NAG Library Function Document

nag_cp_stat (g02ecc)

1 Purpose

nag_cp_stat (g02ecc) calculates R^2 and C_p-values from the residual sums of squares for a series of linear regression models.

2 Specification

```
#include <nag.h>
#include <nagg02.h>
```

```
void nag_cp_stat (Nag_IncludeMean mean, Integer n, double sigsq, double tss,
     Integer nmod, const Integer nterms[], const double rss[], double rsq[],
     double cp[], NagError *fail)
```

3 Description

When selecting a linear regression model for a set of n observations a balance has to be found between the number of independent variables in the model and fit as measured by the residual sum of squares. The more variables included the smaller will be the residual sum of squares. Two statistics can help in selecting the best model.

(a) R^2 represents the proportion of variation in the dependent variable that is explained by the independent variables.

$$R^2 = \frac{\text{Regression Sum of Squares}}{\text{Total Sum of Squares}},$$

where Total Sum of Squares $= \mathbf{tss} = \sum (y - \bar{y})^2$ (if mean is fitted, otherwise $\mathbf{tss} = \sum y^2$) and

Regression Sum of Squares $=$ RegSS $= \mathbf{tss} - \mathbf{rss}$, where
$\mathbf{rss} =$ residual sum of squares $= \sum (y - \hat{y})^2$.

The R^2-values can be examined to find a model with a high R^2-value but with small number of independent variables.

(b) C_p statistic.

$$C_p = \frac{\mathbf{rss}}{\hat{\sigma}^2} - (n - 2p),$$

where p is the number of arguments (including the mean) in the model and $\hat{\sigma}^2$ is an estimate of the true variance of the errors. This can often be obtained from fitting the full model.

A well fitting model will have $C_p \simeq p$. C_p is often plotted against p to see which models are closest to the $C_p = p$ line.

nag_cp_stat (g02ecc) may be called after nag_all_regsn (g02eac) which calculates the residual sums of squares for all possible linear regression models.

4 References

Draper N R and Smith H (1985) *Applied Regression Analysis* (2nd Edition) Wiley

Weisberg S (1985) *Applied Linear Regression* Wiley

5 Arguments

1: **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.

2: **n** – Integer *Input*

On entry: n, the number of observations used in the regression model.

Constraint: **n** must be greater than $2 \times p_{\text{max}}$, where p_{max} is the largest number of independent variables fitted (including the mean if fitted).

3: **sigsq** – double *Input*

On entry: the best estimate of true variance of the errors, $\hat{\sigma}^2$.

Constraint: **sigsq** > 0.0.

4: **tss** – double *Input*

On entry: the total sum of squares for the regression model.

Constraint: **tss** > 0.0.

5: **nmod** – Integer *Input*

On entry: the number of regression models.

Constraint: **nmod** > 0.

6: **nterms**[**nmod**] – const Integer *Input*

On entry: **nterms**$[i-1]$ must contain the number of independent variables (not counting the mean) fitted to the ith model, for $i = 1, 2, \ldots,$ **nmod**.

7: **rss**[**nmod**] – const double *Input*

On entry: **rss**$[i-1]$ must contain the residual sum of squares for the ith model.

Constraint: **rss**$[i-1] \leq$ **tss**, for $i = 1, 2, \ldots,$ **nmod**.

8: **rsq**[**nmod**] – double *Output*

On exit: **rsq**$[i-1]$ contains the R^2-value for the ith model, for $i = 1, 2, \ldots,$ **nmod**.

9: **cp**[**nmod**] – double *Output*

On exit: **cp**$[i-1]$ contains the C_p-value for the ith model, for $i = 1, 2, \ldots,$ **nmod**.

10: **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_INT

On entry, **nmod** $= \langle value \rangle$.
Constraint: **nmod** > 0.

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_MODEL_PARAMETERS

On entry, number of parameters for model $\langle value \rangle$ is too large for **n**. **n** $= \langle value \rangle$, number of parameters $= \langle value \rangle$.

