NAG Library Function Document nag_glm_normal (g02gac)

1 Purpose

nag glm normal (g02gac) fits a generalized linear model with normal errors.

2 Specification

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

3 Description

A generalized linear model with Normal errors consists of the following elements:

(a) a set of n observations, y_i , from a Normal distribution with probability density function:

$$\frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right),\,$$

where μ is the mean and σ^2 is the variance.

- (b) X, a set of p independent variables for each observation, x_1, x_2, \ldots, x_p .
- (c) a linear model:

$$\eta = \sum \beta_j x_j.$$

(d)

a link between the linear predictor, η , and the mean of the distribution, μ , i.e., $\eta = g(\mu)$. The possible link functions are:

- (i) exponent link: $\eta = \mu^a$, for a constant a,
- (ii) identity link: $\eta = \mu$,
- (iii) log link: $\eta = \log \mu$,
- (iv) square root link: $\eta = \sqrt{\mu}$,
- (v) reciprocal link: $\eta = \frac{1}{\mu}$.
- (e) a measure of fit, the residual sum of squares $=\sum (y_i \hat{\mu}_i)^2$

The linear arguments are estimated by iterative weighted least squares. An adjusted dependent variable, z, is formed:

$$z = \eta + (y - \mu) \frac{d\eta}{d\mu}$$

and a working weight, w,

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$$w = \left(\frac{d\eta}{d\mu}\right)^2.$$

At each iteration an approximation to the estimate of β , $\hat{\beta}$, is found by the weighted least squares regression of z on X with weights w.

nag glm normal (g02gac) finds a QR decomposition of $w^{\frac{1}{2}}X$, i.e.,

 $w^{\frac{1}{2}}X=QR$ where R is a p by p triangular matrix and Q is a n by p column orthogonal matrix. If R is of full rank, then $\hat{\beta}$ is the solution to:

$$R\hat{\beta} = Q^{\mathrm{T}}w^{\frac{1}{2}}z$$

If R is not of full rank a solution is obtained by means of a singular value decomposition (SVD) of R.

$$R = Q_* \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} P^{\mathsf{T}},$$

where D is a k by k diagonal matrix with nonzero diagonal elements, k being the rank of R and $w^{\frac{1}{2}}X$. This gives the solution

$$\hat{\beta} = P_1 D^{-1} \begin{pmatrix} Q_* & 0 \\ 0 & I \end{pmatrix} Q^{\mathsf{T}} w^{\frac{1}{2}} z$$

 P_1 being the first k columns of P, i.e., $P = (P_1 P_0)$.

The iterations are continued until there is only a small change in the residual sum of squares.

The initial values for the algorithm are obtained by taking

$$\hat{\eta} = q(y)$$

The fit of the model can be assessed by examining and testing the residual sum of squares, in particular comparing the difference in residual sums of squares between nested models, i.e., when one model is a sub-model of the other.

Let RSS_f be the residual sum of squares for the full model with degrees of freedom ν_f and let RSS_s be the residual sum of squares for the sub-model with degrees of freedom ν_s then:

$$F = \frac{\left(RSS_s - RSS_f\right)/\left(\nu_s - \nu_f\right)}{RSS_f/\nu_f},$$

has, approximately, a F-distribution with $(\nu_s - \nu_f)$, ν_f degrees of freedom.

The parameter estimates, $\hat{\beta}$, are asymptotically Normally distributed with variance-covariance matrix:

$$C = R^{-1}R^{-1^{T}}$$
 in the full rank case, otherwise

$$C = P_1 D^{-2} P_1^{\mathrm{T}}$$

The residuals and influence statistics can also be examined.

The estimated linear predictor $\hat{\eta} = X\hat{\beta}$, can be written as $Hw^{\frac{1}{2}}z$ for an n by n matrix H. The ith diagonal elements of H, h_i , give a measure of the influence of the ith values of the independent variables on the fitted regression model. These are sometimes known as leverages.

