

NAG Library Function Document

nag_regress_confid_interval (g02cbc)

1 Purpose

`nag_regress_confid_interval (g02cbc)` performs a simple linear regression with or without a constant term. The data is optionally weighted, and confidence intervals are calculated for the predicted and average values of y at a given x .

2 Specification

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

void nag_regress_confid_interval (Nag_SumSquare mean, Integer n,
    const double x[], const double y[], const double wt[], double clm,
    double clp, double yhat[], double yml[], double ymu[], double yl[],
    double yu[], double h[], double res[], double *rms, NagError *fail)
```

3 Description

`nag_regress_confid_interval (g02cbc)` fits a straight line model of the form,

$$E(y) = a + bx$$

where $E(y)$ is the expected value of the variable y , to the data points

$$(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n),$$

such that

$$y_i = a + bx_i + e_i, \quad i = 1, 2, \dots, n,$$

where the e_i values are independent random errors. The i th data point may have an associated weight w_i . The values of a and b are estimated by minimizing $\sum w_i e_i^2$ (if the weights option is not selected then $w_i = 1.0$). The fitted values \hat{y}_i are calculated using

$$\hat{y}_i = \hat{a} + \hat{b}x_i$$

where

$$\hat{a} = \bar{y} - \hat{b}\bar{x} \quad \hat{b} = \frac{\sum w_i(x_i - \bar{x})(y_i - \bar{y})}{\sum w_i(x_i - \bar{x})^2}$$

and the weighted means \bar{x} and \bar{y} are given by

$$\bar{y} = \frac{\sum w_i y_i}{\sum w_i} \quad \text{and} \quad \bar{x} = \frac{\sum w_i x_i}{\sum w_i}.$$

The residuals of the regression are calculated using

$$res_i = y_i - \hat{y}_i$$

and the residual mean square about the regression rms , is determined using

$$rms = \frac{\sum w_i(y_i - \hat{y}_i)^2}{df}$$

where df (the number of degrees of freedom) has the following values

$$df = \sum w_i - 2 \text{ where } \mathbf{mean} = \text{Nag_AboutMean}$$

$$df = \sum w_i - 1 \text{ where } \mathbf{mean} = \text{Nag_AboutZero}.$$

Note: the weights should be scaled to give the required degrees of freedom.

The function calculates predicted y estimates for a value of x , x_i^* , is given by

$$y_i^* = \hat{a} + \hat{b}x_i^*$$

this prediction has a standard error

$$serr_pred = \sqrt{rms} \sqrt{1 + \frac{1}{\sum w_i} + \frac{(x_i^* - \bar{x})^2}{\sum w_i(x_i - \bar{x})^2}}.$$

The $(1 - \alpha)$ confidence interval for this estimation of y is given by

$$y_i^* \pm t_{df}(1 - \alpha/2).serr_pred$$

where $t_{df}(1 - \alpha/2)$ refers to the $(1 - \alpha/2)$ point of the t distribution with df degrees of freedom (e.g., when $df = 20$ and $\alpha = 0.1$, $t_{20}(0.95) = 2.086$). If you specify the probability $clp = 0.9$ ($\alpha = 0.1$) then the lower limit of this interval is

$$yl_i = y_{i-t}^* - t_{df}(0.95).serr_pred$$

and the upper limit is

$$yu_i = y_i^* + t_{df}(0.95).serr_pred.$$

The mean value of y at x_i is estimated by the fitted value \hat{y}_i . This has a standard error of

$$serr_arg = \sqrt{rms} \sqrt{\frac{1}{\sum w_i} + \frac{(x_i - \bar{x})^2}{\sum w_i(x_i - \bar{x})^2}}$$

and a $(1 - \alpha)$ confidence interval is given by

$$\hat{y}_i \pm t_{df}(1 - \alpha/2).serr_arg.$$

For example, if you specify the probability $clm = 0.6$ ($\alpha = 0.4$) then the lower limit of this interval is

$$yml_i = \hat{y}_{i-t} - t_{df}(0.8).serr_arg$$

and the upper limit is

$$ymu_i = \hat{y}_i + t_{df}(0.8).serr_arg.$$

The leverage, h_i , is a measure of the influence a value x_i has on the fitted line at that point, \hat{y}_i . The leverage is given by

$$h_i = \frac{w_i}{\sum w_i} + \frac{w_i(x_i - \bar{x})^2}{\sum w_i(x_i - \bar{x})^2}$$

so it can be seen that

$$\begin{aligned} serr_arg &= \sqrt{rms} \sqrt{h_i/w_i} \\ \text{and } serr_pred &= \sqrt{rms} \sqrt{1 + h_i/w_i} \end{aligned}$$

Similar formulae can be derived for the case when the line goes through the origin, that is $a = 0$.

4 References

Snedecor G W and Cochran W G (1967) *Statistical Methods* Iowa State University Press

5 Arguments

1: **mean** – Nag_SumSquare *Input*

On entry: indicates whether nag_regress_confid_interval (g02cbc) is to include a constant term in the regression.

