NAG Library Function Document

nag_lone_fit (e02gac)

1 Purpose

nag_lone_fit (e02gac) calculates an l_1 solution to an over-determined system of linear equations.

2 Specification

```
#include <nag.h>
#include <nage02.h>
```

```
void nag_lone_fit (Nag_OrderType order, Integer m, double a[], double b[],
     Integer nplus2, double toler, double x[], double *resid, Integer *rank,
     Integer *iter, NagError *fail)
```

3 Description

Given a matrix A with m rows and n columns $(m \geq n)$ and a vector b with m elements, the function calculates an l_1 solution to the over-determined system of equations

$$Ax = b.$$

That is to say, it calculates a vector x, with n elements, which minimizes the l_1 norm (the sum of the absolute values) of the residuals

$$r(x) = \sum_{i=1}^{m} |r_i|,$$

where the residuals r_i are given by

$$r_i = b_i - \sum_{j=1}^{n} a_{ij} x_j, \quad i = 1, 2, \ldots, m.$$

Here a_{ij} is the element in row i and column j of A, b_i is the ith element of b and x_j the jth element of x. The matrix A need not be of full rank.

Typically in applications to data fitting, data consisting of m points with coordinates (t_i, y_i) are to be approximated in the l_1 norm by a linear combination of known functions $\phi_j(t)$,

$$\alpha_1 \phi_1(t) + \alpha_2 \phi_2(t) + \cdots + \alpha_n \phi_n(t).$$

This is equivalent to fitting an l_1 solution to the over-determined system of equations

$$\sum_{j=1}^{n} \phi_j(t_i) \alpha_j = y_i, \quad i = 1, 2, \ldots, m.$$

Thus if, for each value of i and j, the element a_{ij} of the matrix A in the previous paragraph is set equal to the value of $\phi_j(t_i)$ and b_i is set equal to y_i, the solution vector x will contain the required values of the α_j. Note that the independent variable t above can, instead, be a vector of several independent variables (this includes the case where each ϕ_i is a function of a different variable, or set of variables).

The algorithm is a modification of the simplex method of linear programming applied to the primal formulation of the l_1 problem (see Barrodale and Roberts (1973) and Barrodale and Roberts (1974)). The modification allows several neighbouring simplex vertices to be passed through in a single iteration, providing a substantial improvement in efficiency.

4 References

Barrodale I and Roberts F D K (1973) An improved algorithm for discrete l_1 linear approximation *SIAM J. Numer. Anal.* **10** 839–848

Barrodale I and Roberts F D K (1974) Solution of an overdetermined system of equations in the l_1-norm *Comm. ACM* **17(6)** 319–320

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: **m** – Integer *Input*

On entry: the number of equations, m (the number of rows of the matrix A).

Constraint: $\mathbf{m} \geq n \geq 1$.

3: **a**[$(\mathbf{m}+\mathbf{2}) \times \mathbf{nplus2}$] – double *Input/Output*

Note: where $\mathbf{A}(i,j)$ appears in this document, it refers to the array element

$\mathbf{a}[(j-1) \times ((\mathbf{m}+2)) + i - 1]$ when **order** = Nag_ColMajor;
$\mathbf{a}[(i-1) \times \mathbf{nplus2} + j - 1]$ when **order** = Nag_RowMajor.

On entry: $\mathbf{A}(i,j)$ must contain a_{ij}, the element in the ith row and jth column of the matrix A, for $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$. The remaining elements need not be set.

On exit: contains the last simplex tableau generated by the simplex method.

4: **b**[**m**] – double *Input/Output*

On entry: $\mathbf{b}[i-1]$ must contain b_i, the ith element of the vector b, for $i = 1, 2, \ldots, m$.

On exit: the ith residual r_i corresponding to the solution vector x, for $i = 1, 2, \ldots, m$.

5: **nplus2** – Integer *Input*

On entry: $n + 2$, where n is the number of unknowns (the number of columns of the matrix A).

Constraint: $3 \leq \mathbf{nplus2} \leq \mathbf{m} + 2$.

6: **toler** – double *Input*

On entry: a non-negative value. In general **toler** specifies a threshold below which numbers are regarded as zero. The recommended threshold value is $\epsilon^{2/3}$ where ϵ is the ***machine precision***. The recommended value can be computed within the function by setting **toler** to zero. If premature termination occurs a larger value for **toler** may result in a valid solution.

Suggested value: 0.0.

7: **x**[**nplus2**] – double *Output*

On exit: $\mathbf{x}[j-1]$ contains the jth element of the solution vector x, for $j = 1, 2, \ldots, n$. The elements $\mathbf{x}[n]$ and $\mathbf{x}[n+1]$ are unused.

8: **resid** – double * *Output*

On exit: the sum of the absolute values of the residuals for the solution vector x.

9: **rank** – Integer * *Output*

On exit: the computed rank of the matrix A.

10: **iter** – Integer * *Output*

On exit: the number of iterations taken by the simplex method.

11: **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.