The fitted values are given by $\hat{\mu} = g^{-1}(\hat{\eta})$.

nag glm normal (g02gac) also computes the residuals, r:

$$r_i = y_i - \hat{\mu}_i$$

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Input

An option allows prior weights, ω_i to be used, this gives a model with:

$$\sigma_i^2 = \frac{\sigma^2}{\omega_i}.$$

In many linear regression models the first term is taken as a mean term or an intercept, i.e., $x_{i,1} = 1$, for $i = 1, 2, \dots, n$; this is provided as an option.

Often only some of the possible independent variables are included in a model, the facility to select variables to be included in the model is provided.

If part of the linear predictor can be represented by a variable with a known coefficient, then this can be included in the model by using an offset, o:

$$\eta = o + \sum \beta_j x_j.$$

If the model is not of full rank the solution given will be only one of the possible solutions. Other estimates be may be obtained by applying constraints to the arguments. These solutions can be obtained by using nag glm tran model (g02gkc) after using nag glm normal (g02gac). Only certain linear combinations of the arguments will have unique estimates; these are known as estimable functions and can be estimated and tested using nag glm est func (g02gnc).

Details of the SVD, are made available, in the form of the matrix P^* :

$$P^* = \begin{pmatrix} D^{-1}P_1^{\mathsf{T}} \\ P_0^{\mathsf{T}} \end{pmatrix}.$$

4 References

Cook R D and Weisberg S (1982) Residuals and Influence in Regression Chapman and Hall McCullagh P and Nelder J A (1983) Generalized Linear Models Chapman and Hall

5 **Arguments**

link - Nag Link 1:

Input

On entry: indicates which link function is to be used.

 $link = Nag_Expo$

An exponent link is used.

link = Nag_Iden

An identity link is used. You are advised not to use nag glm normal (g02gac) with an identity link as nag regsn mult linear (g02dac) provides a more efficient way of fitting such a model.

 $link = Nag_Log$

A log link is used.

 $link = Nag_Sqrt$

A square root link is used.

link = Nag_Reci

A reciprocal link is used.

Constraint: link = Nag_Expo, Nag_Iden, Nag_Log, Nag_Sqrt or Nag_Reci.

2: mean - Nag IncludeMean

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

mean = Nag_MeanInclude

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

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 $mean = Nag_MeanZero$

The model will pass through the origin, zero point.

Constraint: **mean** = Nag_MeanInclude or Nag_MeanZero.

3: \mathbf{n} - Integer Input

On entry: the number of observations, n.

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

4: $\mathbf{x}[\mathbf{n} \times \mathbf{tdx}] - \text{const double}$

Input

On entry: $\mathbf{x}[(i-1) \times \mathbf{tdx} + j - 1]$ must contain the *i*th observation for the *j*th independent variable, for i = 1, 2, ..., n and $j = 1, 2, ..., \mathbf{m}$.

5: tdx – Integer Input

On entry: the stride separating matrix column elements in the array \mathbf{x} .

Constraint: $tdx \ge m$.

6: \mathbf{m} - Integer Input

On entry: the total number of independent variables.

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

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

Input

On entry: indicates which independent variables are to be included in the model. If $\mathbf{sx}[j-1] > 0$, then the variable contained in the *j*th column of \mathbf{x} is included in the regression model.

Constraints:

```
\mathbf{sx}[j-1] \ge 0, for j=1,2,\ldots,\mathbf{m}; if \mathbf{mean} = \text{Nag\_MeanInclude}, then exactly \mathbf{ip} - 1 values of \mathbf{sx} must be > 0; if \mathbf{mean} = \text{Nag\_MeanZero}, then exactly \mathbf{ip} values of \mathbf{sx} must be > 0.
```

8: \mathbf{ip} - Integer Input

On entry: the number p of independent variables in the model, including the mean or intercept if present.

Constraint: ip > 0.

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

Input

On entry: observations on the dependent variable, y_i , for i = 1, 2, ..., n.

10: $\mathbf{wt}[\mathbf{n}]$ – const double

Input

On entry: if weighted estimates are required, then wt must contain the weights to be used. Otherwise wt need not be defined and may be set to NULL.

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 positive weights.