mean = Nag_AboutMean

The constant term, a , is included.

mean = Nag_AboutZero

The constant term, a , is not included, i.e., $a = 0$.

Constraint: **mean** = Nag_AboutMean or Nag_AboutZero.

2: **n** – Integer *Input*

On entry: N , the number of observations.

Constraints:

if **mean** = Nag_AboutMean, $n \geq 2$;
 if **mean** = Nag_AboutZero, $n \geq 1$.

3: **x[n]** – const double *Input*

On entry: observations on the independent variable, x .

Constraint: all the values of x must not be identical.

4: **y[n]** – const double *Input*

On entry: observations on the dependent variable, y .

5: **wt[n]** – const double *Input*

On entry: if weighted estimates are required then **wt** must contain the weights to be used in the weighted regression. Usually **wt**[$i - 1$] will be an integral value corresponding to the number of observations associated with the i th data point, or zero if the i th data point is to be ignored. The sum of the weights therefore represents the effective total number of observations used to create the regression line.

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 $i = 1, 2, \dots, n$.

6: **clm** – double *Input*

On entry: the confidence level for the confidence intervals for the mean.

Constraint: $0.0 < \text{clm} < 1.0$.

7: **clp** – double *Input*

On entry: the confidence level for the prediction intervals.

Constraint: $0.0 < \text{clp} < 1.0$.

8: **yhat[n]** – double *Output*

On exit: the fitted values, \hat{y}_i .

9: **yml[n]** – double *Output*

On exit: **yml**[$i - 1$] contains the lower limit of the confidence interval for the regression line at **x**[$i - 1$].

10:	ymu[n] – double	<i>Output</i>
<i>On exit: ymu[i – 1]</i> contains the upper limit of the confidence interval for the regression line at $\mathbf{x}[i – 1]$.		
11:	yl[n] – double	<i>Output</i>
<i>On exit: yl[i – 1]</i> contains the lower limit of the confidence interval for the individual y value at $\mathbf{x}[i – 1]$.		
12:	yu[n] – double	<i>Output</i>
<i>On exit: yu[i – 1]</i> contains the upper limit of the confidence interval for the individual y value at $\mathbf{x}[i – 1]$.		
13:	h[n] – double	<i>Output</i>
<i>On exit: h[i]</i> contains the leverage of each observation on the regression.		
14:	res[n] – double	<i>Output</i>
<i>On exit: res[i]</i> contains the residuals of the regression.		
15:	rms – double *	<i>Output</i>
<i>On exit: rms</i> contains the residual mean square about the regression.		
16:	fail – NagError *	<i>Input/Output</i>
The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).		

6 Error Indicators and Warnings

NE_BAD_PARAM

On entry, argument **mean** had an illegal value.

NE_INT_ARG_LT

On entry, **n** = $\langle \text{value} \rangle$.
 Constraint: if **mean** = Nag_AboutMean, **n** ≥ 2 .

On entry, **n** = $\langle \text{value} \rangle$.
 Constraint: if **mean** = Nag_AboutZero, **n** ≥ 1 .

NE_NEG_WEIGHT

On entry, at least one of the weights is negative.

NE_REAL_ARG_GE

On entry, **clm** must not be greater than or equal to 1.0: **clm** = $\langle \text{value} \rangle$.
 On entry, **clp** must not be greater than or equal to 1.0: **clp** = $\langle \text{value} \rangle$.

NE_REAL_ARG_LE

On entry, **clm** must not be less than or equal to 0.0: **clm** = $\langle \text{value} \rangle$.
 On entry, **clp** must not be less than or equal to 0.0: **clp** = $\langle \text{value} \rangle$.

NE_SW_LOW

On entry, the sum of elements of **wt** must be greater than 1.0 if **mean** = Nag_AboutZero and 2.0 if **mean** = Nag_AboutMean.

NE_WT_LOW

On entry, **wt** must contain at least 1 positive element if **mean** = Nag_AboutZero or at least 2 positive elements if **mean** = Nag_AboutMean.

NE_X_IDEN

On entry, all elements of **x** are equal.

NW_RMS_EQ_ZERO

Residual mean sum of squares is zero, i.e., a perfect fit was obtained.

7 Accuracy

The computations are believed to be stable.

8 Parallelism and Performance

`nag_regress_confid_interval` (g02cbc) is not threaded in any implementation.

9 Further Comments

None.

10 Example

A program to calculate the fitted value of y and the upper and lower limits of the confidence interval for the regression line as well as the individual y values.

10.1 Program Text

