# NAG Library Function Document nag\_all\_regsn (g02eac)

## 1 Purpose

nag\_all\_regsn (g02eac) calculates the residual sums of squares for all possible linear regressions for a given set of independent variables.

## 2 Specification

# 3 Description

For a set of k possible independent variables there are  $2^k$  linear regression models with from zero to k independent variables in each model. For example if k = 3 and the variables are A, B and C then the possible models are:

- (i) null model
- (ii) A
- (iii) B
- (iv) C
- (v) A and B
- (vi) A and C
- (vii) B and C
- (viii) A, B and C.

nag\_all\_regsn (g02eac) calculates the residual sums of squares from each of the  $2^k$  possible models. The method used involves a QR decomposition of the matrix of possible independent variables. Independent variables are then moved into and out of the model by a series of Givens rotations and the residual sums of squares computed for each model; see Clark (1981) and Smith and Bremner (1989).

The computed residual sums of squares are then ordered first by increasing number of terms in the model, then by decreasing size of residual sums of squares. So the first model will always have the largest residual sum of squares and the  $2^k$ th will always have the smallest. This aids you in selecting the best possible model from the given set of independent variables.

nag\_all\_regsn (g02eac) allows you to specify some independent variables that must be in the model, the forced variables. The other independent variables from which the possible models are to be formed are the free variables.

#### 4 References

Clark M R B (1981) A Givens algorithm for moving from one linear model to another without going back to the data *Appl. Statist.* **30** 198–203

Smith D M and Bremner J M (1989) All possible subset regressions using the QR decomposition Comput. Statist. Data Anal. 7 217–236

Weisberg S (1985) Applied Linear Regression Wiley

# 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: **mean** – Nag\_IncludeMean

Input

On entry: indicates if a mean term is to be included.

mean = Nag\_MeanInclude

A mean term, intercept, will be included in the model.

mean = Nag\_MeanZero

The model will pass through the origin, zero-point.

Constraint: mean = Nag\_MeanInclude or Nag\_MeanZero.

3:  $\mathbf{n}$  – Integer

On entry: n, the number of observations.

Constraints:

 $n \ge 2$ ;

 $n \ge m$ , is the number of independent variables to be considered (forced plus free plus mean if included), as specified by **mean** and **sx**.

4: **m** – Integer

Input

Input

On entry: the number of variables contained in x.

Constraint:  $\mathbf{m} \geq 2$ .

5:  $\mathbf{x}[dim]$  – const double

Input

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

```
\max(1, \mathbf{pdx} \times \mathbf{m}) when \mathbf{order} = \text{Nag\_ColMajor}; \max(1, \mathbf{n} \times \mathbf{pdx}) when \mathbf{order} = \text{Nag\_RowMajor}.
```

Where X(i, j) appears in this document, it refers to the array element

$$\mathbf{x}[(j-1) \times \mathbf{pdx} + i - 1]$$
 when  $\mathbf{order} = \text{Nag\_ColMajor};$   
 $\mathbf{x}[(i-1) \times \mathbf{pdx} + j - 1]$  when  $\mathbf{order} = \text{Nag\_RowMajor}.$ 

On entry:  $\mathbf{X}(i,j)$  must contain the *i*th observation for the *j*th independent variable, for  $i=1,2,\ldots,\mathbf{n}$  and  $j=1,2,\ldots,\mathbf{m}$ .

6:  $\mathbf{pdx}$  - Integer Input

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

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Constraints:

if order = Nag\_ColMajor,  $pdx \ge n$ ; if order = Nag\_RowMajor,  $pdx \ge m$ .

7: **var\_names**[**m**] - const char \*

Input

On entry:  $\mathbf{var\_names}[i-1]$  must contain the name of the independent variable in row i of  $\mathbf{x}$ , for  $i=1,2,\ldots,\mathbf{m}$ .

8:  $\mathbf{sx}[\mathbf{m}]$  – const Integer

Input

On entry: indicates which independent variables are to be considered in the model.

$$sx[i-1] > 2$$

The variable contained in the jth column of X is included in all regression models, i.e., is a forced variable.

$$\mathbf{sx}[j-1] = 1$$

The variable contained in the jth column of X is included in the set from which the regression models are chosen, i.e., is a free variable.

$$\mathbf{sx}[j-1] = 0$$

The variable contained in the *i*th column of **X** is not included in the models.

