

## nag\_mv\_discrim (g03dac)

### 1. Purpose

**nag\_mv\_discrim (g03dac)** computes a test statistic for the equality of within-group covariance matrices and also computes matrices for use in discriminant analysis.

### 2. Specification

```
#include <nag.h>
#include <nagg03.h>

void nag_mv_discrim(Integer n, Integer m, double x[],
                   Integer tdx, Integer isx[], Integer nvar, Integer ing[],
                   Integer ng, double wt[], Integer nig[], double gmean[],
                   Integer tdg, double det[], double gc[], double *stat,
                   double *df, double *sig, NagError *fail)
```

### 3. Description

Let a sample of  $n$  observations on  $p$  variables come from  $n_g$  groups with  $n_j$  observations in the  $j$ th group and  $\sum n_j = n$ . If the data is assumed to follow a multivariate Normal distribution with the variance-covariance matrix of the  $j$ th group  $\Sigma_j$ , then to test for equality of the variance-covariance matrices between groups, that is,  $\Sigma_1 = \Sigma_2 = \dots = \Sigma_{n_g} = \Sigma$ , the following likelihood-ratio test statistic,  $G$ , can be used;

$$G = C \left\{ (n - n_g) \log |S| - \sum_{j=1}^{n_g} (n_j - 1) \log |S_j| \right\},$$

where

$$C = 1 - \frac{2p^2 + 3p - 1}{6(p+1)(n_g - 1)} \left( \sum_{j=1}^{n_g} \frac{1}{(n_j - 1)} - \frac{1}{(n - n_g)} \right),$$

and  $S_j$  are the within-group variance-covariance matrices and  $S$  is the pooled variance-covariance matrix given by

$$S = \frac{\sum_{j=1}^{n_g} (n_j - 1) S_j}{(n - n_g)}.$$

For large  $n$ ,  $G$  is approximately distributed as a  $\chi^2$  variable with  $\frac{1}{2}p(p+1)(n_g - 1)$  degrees of freedom, see Morrison (1967) for further comments. If weights are used, then  $S$  and  $S_j$  are the weighted pooled and within-group variance-covariance matrices and  $n$  is the effective number of observations, that is, the sum of the weights.

Instead of calculating the within-group variance-covariance matrices and then computing their determinants in order to calculate the test statistic, **nag\_mv\_discrim** uses a  $QR$  decomposition. The group means are subtracted from the data and then for each group, a  $QR$  decomposition is computed to give an upper triangular matrix  $R_j^*$ . This matrix can be scaled to give a matrix  $R_j$  such that  $S_j = R_j^T R_j$ . The pooled  $R$  matrix is then computed from the  $R_j$  matrices. The values of  $|S|$  and the  $|S_j|$  can then be calculated from the diagonal elements of  $R$  and the  $R_j$ .

This approach means that the Mahalanobis squared distances for a vector observation  $x$  can be computed as  $z^T z$ , where  $R_j z = (x - \bar{x}_j)$ ,  $\bar{x}_j$  being the vector of means of the  $j$ th group. These distances can be calculated by **nag\_mv\_discrim\_mahaldist** (g03dbc). The distances are used in discriminant analysis and **nag\_mv\_discrim\_group** (g03dcc) uses the results of **nag\_mv\_discrim** to perform several different types of discriminant analysis. The differences between the discriminant methods are, in part, due to whether or not the within-group variance-covariance matrices are equal.