```
/* nag_regress_confid_interval (g02cbc) Example Program.
*
* NAGPRODCODE Version.
*
* Copyright 2016 Numerical Algorithms Group.
*
* Mark 26, 2016.
*/
#include <nag.h>
#include <stdio.h>
#include <nag_stdlb.h>
#include <nagg02.h>

int main(void)
{
    Integer exit_status = 0, i, n;
    double clm, clp;
    double *h = 0, *res = 0, rms, *wt = 0, *x = 0, *y = 0, *yhat = 0;
    double *yl = 0, *yml = 0, *ymu = 0, *yu = 0;
    char nag_enum_arg[40];
    Nag_SumSquare mean;
    Nag_Boolean weight;
    NagError fail;

    INIT_FAIL(fail);

    /* Input data: n = 3, x = [1, 2, 3], y = [1, 2, 3], wt = [1, 1, 1] */
    n = 3;
    x = (double *)malloc(n * sizeof(double));
    y = (double *)malloc(n * sizeof(double));
    wt = (double *)malloc(n * sizeof(double));
    for (i = 0; i < n; i++)
        x[i] = i + 1, y[i] = i + 1, wt[i] = 1.0;
    /* Call nag_regress_confid_interval to calculate fitted values and
       confidence intervals for the regression line. */
    res = nag_regress_confid_interval(n, x, y, h, clm, clp, rms, yhat, yl, yml, ymu, yu, wt, mean, weight, &fail);
    if (fail.code != NE_NOERROR)
        printf("NagError returned from nag_regress_confid_interval\n");
    else
        printf("Estimated parameters: mean = %f, clm = %f, clp = %f\n", mean, clm, clp);
        printf("Root mean square residual = %f\n", rms);
        printf("Fitted values: yhat = %f, lower limit = %f, middle limit = %f, upper limit = %f\n", yhat, yl, yml, yu);
    /* Free memory allocated for arrays x, y and wt. */
    free(x);
    free(y);
    free(wt);
}
```