Constraints:

$$\mathbf{sx}[j-1] \ge 0$$
, for  $j = 1, 2, \dots, \mathbf{m}$ ; at least one value of  $\mathbf{sx} = 1$ .

9:  $\mathbf{y}[\mathbf{n}]$  – const double

Input

On entry:  $\mathbf{y}[i-1]$  must contain the *i*th observation on the dependent variable,  $y_i$ , for  $i=1,2,\ldots,n$ .

10:  $\mathbf{wt}[n]$  – const double

Input

On entry: optionally, the weights to be used in the weighted regression.

If  $\mathbf{wt}[i-1] = 0.0$ , then the *i*th observation is not included in the model, in which case the effective number of observations is the number of observations with nonzero weights.

If weights are not provided then wt must be set to NULL and the effective number of observations is n.

Constraint: if wt is not NULL, wt[i-1] = 0.0, for i = 1, 2, ..., n.

11: **nmod** – Integer \*

Output

On exit: the total number of models for which residual sums of squares have been calculated.

12: model[dim] - const char \*

Output

**Note**: the dimension, dim, of the array **model** must be at least big enough to hold the names of all the free independent variables which appear in all the models. This will never exceed  $2^k \times \mathbf{m}$ , where k is the number of free variables in the model.

On exit: the names of the independent variables in each model, represented as pointers to the names provided by you in var names. The model names are stored as follows:

if the first model has three names, i.e., nterms[0] = 3; then model[0], model[1] and model[2] will contain these three names;

if the second model has two names, i.e., nterms[1] = 2; then model[3], model[4] will contain these two names.

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13:  $rss[max(2^k, m)] - double$ 

Output

On exit: rss[i-1] contains the residual sum of squares for the ith model, for  $i=1,2,\ldots,n$  mod.

14:  $\mathbf{nterms}[\mathbf{max}(\mathbf{2}^k, \mathbf{m})] - \mathbf{Integer}$ 

Output

On exit: nterms[i-1] contains the number of independent variables in the *i*th model, not including the mean if one is fitted, for i = 1, 2, ..., nmod.

15:  $mrank[max(2^k, m)] - Integer$ 

Output

On exit: mrank[i-1] contains the rank of the residual sum of squares for the ith model.

16: **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.

See Section 3.2.1.2 in the Essential Introduction for further information.

## NE\_BAD\_PARAM

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

#### NE FREE VARS

There are no free x variables.

#### NE FULL RANK

Full model is not of full rank.

#### **NE INDEP VARS OBS**

Number of requested x-variables  $\geq$  number of observations.

#### NE INT

On entry,  $\mathbf{m} = \langle value \rangle$ .

Constraint:  $\mathbf{m} \geq 2$ .

On entry,  $\mathbf{n} = \langle value \rangle$ .

Constraint:  $n \ge 2$ .

On entry,  $\mathbf{pdx} = \langle value \rangle$ .

Constraint:  $\mathbf{pdx} > 0$ .

## NE\_INT\_2

On entry,  $\mathbf{pdx} = \langle value \rangle$  and  $\mathbf{m} = \langle value \rangle$ .

Constraint:  $pdx \ge m$ .

On entry,  $\mathbf{pdx} = \langle value \rangle$  and  $\mathbf{n} = \langle value \rangle$ .

Constraint:  $pdx \ge n$ .

#### NE INT ARRAY ELEM CONS

On entry,  $\mathbf{sx}[\langle value \rangle] < 0$ .

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#### 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 the Essential Introduction 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 the Essential Introduction for further information.

#### NE REAL ARRAY ELEM CONS

On entry,  $\mathbf{wt}[\langle value \rangle] < 0.0$ .

## 7 Accuracy

For a discussion of the improved accuracy obtained by using a method based on the QR decomposition see Smith and Bremner (1989).

## 8 Parallelism and Performance

nag\_all\_regsn (g02eac) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag\_all\_regsn (g02eac) 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

nag\_cp\_stat (g02ecc) may be used to compute  $\mathbb{R}^2$  and  $\mathbb{C}_p$ -values from the results of nag\_all\_regsn (g02eac).