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

On entry, **sigsq** $= \langle value \rangle$.
Constraint: **sigsq** > 0.0.

On entry, **tss** $= \langle value \rangle$.
Constraint: **tss** > 0.0.

NE_REAL_ARRAY_ELEM_CONS

On entry, **cp**$[\langle value \rangle] = \langle value \rangle$.
Constraint: **cp**$[i] \geq 0.0$, for all i.

On entry, **rss**$[\langle value \rangle] = \langle value \rangle$ and **tss** $= \langle value \rangle$.
Constraint: **rss**$[i] \leq$ **tss**, for all i.

7 Accuracy

Accuracy is sufficient for all practical purposes.

8 Parallelism and Performance

Not applicable.

9 Further Comments

None.

10 Example

The data, from an oxygen uptake experiment, is given by Weisberg (1985). The independent and dependent variables are read and the residual sums of squares for all possible models computed using nag_all_regsn (g02eac). The values of R^2 and C_p are then computed and printed along with the names of variables in the models.

10.1 Program Text

```
/* nag_cp_stat (g02ecc) Example Program.
 *
 * Copyright 2014 Numerical Algorithms Group.
 *
 * Mark 7, 2002.
 * Mark 7b revised, 2004.
 */

#include <math.h>
#include <stdio.h>
#include <string.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagg02.h>

int main(void)
{

  /* Scalars */
  double        sigsq, tss;
  Integer       exit_status, num_models, i, ii, j, m, n, nmod, pdx;
  NagError      fail;
  Nag_OrderType order;

  /* Arrays */
  char          **model = 0;
  double        *cp = 0, *rsq = 0, *rss = 0, *wtptr = 0, *x = 0, *y = 0;
  Integer       *sx = 0, *mrank = 0, *nterms = 0;
  const char    *var_names[] = { "DAY", "BOD", "TKN", "TS", "TVS", "COD" };

  /* For iteration over model */
  Integer       model_index = 0;

#ifdef NAG_COLUMN_MAJOR
#define X(I, J) x[(J-1)*pdx + I - 1]
  order = Nag_ColMajor;
#else
#define X(I, J) x[(I-1)*pdx + J - 1]
  order = Nag_RowMajor;
#endif

  INIT_FAIL(fail);

  exit_status = 0;
  printf("nag_cp_stat (g02ecc) Example Program Results\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, &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 <= n; ++i)
    {
      for (j = 1; j <= m; ++j)
#ifdef _WIN32
        scanf_s("%lf", &X(i, j));
#else
        scanf("%lf", &X(i, j));
#endif
#ifdef _WIN32
      scanf_s("%lf%*[^\n] ", &y[i - 1]);
#else
      scanf("%lf%*[^\n] ", &y[i - 1]);
#endif
    }

  num_models = 1;
  for (j = 1; j <= m; ++j)
    {
#ifdef _WIN32
      scanf_s("%"NAG_IFMT"", &sx[j - 1]);
#else
      scanf("%"NAG_IFMT"", &sx[j - 1]);
#endif
      if (sx[j - 1] == 1)
        num_models <<= 1;
    }
#ifdef _WIN32
  scanf_s("%*[^\n] ");
#else
  scanf("%*[^\n] ");
#endif

  /* Allocate memory */
  if (!(model = NAG_ALLOC(num_models*m, char *)) ||
      !(cp = NAG_ALLOC(num_models, double)) ||
      !(rsq = NAG_ALLOC(num_models, double)) ||
      !(rss = NAG_ALLOC(num_models, double)) ||
      !(mrank = NAG_ALLOC(num_models, Integer)) ||
      !(nterms = NAG_ALLOC(num_models, Integer)))
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }

  /* Calculate residual sums of squares using nag_all_regsn (g02eac) */

  /* 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;
    }

  tss = rss[0];
  sigsq = rss[nmod - 1] / (n - nterms[nmod - 1] - 1);
  /* nag_cp_stat (g02ecc).
   * Calculates R^2 and C_P values from residual sums of
   * squares
   */
  nag_cp_stat(Nag_MeanInclude, n, sigsq, tss, nmod, nterms, rss, rsq, cp,
              &fail);
  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_cp_stat (g02ecc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }

  printf("\n");
  printf("Number of     CP      RSQ         MODEL\n");
  printf("parameters\n");
  for (i = 1; i <= nmod; ++i)
    {
      ii = nterms[i - 1];
      printf(" %7"NAG_IFMT"%11.2f%8.4f  ", ii, cp[i - 1], rsq[i - 1]);
      for (j = 1; j <= ii; ++j)
        printf("%-3.3s %s", model[model_index++],
                j%5 == 0 || j == 5?"\n":" ");
      printf("\n");
    }
 END:
  NAG_FREE(model);
  NAG_FREE(cp);
  NAG_FREE(rsq);
  NAG_FREE(rss);
  NAG_FREE(x);
  NAG_FREE(y);
  NAG_FREE(sx);
  NAG_FREE(mrank);
  NAG_FREE(nterms);

  return exit_status;
}
```