```

printf("nag_regress_confid_interval (g02cbc) Example Program Results\n");
/* Skip heading in data file */
#ifndef _WIN32
scanf_s("%*[^\n]");
#else
scanf("%*[^\n]");
#endif
#ifndef _WIN32
scanf_s("%" NAG_IFMT "\n", &n);
#else
scanf("%" NAG_IFMT "\n", &n);
#endif
#ifndef _WIN32
scanf_s("%lf%lf\n", &clm, &clp);
#else
scanf("%lf%lf\n", &clm, &clp);
#endif
#ifndef _WIN32
scanf_s(" %39s", nag_enum_arg, (unsigned)_countof(nag_enum_arg));
#else
scanf(" %39s", nag_enum_arg);
#endif
/* nag_enum_name_to_value (x04nac).
 * Converts NAG enum member name to value
 */
mean = (Nag_SumSquare) nag_enum_name_to_value(nag_enum_arg);
#ifndef _WIN32
scanf_s(" %39s", nag_enum_arg, (unsigned)_countof(nag_enum_arg));
#else
scanf(" %39s", nag_enum_arg);
#endif
weight = (Nag_Boolean) nag_enum_name_to_value(nag_enum_arg);
if (n >= (mean == Nag_AboutMean ? 2 : 1)) {
    if (!(x = NAG_ALLOC(n, double)) ||
        !(y = NAG_ALLOC(n, double)) ||
        !(wt = NAG_ALLOC(n, double)) ||
        !(yhat = NAG_ALLOC(n, double)) ||
        !(yml = NAG_ALLOC(n, double)) ||
        !(ymu = NAG_ALLOC(n, double)) ||
        !(yl = NAG_ALLOC(n, double)) ||
        !(yu = NAG_ALLOC(n, double)) ||
        !(h = NAG_ALLOC(n, double)) || !(res = NAG_ALLOC(n, double)))
    )
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }
}
else {
    printf("Invalid n.\n");
    exit_status = 1;
    return exit_status;
}
if (weight)
    for (i = 0; i < n; i++)
#ifndef _WIN32
scanf_s("%lf%lf%lf\n", &x[i], &y[i], &wt[i]);
#else
scanf("%lf%lf%lf\n", &x[i], &y[i], &wt[i]);
#endif
else
    for (i = 0; i < n; ++i)
#ifndef _WIN32
scanf_s("%lf%lf\n", &x[i], &y[i]);
#else
scanf("%lf%lf\n", &x[i], &y[i]);
#endif
/* nag_regress_confid_interval (g02cbc).
 * Simple linear regression confidence intervals for the

```

```

* regression line and individual points
*/
nag_regress_confid_interval(mean, n, x, y, wt, clm, clp, yhat, yml, ymu, yl,
                            yu, h, res, &rms, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_regress_confid_interval (g02cbc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
}

printf("\ni      yhat[i]      yml[i]      ymu[i]      yl[i]      yu[i]"
      "\n\n");
for (i = 0; i < n; ++i) {
    printf("%" NAG_IFMT " %10.2f %10.2f", i, yhat[i], yml[i]);
    printf("%10.2f %10.2f %10.2f\n", ymu[i], yl[i], yu[i]);
}

END:
NAG_FREE(x);
NAG_FREE(y);
NAG_FREE(wt);
NAG_FREE(yhat);
NAG_FREE(yml);
NAG_FREE(ymu);
NAG_FREE(yl);
NAG_FREE(yu);
NAG_FREE(h);
NAG_FREE(res);

return exit_status;
}

```

10.2 Program Data

```

nag_regress_confid_interval (g02cbc) Example Program Data
9
0.95 0.95
Nag_AboutMean Nag_TRUE
1.0 4.0 1.0
2.0 4.0 2.0
4.0 5.1 1.0
2.0 4.0 1.0
2.0 6.0 1.0
3.0 5.2 1.0
7.0 9.1 1.0
4.0 2.0 1.0
2.0 4.1 1.0

```

10.3 Program Results

```

nag_regress_confid_interval (g02cbc) Example Program Results

```

i	yhat[i]	yml[i]	ymu[i]	yl[i]	yu[i]
0	3.47	1.76	5.18	-0.46	7.40
1	4.14	2.87	5.42	0.38	7.90
2	5.49	4.15	6.84	1.71	9.27
3	4.14	2.87	5.42	0.38	7.90
4	4.14	2.87	5.42	0.38	7.90
5	4.82	3.70	5.94	1.11	8.53
6	7.52	4.51	10.53	2.87	12.16
7	5.49	4.15	6.84	1.71	9.27
8	4.14	2.87	5.42	0.38	7.90