If wt is NULL, then the effective number of observations is n.

Constraint: wt is NULL or wt $[i-1] \ge 0.0$, for i = 1, 2, ..., n.

11: offset[n] - const double

Input

On entry: if an offset is required then **offset** must contain the values of the offset o. Otherwise **offset** must be supplied as **NULL**.

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12: **scale** – double *

Input/Output

On entry: indicates the scale argument for the model, σ^2 . If **scale** = 0.0, then the scale argument is estimated using the residual mean square.

On exit: if on input scale = 0.0, then scale contains the estimated value of the scale argument, $\hat{\sigma}^2$. If on input scale \neq 0.0, then scale is unchanged on exit.

Constraint: scale ≥ 0.0 .

13: **ex_power** – double

Input

On entry: if link = Nag. Expo then ex power must contain the power a of the exponential.

If $link \neq Nag$. Expo, ex power is not referenced.

Constraint: If $link = Nag_Expo$, $ex_power \neq 0.0$.

14: **rss** – double *

Output

On exit: the residual sum of squares for the fitted model.

15: **df** – double *

Output

On exit: the degrees of freedom associated with the residual sum of squares for the fitted model.

16: **b**[**ip**] – double

Output

On exit: $\mathbf{b}[i-1]$, $i=1,2,\ldots,\mathbf{ip}$ contains the estimates of the arguments of the generalized linear model, $\hat{\beta}$.

If **mean** = Nag_MeanInclude, then $\mathbf{b}[0]$ will contain the estimate of the mean argument and $\mathbf{b}[i]$ will contain the coefficient of the variable contained in column j of \mathbf{x} , where $\mathbf{s}\mathbf{x}[j-1]$ is the ith positive value in the array $\mathbf{s}\mathbf{x}$.

If **mean** = Nag_MeanZero, then $\mathbf{b}[i-1]$ will contain the coefficient of the variable contained in column j of \mathbf{x} , where $\mathbf{sx}[j-1]$ is the ith positive value in the array \mathbf{sx} .

17: rank – Integer *

Output

On exit: the rank of the independent variables.

If the model is of full rank, then rank = ip.

If the model is not of full rank, then \mathbf{rank} is an estimate of the rank of the independent variables. \mathbf{rank} is calculated as the number of singular values greater than $\mathbf{eps} \times$ (largest singular value). It is possible for the SVD to be carried out but \mathbf{rank} to be returned as \mathbf{ip} .

18: $\mathbf{se}[\mathbf{ip}]$ – double

Output

On exit: the standard errors of the linear arguments.

 $\mathbf{se}[i-1]$ contains the standard error of the parameter estimate in $\mathbf{b}[i-1]$, for $i=1,2,\ldots,\mathbf{ip}$.

19: $\operatorname{cov}[\operatorname{ip} \times (\operatorname{ip} + 1)/2] - \operatorname{double}$

Output

On exit: the $i\mathbf{p} \times (i\mathbf{p}+1)/2$ elements of \mathbf{cov} contain the upper triangular part of the variance-covariance matrix of the $i\mathbf{p}$ parameter estimates given in \mathbf{b} . They are stored packed by column, i.e., the covariance between the parameter estimate given in $\mathbf{b}[i]$ and the parameter estimate given in $\mathbf{b}[j]$, $j \ge i$, is stored in $\mathbf{cov}[j(j+1)/2+i]$, for $i=0,1,\ldots,i\mathbf{p}-1$ and $j=i,\ldots,i\mathbf{p}-1$.

20: $\mathbf{v}[\mathbf{n} \times \mathbf{tdv}] - \text{double}$

Output

On exit: auxiliary information on the fitted model.

 $\mathbf{v}[(i-1) \times \mathbf{tdv}]$, contains the linear predictor value, η_i , for $i = 1, 2, \dots, n$.

 $\mathbf{v}[(i-1) \times \mathbf{tdv} + 1]$, contains the fitted value, $\hat{\mu}_i$, for $i = 1, 2, \dots, n$.