10.2 Program Data

```
nag_cp_stat (g02ecc) 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
  72.  583.0 165.0 5012.0 79.3 4461.0 -0.1549
  80.  570.0 151.0 4825.0 78.7 3901.0  0.0000
  86.  570.0 171.0 4391.0 78.0 5002.0  0.0000
  93.  510.0 243.0 4320.0 72.3 4665.0 -0.0969
 100.  555.0 147.0 3709.0 74.9 4642.0 -0.2218
 107.  460.0 286.0 3969.0 74.4 4840.0 -0.3979
 122.  275.0 198.0 3558.0 72.5 4479.0 -0.1549
```

```
 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
 171.   244.0 327.0 2964.0 72.5 3360.0 -0.5229
 220.    79.0 334.0 2777.0 71.9 2599.0 -0.0458
  0      1    1      1     1    1
```

10.3 Program Results

```
nag_cp_stat (g02ecc) Example Program Results

Number of      CP      RSQ         MODEL
parameters
       0      55.45  0.0000
       1      56.84  0.0082  TKN
       1      20.33  0.5054  TVS
       1      13.50  0.5983  BOD
       1       6.57  0.6926  COD
       1       6.29  0.6965  TS
       2      21.36  0.5185  TKN  TVS
       2      11.33  0.6551  BOD  TVS
       2       9.09  0.6856  BOD  TKN
       2       7.70  0.7045  BOD  COD
       2       7.33  0.7095  TKN  TS
       2       7.16  0.7119  TS   TVS
       2       6.88  0.7157  BOD  TS
       2       6.87  0.7158  TKN  COD
       2       5.27  0.7376  TVS  COD
       2       1.74  0.7857  TS   COD
       3       8.68  0.7184  BOD  TKN  TVS
       3       8.16  0.7255  TKN  TS   TVS
       3       8.15  0.7256  BOD  TS   TVS
       3       7.15  0.7392  BOD  TVS  COD
       3       6.51  0.7479  BOD  TKN  COD
       3       6.25  0.7515  BOD  TKN  TS
       3       5.67  0.7595  TKN  TVS  COD
       3       3.44  0.7898  BOD  TS   COD
       3       3.42  0.7900  TS   TVS  COD
       3       2.32  0.8050  TKN  TS   COD
       4       7.70  0.7591  BOD  TKN  TS   TVS
       4       6.78  0.7716  BOD  TKN  TVS  COD
       4       5.07  0.7948  BOD  TS   TVS  COD
       4       4.32  0.8050  BOD  TKN  TS   COD
       4       4.00  0.8094  TKN  TS   TVS  COD
       5       6.00  0.8094  BOD  TKN  TS   TVS  COD
```