13: **b**[dim] – const double *Input*

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

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

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

15: **x**[dim] – double *Input/Output*

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

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

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

x$[(j-1) \times \mathbf{pdx} + i - 1]$ when **order** = Nag_ColMajor;
x$[(i-1) \times \mathbf{pdx} + j - 1]$ when **order** = Nag_RowMajor.

On entry: the n by r initial solution matrix X.

On exit: the n by r refined solution matrix X.

16: **pdx** – Integer *Input*

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

Constraints:

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

17: **ferr**[**nrhs**] – double *Output*

On exit: estimate of the forward error bound for each computed solution vector, such that $\left\|\hat{x}_j - x_j\right\|_\infty / \left\|\hat{x}_j\right\|_\infty \leq$ **ferr**$[j-1]$, where $\hat{x}_j$ is the jth column of the computed solution returned in the array **x** and x_j is the corresponding column of the exact solution X. The estimate is almost always a slight overestimate of the true error.

18: **berr**[**nrhs**] – double *Output*

On exit: estimate of the component-wise relative backward error of each computed solution vector $\hat{x}_j$ (i.e., the smallest relative change in any element of A or B that makes $\hat{x}_j$ an exact solution).

19: **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 ⟨*value*⟩ had an illegal value.

NE_INT

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

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

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

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

NE_INT_2

On entry, **pdb** = ⟨*value*⟩ and **n** = ⟨*value*⟩.
Constraint: **pdb** $\geq \max(1, \mathbf{n})$.

On entry, **pdb** = ⟨*value*⟩ and **nrhs** = ⟨*value*⟩.
Constraint: **pdb** $\geq \max(1, \mathbf{nrhs})$.

On entry, **pdx** = ⟨*value*⟩ and **n** = ⟨*value*⟩.
Constraint: **pdx** $\geq \max(1, \mathbf{n})$.

On entry, **pdx** = ⟨*value*⟩ and **nrhs** = ⟨*value*⟩.
Constraint: **pdx** $\geq \max(1, \mathbf{nrhs})$.

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

7 Accuracy

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

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

where

$$\|E\|_\infty = O(\epsilon)\|A\|_\infty$$

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

$$\frac{\|\hat{x} - x\|_\infty}{\|x\|_\infty} \leq \kappa(A)\frac{\|E\|_\infty}{\|A\|_\infty},$$

where $\kappa(A) = \left\|A^{-1}\right\|_\infty \|A\|_\infty$, 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.

Function nag_dgtcon (f07cgc) can be used to estimate the condition number of A.

8 Parallelism and Performance

nag_dgtrfs (f07chc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_dgtrfs (f07chc) 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

The total number of floating-point operations required to solve the equations $AX = B$ or $A^{\mathrm{T}}X = B$ is proportional to nr. At most five steps of iterative refinement are performed, but usually only one or two steps are required.

The complex analogue of this function is nag_zgtrfs (f07cvc).

10 Example

This example solves the equations

$$AX = B,$$

where A is the tridiagonal matrix

$$A = \begin{pmatrix} 3.0 & 2.1 & 0 & 0 & 0 \\ 3.4 & 2.3 & -1.0 & 0 & 0 \\ 0 & 3.6 & -5.0 & 1.9 & 0 \\ 0 & 0 & 7.0 & -0.9 & 8.0 \\ 0 & 0 & 0 & -6.0 & 7.1 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 2.7 & 6.6 \\ -0.5 & 10.8 \\ 2.6 & -3.2 \\ 0.6 & -11.2 \\ 2.7 & 19.1 \end{pmatrix}.$$

Estimates for the backward errors and forward errors are also output.