## 4. Parameters

**n**Input: the number of observations,  $n$ .Constraint:  $n \geq 1$ .**m**Input: the number of variables in the data array  $\mathbf{x}$ .Constraint:  $m \geq \mathbf{nvar}$ .**x[n][tdx]**Input:  $\mathbf{x}[k-1][l-1]$  must contain the  $k$ th observation for the  $l$ th variable, for  $k = 1, 2, \dots, n$ ;  $l = 1, 2, \dots, m$ .**tdx**Input: the last dimension of the array  $\mathbf{x}$  as declared in the calling program.Constraint:  $\mathbf{tdx} \geq m$ .**isx[m]**Input:  $\mathbf{isx}[l-1]$  indicates whether or not the  $l$ th variable in  $\mathbf{x}$  is to be included in the variance-covariance matrices.If  $\mathbf{isx}[l-1] > 0$  the  $l$ th variable is included, for  $l = 1, 2, \dots, m$ ; otherwise it is not referenced.Constraint:  $\mathbf{isx}[l-1] > 0$  for  $\mathbf{nvar}$  values of  $l$ .**nvar**Input: the number of variables in the variance-covariance matrices,  $p$ .Constraint:  $\mathbf{nvar} \geq 1$ .**ing[n]**Input:  $\mathbf{ing}[k-1]$  indicates to which group the  $k$ th observation belongs, for  $k = 1, 2, \dots, n$ .Constraint:  $1 \leq \mathbf{ing}[k-1] \leq \mathbf{ng}$  for  $k = 1, 2, \dots, n$  and the values of  $\mathbf{ing}$  must be such that each group has at least  $\mathbf{nvar}$  members.**ng**Input: the number of groups,  $n_g$ .Constraint:  $\mathbf{ng} \geq 2$ .**wt[n]**Input: the elements of  $\mathbf{wt}$  must contain the weights to be used in the analysis and the effective number of observations for a group is the sum of the weights of the observations in that group. If  $\mathbf{wt}[k-1] = 0.0$  then the  $k$ th observation is excluded from the calculations.Constraint:  $\mathbf{wt}[k-1] \geq 0.0$  for  $k = 1, 2, \dots, n$  and the effective number of observations for each group must be greater than 1.Note: If  $\mathbf{wt}$  is set to the null pointer **NULL**, i.e., (double \*)0, then  $\mathbf{wt}$  is not referenced and the effective number of observations for a group is the number of observations in that group.**nig[ng]**Output:  $\mathbf{nig}[j-1]$  contains the number of observations in the  $j$ th group, for  $j = 1, 2, \dots, n_g$ .**gmean[ng][tdg]**Output: the  $j$ th row of  $\mathbf{gmean}$  contains the means of the  $p$  selected variables for the  $j$ th group, for  $j = 1, 2, \dots, n_g$ .**tdg**Input: the last dimension of the array  $\mathbf{gmean}$  as declared in the calling program.Constraint:  $\mathbf{tdg} \geq \mathbf{nvar}$ .**det[ng]**

Output: the logarithm of the determinants of the within-group variance-covariance matrices.

**gc**[(ng+1)\*nvar\*(nvar+1)/2]

Output: the first  $p(p+1)/2$  elements of **gc** contain  $R$  and the remaining  $n_g$  blocks of  $p(p+1)/2$  elements contain the  $R_j$  matrices. All are stored in packed form by columns.

**stat**

Output: the likelihood-ratio test static,  $G$ .

**df**

Output: the degrees of freedom for the distribution of  $G$ .

**sig**

Output: the significance level for  $G$ .

**fail**

The NAG error parameter, see the Essential Introduction to the NAG C Library.

## 5. Error Indications and Warnings

### NE\_INT\_ARG\_LT

On entry, **n** must not be less than 1: **n** =  $\langle value \rangle$ .

On entry, **nvar** must not be less than 1: **nvar** =  $\langle value \rangle$ .

On entry, **ng** must not be less than 2: **ng** =  $\langle value \rangle$ .

### NE\_2\_INT\_ARG\_LT

On entry, **m** =  $\langle value \rangle$  while **nvar** =  $\langle value \rangle$ .

These parameters must satisfy **m**  $\geq$  **nvar**.

On entry, **tdx** =  $\langle value \rangle$  while **m** =  $\langle value \rangle$ .

These parameters must satisfy **tdx**  $\geq$  **m**.

On entry, **tdg** =  $\langle value \rangle$  while **nvar** =  $\langle value \rangle$ .

These parameters must satisfy **tdg**  $\geq$  **nvar**.

### NE\_INTARR\_INT

On entry, **ing**[ $\langle value \rangle$ ] =  $\langle value \rangle$ , **ng** =  $\langle value \rangle$ .

Constraint:  $1 \leq \mathbf{ing}[i - 1] \leq \mathbf{ng}$ ,  $i = 1, 2, \dots, n$ .

### NE\_NEG\_WEIGHT\_ELEMENT

On entry, **wt**[ $\langle value \rangle$ ] =  $\langle value \rangle$ .

Constraint: when referenced, all elements of **wt** must be non-negative.

### NE\_VAR\_INCL\_INDICATED

The number of variables, **nvar** in the analysis =  $\langle value \rangle$ , while number of variables included in the analysis via array **isx** =  $\langle value \rangle$ .

Constraint: these two numbers must be the same.

### NE\_GROUP\_OBSERV

On entry, group  $\langle value \rangle$  has  $\langle value \rangle$  effective observations.