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 $\mathbf{v}[(i-1) \times \mathbf{tdv} + 2]$, is only included for consistency with other functions. $\mathbf{v}[(i-1) \times \mathbf{tdv} + 2] = 1.0$, for $i = 1, 2, \dots, n$.

 $\mathbf{v}[(i-1) \times \mathbf{tdv} + 3]$, contains the working weight, w_i , for $i = 1, 2, \dots, n$.

 $\mathbf{v}[(i-1) \times \mathbf{tdv} + 4]$, contains the standardized residual, r_i , for $i = 1, 2, \dots, n$.

 $\mathbf{v}[(i-1) \times \mathbf{tdv} + 5]$, contains the leverage, h_i , for $i = 1, 2, \dots, n$.

 $\mathbf{v}[(i-1) \times \mathbf{tdv} + j - 1]$, for $j = 7, 8, \dots, \mathbf{ip} + 6$, contains the results of the QR decomposition or the singular value decomposition.

If the model is not of full rank, i.e., rank < ip, then the first ip rows of columns 7 to ip + 6 contain the P^* matrix.

21: **tdv** – Integer Input

On entry: the stride separating matrix column elements in the array v.

Constraint: $\mathbf{tdv} > \mathbf{ip} + 6$.

22: **tol** – double *Input*

On entry: indicates the accuracy required for the fit of the model.

The iterative weighted least squares procedure is deemed to have converged if the absolute change in deviance between interactions is less than $tol \times (1.0+current residual sum of squares)$. This is approximately an absolute precision if the residual sum of squares is small and a relative precision if the residual sum of squares is large.

If $0.0 \le \text{tol} < \text{machine precision}$, then the function will use $10 \times \text{machine precision}$.

Constraint: tol > 0.0.

23: max_iter - Integer Input

On entry: the maximum number of iterations for the iterative weighted least squares. If $max_iter = 0$, then a default value of 10 is used.

Constraint: \max_{\cdot} iter ≥ 0 .

24: **print_iter** – Integer Input

On entry: indicates if the printing of information on the iterations is required and the rate at which printing is produced. The following values are available:

 $print_iter \le 0$

There is no printing.

print_iter > 0

The following items are printed every **print iter** iterations:

- (i) the deviance,
- (ii) the current estimates, and
- (iii) if the weighted least squares equations are singular then this is indicated.

25: **outfile** – const char *

Input

On entry: a null terminated character string giving the name of the file to which results should be printed. If **outfile** is **NULL** or an empty string then the stdout stream is used. Note that the file will be opened in the append mode.

26: **eps** – double *Input*

On entry: the value of **eps** is used to decide if the independent variables are of full rank and, if not, what the rank of the independent variables is. The smaller the value of **eps** the stricter the criterion for selecting the singular value decomposition.

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If $0.0 \le eps < machine precision$, then the function will use machine precision instead.

Constraint: $eps \ge 0.0$.

27: **fail** – NagError *

Input/Output

The NAG error argument (see Section 3.6 in the Essential Introduction).

6 Error Indicators and Warnings

NE 2 INT ARG LT

```
On entry, \mathbf{tdv} = \langle value \rangle while \mathbf{ip} = \langle value \rangle. These arguments must satisfy \mathbf{tdv} \geq \mathbf{ip} + 6. On entry, \mathbf{tdx} = \langle value \rangle while \mathbf{m} = \langle value \rangle. These arguments must satisfy \mathbf{tdx} \geq \mathbf{m}.
```

NE ALLOC FAIL

Dynamic memory allocation failed.

NE BAD PARAM

On entry, argument link had an illegal value.

On entry, argument mean had an illegal value.

NE_INT_ARG_LT

```
On entry, \mathbf{ip} = \langle value \rangle.

Constraint: \mathbf{ip} \geq 1.

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

Constraint: \mathbf{m} \geq 1.

On entry, \mathbf{max\_iter} must not be less than 0: \mathbf{max\_iter} = \langle value \rangle.

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

Constraint: \mathbf{n} \geq 2.

On entry, \mathbf{sx}[\langle value \rangle] must not be less than 0: \mathbf{sx}[\langle value \rangle] = \langle value \rangle.
```

NE IP GT OBSERV

Argument **ip** is greater than the effective number of observations.