10.1 Program Text

```
/* nag_dgtrfs (f07chc) 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 <nagf16.h>

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

  /* Arrays */
  double *b = 0, *berr = 0, *d = 0, *df = 0, *dl = 0, *dlf = 0, *du = 0;
  double *du2 = 0, *duf = 0, *ferr = 0, *x = 0;
  Integer *ipiv = 0;

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

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

  INIT_FAIL(fail);

  printf("nag_dgtrfs (f07chc) 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;
    goto END;
  }
  /* Allocate memory */
  if (!(b = NAG_ALLOC(n * nrhs, double)) ||
      !(berr = NAG_ALLOC(nrhs, double)) ||
      !(d = NAG_ALLOC(n, double)) ||
      !(df = NAG_ALLOC(n, double)) ||
      !(dl = NAG_ALLOC(n - 1, double)) ||
      !(dlf = NAG_ALLOC(n - 1, double)) ||
      !(du = NAG_ALLOC(n - 1, double)) ||
      !(du2 = NAG_ALLOC(n - 2, double)) ||
      !(duf = NAG_ALLOC(n - 1, double)) ||
      !(ferr = NAG_ALLOC(nrhs, double)) ||
```

```
      !(x = NAG_ALLOC(n * nrhs, double)) || !(ipiv = NAG_ALLOC(n, Integer)))
  {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }

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

  /* Read the tridiagonal matrix A from data file */

#ifdef _WIN32
  for (i = 0; i < n - 1; ++i)
    scanf_s("%lf", &du[i]);
#else
  for (i = 0; i < n - 1; ++i)
    scanf("%lf", &du[i]);
#endif
#ifdef _WIN32
  scanf_s("%*[^\n]");
#else
  scanf("%*[^\n]");
#endif
#ifdef _WIN32
  for (i = 0; i < n; ++i)
    scanf_s("%lf", &d[i]);
#else
  for (i = 0; i < n; ++i)
    scanf("%lf", &d[i]);
#endif
#ifdef _WIN32
  scanf_s("%*[^\n]");
#else
  scanf("%*[^\n]");
#endif
#ifdef _WIN32
  for (i = 0; i < n - 1; ++i)
    scanf_s("%lf", &dl[i]);
#else
  for (i = 0; i < n - 1; ++i)
    scanf("%lf", &dl[i]);
#endif
#ifdef _WIN32
  scanf_s("%*[^\n]");
#else
  scanf("%*[^\n]");
#endif

  /* Read the right hand matrix B */
  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

  /* Copy A into arrays duf, df and dlf. */
  for (i = 0; i < n - 1; ++i) {
```

```
    duf[i] = du[i], df[i] = d[i], dlf[i] = dl[i];
  }
  df[n - 1] = d[n - 1];

  /* Copy B into X using nag_dge_copy (f16qfc). */
  nag_dge_copy(order, Nag_NoTrans, n, nrhs, b, pdb, x, pdx, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_dge_copy (f16qfc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  /* Factorize the copy of the tridiagonal matrix A
   * using nag_dgttrf (f07cdc).
   */
  nag_dgttrf(n, dlf, df, duf, du2, ipiv, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_dgttrf (f07cdc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  /* Solve the equations AX = B using  nag_dgttrs (f07cec). */
  nag_dgttrs(order, Nag_NoTrans, n, nrhs, dlf, df, duf, du2, ipiv, x,
             pdx, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_dgttrs (f07cec).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  /* Improve the solution and compute error estimates using
   * nag_dgtrfs (f07chc).
   */
  nag_dgtrfs(order, Nag_NoTrans, n, nrhs, dl, d, du, dlf, df, duf, du2,
             ipiv, b, pdb, x, pdx, ferr, berr, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_dgtrfs (f07chc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  /* Print the solution using nag_gen_real_mat_print (x04cac). */
  fflush(stdout);
  nag_gen_real_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, nrhs,
                         x, pdx, "Solution(s)", 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 the forward and backward error estimates */
  printf("\nBackward errors (machine-dependent)\n");
  for (j = 0; j < nrhs; ++j)
    printf("%11.1e%s", berr[j], j % 7 == 6 ? "\n" : " ");

  printf("\n\nEstimated forward error bounds (machine-dependent)\n");
  for (j = 0; j < nrhs; ++j)
    printf("%11.1e%s", ferr[j], j % 7 == 6 ? "\n" : " ");
  printf("\n");

END:
  NAG_FREE(b);
  NAG_FREE(berr);
  NAG_FREE(d);
  NAG_FREE(df);
  NAG_FREE(dl);
  NAG_FREE(dlf);
  NAG_FREE(du);
  NAG_FREE(du2);
```

```
  NAG_FREE(duf);
  NAG_FREE(ferr);
  NAG_FREE(x);
  NAG_FREE(ipiv);

  return exit_status;
}

#undef B
```

10.2 Program Data

```
nag_dgtrfs (f07chc) Example Program Data
  5     2                        : n and nrhs
        2.1  -1.0   1.9   8.0
  3.0   2.3  -5.0  -0.9   7.1
  3.4   3.6   7.0  -6.0         : matrix A
  2.7   6.6
 -0.5  10.8
  2.6  -3.2
  0.6 -11.2
  2.7  19.1                     : matrix B
```

10.3 Program Results

```
nag_dgtrfs (f07chc) Example Program Results

 Solution(s)
              1           2
 1     -4.0000     5.0000
 2      7.0000    -4.0000
 3      3.0000    -3.0000
 4     -4.0000    -2.0000
 5     -3.0000     1.0000

Backward errors (machine-dependent)
    7.2e-17    5.9e-17

Estimated forward error bounds (machine-dependent)
    1.4e-14    0.0e+00
```