NE_BAD_PARAM

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

NE_INT

On entry, **nplus2** $= \langle value\rangle$.
Constraint: **nplus2** ≥ 3.

NE_INT_2

On entry, **nplus2** $= \langle value\rangle$ and **m** $= \langle value\rangle$.
Constraint: $3 \leq$ **nplus2** $\leq$ **m** $+ 2$.

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.

NE_NON_UNIQUE

An optimal solution has been obtained, but may not be unique.

NE_TERMINATION_FAILURE

Premature termination due to rounding errors. Try using larger value of **toler**: **toler** $= \langle value\rangle$.

7 Accuracy

Experience suggests that the computational accuracy of the solution x is comparable with the accuracy that could be obtained by applying Gaussian elimination with partial pivoting to the n equations satisfied by this algorithm (i.e., those equations with zero residuals). The accuracy therefore varies with the conditioning of the problem, but has been found generally very satisfactory in practice.

8 Parallelism and Performance

Not applicable.

9 Further Comments

The effects of m and n on the time and on the number of iterations in the Simplex Method vary from problem to problem, but typically the number of iterations is a small multiple of n and the total time taken is approximately proportional to mn^2.

It is recommended that, before the function is entered, the columns of the matrix A are scaled so that the largest element in each column is of the order of unity. This should improve the conditioning of the matrix, and also enable the argument **toler** to perform its correct function. The solution x obtained will then, of course, relate to the scaled form of the matrix. Thus if the scaling is such that, for each $j = 1, 2, \ldots, n$, the elements of the jth column are multiplied by the constant k_j, the element x_j of the solution vector x must be multiplied by k_j if it is desired to recover the solution corresponding to the original matrix A.

10 Example

Suppose we wish to approximate a set of data by a curve of the form

$$y = Ke^t + Le^{-t} + M$$

where K, L and M are unknown. Given values y_i at 5 points t_i we may form the over-determined set of equations for K, L and M

$$e^{x_i}K + e^{-x_i}L + M = y_i, \quad i = 1, 2, \ldots, 5.$$

nag_lone_fit (e02gac) is used to solve these in the l_1 sense.

10.1 Program Text

```
/* nag_lone_fit (e02gac) Example Program.
 *
 * Copyright 2001 Numerical Algorithms Group.
 *
 * Mark 7, 2001.
 */

#include <stdio.h>
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nage02.h>

int main(void)
{
  /* Scalars */
  double        resid, t, tol;
  Integer       exit_status, i, iter, m, rank, n, nplus2, pda;
  NagError      fail;
  Nag_OrderType order;

  /* Arrays */
  double        *a = 0, *b = 0, *x = 0;

#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);

  exit_status = 0;
  printf("nag_lone_fit (e02gac) Example Program Results\n");

  /* Skip heading in data file */
  scanf("%*[^\n] ");

  n = 3;
  nplus2 = n + 2;
  scanf("%ld%*[^\n] ", &m);
  if (m > 0)
```

```
    {
      /* Allocate memory */
      if (!(a = NAG_ALLOC((m + 2) * nplus2, double)) ||
          !(b = NAG_ALLOC(m, double)) ||
          !(x = NAG_ALLOC(nplus2, double)))
        {
          printf("Allocation failure\n");
          exit_status = -1;
          goto END;
        }

      if (order == Nag_ColMajor)
        pda = m + 2;
      else
        pda = nplus2;

      for (i = 1; i <= m; ++i)
        {
          scanf("%lf%lf%*[^\n] ", &t, &b[i-1]);
          A(i, 1) = exp(t);
          A(i, 2) = exp(-t);
          A(i, 3) = 1.0;
        }
      tol = 0.0;
      /* nag_lone_fit (e02gac).
       * L_1-approximation by general linear function
       */
      nag_lone_fit(order, m, a, b, nplus2, tol, x, &resid,
                   &rank, &iter, &fail);
      if (fail.code == NE_INT || fail.code == NE_INT_2 ||
          fail.code == NE_NO_LICENCE)
        {
          printf("Error from nag_lone_fit (e02gac).\n%s\n",
                 fail.message);
          exit_status = 1;
          goto END;
        }
      else
        {
          printf("\n");
          printf("resid = %11.2e  Rank = %5ld  Iterations ="
                 " %5ld\n", resid, rank, iter);

          printf("\n");
          printf("Solution\n");

          for (i = 1; i <= n; ++i)
            printf("%10.4f", x[i-1]);
          printf("\n");
        }
    }

 END:
  NAG_FREE(a);
  NAG_FREE(b);
  NAG_FREE(x);

  return exit_status;
}
```

10.2 Program Data

```
nag_lone_fit (e02gac) Example Program Data
  5
   0.0 4.501
   0.2 4.360
   0.4 4.333
   0.6 4.418
   0.8 4.625
```

10.3 Program Results

```
nag_lone_fit (e02gac) Example Program Results

resid =   2.78e-03  Rank =     3  Iterations =     5

Solution
    1.0014    2.0035    1.4960
```