NE IP INCOMP SX

Argument **ip** is incompatible with arguments **mean** and **sx**.

NE_LSQ_ITER_NOT_CONV

The iterative weighted least squares has failed to converge in $max_iter = \langle value \rangle$ iterations. The value of max_iter could be increased but it may be advantageous to examine the convergence using the **print_iter** option. This may indicate that the convergence is slow because the solution is at a boundary in which case it may be better to reformulate the model.

NE NOT APPEND FILE

Cannot open file $\langle string \rangle$ for appending.

NE NOT CLOSE FILE

Cannot close file $\langle string \rangle$.

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NE RANK CHANGED

The rank of the model has changed during the weighted least squares iterations. The estimate for β returned may be reasonable, but you should check how the deviance has changed during iterations.

NE REAL ARG LT

On entry, **eps** must not be less than 0.0: **eps** = $\langle value \rangle$.

On entry, scale must not be less than 0.0: scale = $\langle value \rangle$.

On entry, **tol** must not be less than 0.0: **tol** = $\langle value \rangle$.

On entry, $\mathbf{wt}[\langle value \rangle]$ must not be less than 0.0: $\mathbf{wt}[\langle value \rangle] = \langle value \rangle$.

NE_REAL_ENUM_ARG_CONS

On entry, $ex_power = 0.0$, $link = Nag_Expo$. These arguments must satisfy $link = Nag_Expo$ and $ex_power \neq 0.0$.

NE SVD NOT CONV

The singular value decomposition has failed to converge.

NE VALUE AT BOUNDARY A

A fitted value is at a boundary. This will only occur with $link = Nag_Expo$, Nag_Log or Nag_Reci . This may occur if there are small values of y and the model is not suitable for the data. The model should be reformulated with, perhaps, some observations dropped.

NE ZERO DOF ERROR

The degrees of freedom for error are 0. A saturated model has been fitted.

7 Accuracy

The accuracy is determined by **tol** as described in Section 5. As the residual sum of squares is a function of μ^2 the accuracy of the $\hat{\beta}$'s will depend on the link used and may be of the order $\sqrt{\text{tol}}$.

8 Parallelism and Performance

Not applicable.

9 Further Comments

None.

10 Example

The model:

$$y = \frac{1}{\beta_1 + \beta_2 x} + \epsilon$$

for a sample of five observations.

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10.1 Program Text

```
/* nag_glm_normal (g02gac) Example Program.
* Copyright 1996 Numerical Algorithms Group.
* Mark 4, 1996.
* Mark 8 revised, 2004.
 */
#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <ctype.h>
#include <nagg02.h>
\#define X(I, J) \times [(I) *tdx + J]
\#define\ V(I,\ J)\ v[(I)\ *tdv\ +\ J]
int main(void)
                   exit_status = 0, i, ip, j, m, max_iter, n, print_iter, rank;
  Integer
                   *sx = 0;
  Integer
                   tdv, tdx;
  Integer
 Nag_IncludeMean mean;
  Nag_Link
                   link;
  Nag_Boolean
                   weight;
  char
                   nag_enum_arg[40];
                   df, eps, ex_power, rss, scale, tol;
*b = 0, *cov = 0, *offsetptr = 0, *se = 0, *v = 0, *wt = 0;
  double
  double
                   *wtptr, *x = 0, *y = 0;
  double
  NagError
                   fail;
  INIT_FAIL(fail);
  printf("nag_glm_normal (g02gac) Example Program Results\n");
  /* Skip heading in data file */
  scanf("%*[^\n]");
  scanf("%39s", nag_enum_arg);
  /* nag_enum_name_to_value (x04nac).
   * Converts NAG enum member name to value
  * /
  link = (Nag_Link) nag_enum_name_to_value(nag_enum_arg);
  scanf("%39s", nag_enum_arg);
  mean = (Nag_IncludeMean) nag_enum_name_to_value(nag_enum_arg);
  scanf("%39s", nag_enum_arg);
  weight = (Nag_Boolean) nag_enum_name_to_value(nag_enum_arg);
scanf("%ld %ld %ld %lf", &n, &m, &print_iter,
         &scale);
  if (n \ge 2 \&\& m \ge 1)
      if (!(wt = NAG_ALLOC(n, double)) ||
           !(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;
      tdx = m;
    }
  else
    {
      printf("Invalid n or m.\n");
      exit_status = 1;
      return exit_status;
  if (weight)
```