If a mean has been included in the model and no variables are forced in then rss[0] contains the total sum of squares and in many situations a reasonable estimate of the variance of the errors is given by rss[nmod - 1]/(n - 1 - nterms[nmod - 1]).

## 10 Example

The data for this example is given in Weisberg (1985). The independent variables and the dependent variable are read, as are the names of the variables. These names are as given in Weisberg (1985). The residual sums of squares computed and printed with the names of the variables in the model.

#### 10.1 Program Text

```
/* nag_all_regsn (g02eac) Example Program.
    * Copyright 2014 Numerical Algorithms Group.
    * Mark 7, 2002.
    */
#include <math.h>
#include <stdio.h>
#include <string.h>
#include <nag.h>
```

```
#include <nag_stdlib.h>
#include <nagg02.h>
int main(void)
  /* Scalars */
                exit_status, free_vars, i, ii, j, m, n, nmod, pdx;
  Integer
  NagError
                fail;
  Nag_OrderType order;
  /* Arrays */
                 **model = 0;
                 *var_names[] = { "DAY", "BOD", "TKN", "TS", "TVS", "COD" };
  const char
                 *rss = 0, *x = 0, *y = 0, *wtptr = 0;
*sx = 0, *mrank = 0, *nterms = 0;
  double
  Integer
  /* For iteration over model */
  Integer
                model_index = 0;
#ifdef NAG COLUMN MAJOR
#define X(I, J) \times [(J-1) * pdx + I - 1]
 order = Nag_ColMajor;
#else
#define X(I, J) \times [(I-1)*pdx + J - 1]
 order = Nag_RowMajor;
#endif
  INIT_FAIL(fail);
  exit_status = 0;
 printf("nag_all_regsn (g02eac) Example Program Results\n");
  /* Skip heading in data file */
#ifdef _WIN32
scanf_s("%*[^\n] ");
 scanf("%*[^\n] ");
#endif
#ifdef _WIN32
 scanf_s("%"NAG_IFMT"%"NAG_IFMT"%*[^\n] ", &n, &m);
#else
  scanf("%"NAG_IFMT"%"NAG_IFMT"%*[^\n] ", &n, &m);
#endif
  /* Allocate memory */
  if (!(x = NAG_ALLOC(n * m, double)) ||
    !(y = NAG_ALLOC(n, double)) ||
      !(sx = NAG_ALLOC(m, Integer)))
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
#ifdef NAG_COLUMN_MAJOR
  pdx = n;
  order = Nag_ColMajor;
#else
 pdx = m;
 order = Nag_RowMajor;
#endif
  for (i = 1; i \le n; ++i)
      for (j = 1; j \le m; ++j)
#ifdef _WIN32
        scanf_s("%lf", &X(i, j));
#else
        scanf("%lf", &X(i, j));
```

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```
#endif
#ifdef _WIN32
     scanf_s("%lf%*[^\n] ", &y[i - 1]);
      scanf("%lf%*[^\n] ", &y[i - 1]);
#endif
    }
 free\_vars = 1;
 for (j = 1; j \le m; ++j)
#ifdef _WIN32
     scanf_s("%"NAG_IFMT"", &sx[j - 1]);
#else
      scanf("%"NAG_IFMT"", &sx[j - 1]);
#endif
      if (sx[j - 1] == 1)
         free_vars <<= 1;</pre>
    }
#ifdef _WIN32
 scanf_s("%*[^\n] ");
 scanf("%*[^\n] ");
#endif
  if (!(model = NAG_ALLOC(free_vars*m, char *)) ||
      !(rss = NAG_ALLOC(free_vars, double)) ||
      !(mrank = NAG_ALLOC(free_vars, Integer)) ||
      !(nterms = NAG_ALLOC(free_vars, Integer)))
     printf("Allocation failure\n");
      exit_status = -1;
      goto END;
  /* nag_all_regsn (g02eac).
  * Computes residual sums of squares for all possible linear
   * regressions for a set of independent variables
 nag_all_regsn(order, Nag_MeanInclude, n, m, x, pdx, var_names, sx, y, wtptr,
                &nmod, (const char **) model, rss, nterms, mrank, &fail);
  if (fail.code != NE_NOERROR)
     printf("Error from nag_all_regsn (g02eac).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
 printf("\n");
 printf("Number of
                               Rank
                                           Model\n");
                       Rss
 printf("parameters\n");
 for (i = 1; i <= nmod; ++i)
      ii = nterms[i - 1];
     printf("%8"NAG_IFMT"%11.4f%4"NAG_IFMT" ", ii, rss[i-1],
              mrank[i-1]);
      for (j = 1; j \le ii; ++j)
       printf("%-3.3s %s", model[model_index++],
                j%5 == 0 \mid \mid j == 5?" \n":" ");
     printf("\n");
   3
END:
 NAG_FREE(rss);
 NAG_FREE(x);
 NAG_FREE(y);
 NAG_FREE(sx);
```

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```
NAG_FREE(mrank);
NAG_FREE(nterms);
NAG_FREE(model);
return exit_status;
}
```

#### 10.2 Program Data

```
nag_all_regsn (g02eac) Example Program Data
  20 6
   0. 1125.0 232.0 7160.0 85.9 8905.0
                                          1.5563
   7. 920.0 268.0 8804.0 86.5 7388.0
                                         0.8976
  15. 835.0 271.0 8108.0 85.2 5348.0 0.7482
  22. 1000.0 237.0 6370.0 83.8 8056.0
                                         0.7160
  29. 1150.0 192.0 6441.0 82.1 6960.0
                                         0.3010
  37.
       990.0 202.0 5154.0 79.2 5690.0
                                          0.3617
  44.
       840.0 184.0 5896.0 81.2 6932.0
                                         0.1139
  58.
       650.0 200.0 5336.0 80.6 5400.0
                                         0.1139
  65.
       640.0 180.0 5041.0 78.4 3177.0 -0.2218
       583.0 165.0 5012.0 79.3 4461.0 -0.1549
570.0 151.0 4825.0 78.7 3901.0 0.0000
  72.
  80.
       570.0 171.0 4391.0 78.0 5002.0 0.0000
  86.
       510.0 243.0 4320.0 72.3 4665.0 -0.0969
  93.
 100.
       555.0 147.0 3709.0 74.9 4642.0 -0.2218
       460.0 286.0 3969.0 74.4 4840.0 -0.3979
 107.
       275.0 198.0 3558.0 72.5 4479.0 -0.1549
 122.
 129.
       510.0 196.0 4361.0 57.7 4200.0 -0.2218
 151.
       165.0 210.0 3301.0 71.8 3410.0 -0.3979
       244.0 327.0 2964.0 72.5 3360.0 -0.5229 79.0 334.0 2777.0 71.9 2599.0 -0.0458
 171.
 220.
                     1
```

#### 10.3 Program Results

nag\_all\_regsn (g02eac) Example Program Results

Number o		Rss	Rank		Мс	Model		
paramete 0 1 1 1 1 1 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3	rs 5 5 2 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	.0634 .0219 .5044 .0338 .5563 .5370 .4381 .7462 .5921 .4963 .4707 .4590 .4397 .4388 .3287 .0850 .4257 .3900 .3894 .2764 .2582 .2179 .0644 .0634	32 31 30 28 25 24 29 27 26 23 22 21 20 19 15 8 8 17 16 14 13 12 10 7 6	TKN TVS BOD COD TS TKN BOD BOD TKN TS BOD TKN TVS BOD TKN TVS BOD TKN BOD	TVS TVS TKN COD TS TVS COD COD TKN TS TS TVS TVS TVS TVS TVS TVS TVS	TVS TVS TVS COD COD TS COD COD COD		
3		.9871	4	TKN	TVS	COD		
4		.2199	11	BOD	TKN	TS	TVS	
4		.1565	9	BOD	TKN	TVS	COD	

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4	1.0388	5	BOD	TS	TVS	COD	
4	0.9871	3	BOD	TKN	TS	COD	
4	0.9653	2	TKN	TS	TVS	COD	
5	0.9652	1	BOD	TKN	TS	TVS	COD

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