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```
wtptr = wt;
    for (i = 0; i < n; i++)
        for (j = 0; j < m; j++)
  scanf("%lf", &X(i, j));
scanf("%lf%lf", &y[i], &wt[i]);</pre>
  }
else
  {
    wtptr = (double *) 0;
    for (i = 0; i < n; i++)
        for (j = 0; j < m; j++)
  scanf("%lf", &X(i, j));</pre>
        scanf("%lf", &y[i]);
for (j = 0; j < m; j++)
  scanf("%ld", &sx[j]);
/* Calculate ip */
ip = 0;
for (j = 0; j < m; j++)
  if (sx[j] > 0) ip += 1;
if (mean == Nag_MeanInclude)
  ip += 1;
if (link == Nag_Expo)
 scanf("%lf", &ex_power);
else
 ex_power = 0.0;
if (!(b = NAG_ALLOC(ip, double)) ||
    !(v = NAG\_ALLOC(n*(ip+6), double)) | |
    !(se = NAG_ALLOC(ip, double)) ||
    !(cov = NAG\_ALLOC(ip*(ip+1)/2, double)))
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
tdv = ip+6;
/* Set other control parameters */
max_iter = 10;
tol = 5e-5;
eps = 1e-6;
/* nag_glm_normal (g02gac).
* Fits a generalized linear model with Normal errors
print_iter, "", eps, &fail);
if (fail.code == NE_NOERROR || fail.code == NE_LSQ_ITER_NOT_CONV ||
    fail.code == NE_RANK_CHANGED || fail.code == NE_ZERO_DOF_ERROR)
    if (fail.code != NE_NOERROR) {
      printf("Error from nag_glm_normal (g02gac).\n%s\n",
              fail.message);
    printf("\nResidual sum of squares = %13.4e\n", rss);
    printf("Degrees of freedom = %3.1f\n\n", df);
    printf("
                 Estimate
                                Standard error\n\n");
    for (i = 0; i < ip; i++)
      printf("%14.4f%\bar{1}4.4f\n", b[i], se[i]);
    printf("\n");
```

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```
y fitted value Residual Leverage\n\n");
      printf("
      for (i = 0; i < n; ++i)
          printf("%7.1f%10.2f%12.4f%10.3f\n", y[i], V(i, 1), V(i, 4),
                  V(i, 5));
 else
      printf("Error from nag_glm_normal (g02gac).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
END:
 NAG_FREE(wt);
 NAG_FREE(x);
NAG_FREE(y);
 NAG_FREE(sx);
 NAG_FREE(b);
 NAG_FREE(v);
 NAG_FREE(se);
 NAG_FREE(cov);
 return exit_status;
}
```

10.2 Program Data

```
nag_glm_normal (g02gac) Example Program Data
Nag_Reci Nag_MeanInclude Nag_FALSE 5 1 0 0.0
1.0 25.0
2.0 10.0
3.0 6.0
4.0 4.0
5.0 3.0
```

10.3 Program Results

4.0

3.0

4.32

3.39

```
nag_glm_normal (g02gac) Example Program Results
Residual sum of squares =
                            3.8717e-01
Degrees of freedom = 3.0
       Estimate
                    Standard error
       -0.0239
                      0.0028
                     0.0026
        0.0638
       fitted value Residual
                                 Leverage
   25.0
            25.04
                     -0.0387
                                  0.995
   10.0
             9.64
                                  0.458
                      0.3613
    6.0
             5.97
                      0.0320
                                  0.268
```

-0.3221

-0.3878

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0.167

0.112