Constraint: in each group the effective number of observations must be  $\geq 1$ .

### NE\_GROUP\_VAR

On entry, group  $\langle value \rangle$  has  $\langle value \rangle$  members, while **nvar** =  $\langle value \rangle$ .

Constraint: number of members in each group  $\geq$  **nvar**

### NE\_GROUP\_VAR\_RANK

The variables in group  $\langle value \rangle$  are not of full rank.

### NE\_VAR\_RANK

The variables are not of full rank.

### NE\_ALLOC\_FAIL

Memory allocation failed.

### 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 consult NAG for assistance.

## 6. Further Comments

The time will be approximately proportional to  $np^2$ .

### 6.1. Accuracy

The accuracy is dependent on the accuracy of the computation of the  $QR$  decomposition. See nag\_real\_qr (f01qcc) for further details.

### 6.2. References

Aitchison J and Dunsmore I R (1975) *Statistical Prediction Analysis* Cambridge.

Kendall M G and Stuart A (1976) *The Advanced Theory of Statistics (Volume 3)* Griffin (3rd Edition).

Krzanowski W J (1990) *Principles of Multivariate Analysis* Oxford University Press.

Morrison D F (1967) *Multivariate Statistical Methods* McGraw-Hill.

## 7. See Also

nag\_mv\_discrim\_mahaldist (g03dbc)

nag\_mv\_discrim\_group (g03dcc)

nag\_real\_qr (f01qcc)

## 8. Example

The data, taken from Aitchison and Dunsmore (1975), is concerned with the diagnosis of three 'types' of Cushing's syndrome. The variables are the logarithms of the urinary excretion rates (mg/24hr) of two steroid metabolites. Observations for a total of 21 patients are input and the statistics computed by nag\_mv\_discrim (g03dac). The printed results show that there is evidence that the within-group variance-covariance matrices are not equal.

### 8.1. Program Text

```

/* nag_mv_discrim (g03dac) Example Program.
 *
 * Copyright 1998 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 *
 */
#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nagg03.h>

#define NMAX 21
#define MMAX 2
#define GPMAX 3

main()
{
    double stat;
    double det[GPMAX], gc[(GPMAX+1)*MMAX*(MMAX+1)/2],
    gmean[GPMAX][MMAX], wt[NMAX],
    x[NMAX][MMAX];
    double df;
    double *wtptr = 0;
    double sig;

    Integer nvar;
    Integer i, j, m, n;
    Integer ing[NMAX], isx[MMAX], nig[GPMAX];
    Integer ng;
    Integer tdgmean=MMAX, tdx= MMAX;

    char weight[2];

    Vprintf("g03dac Example Program Results\n\n");

```

```

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

Vscanf("%ld",&n);
Vscanf("%ld",&m);
Vscanf("%ld",&nvar);
Vscanf("%ld",&ng);
Vscanf("%s",weight);
if (n <= NMAX && m <= MMAX)
{
    if (*weight == 'W')
    {
        for (i = 0; i < n; ++i)
        {
            for (j = 0; j < m; ++j)
                Vscanf("%lf",&x[i][j]);
            Vscanf("%ld",&ing[i]);
            Vscanf("%lf",&wt[i]);
        }
        wtptr = wt;
    }
    else
    {
        for (i = 0; i < n; ++i)
        {
            for (j = 0; j < m; ++j)
                Vscanf("%lf",&x[i][j]);
            Vscanf("%ld",&ing[i]);
        }
    }
    for (j = 0; j < m; ++j)
        Vscanf("%ld",&isx[j]);

    g03dac(n, m, (double *)x, tdx, isx, nvar, ing, ng, wtptr, nig,
           (double *)gmean, tdgmean, det, gc, &stat, &df, &sig, NAGERR_DEFAULT);

    Vprintf("\\nGroup means\\n\\n");
    for (i = 0; i < ng; ++i)
    {
        for (j = 0; j < nvar; ++j)
            Vprintf("%10.4f",gmean[i][j]);
        Vprintf("\\n");
    }
    Vprintf("\\nLOG of determinants\\n\\n");
    for (j = 0; j < ng; ++j)
        Vprintf("%10.4f",det[j]);
    Vprintf("\\n\\n%s%7.4f\\n","stat = ",stat);
    Vprintf("%s%7.4f\\n"," df = ",df);
    Vprintf("%s%7.4f\\n"," sig = ",sig);
    exit(EXIT_SUCCESS);
}
else
{
    Vprintf("Incorrect input value of n or m.\\n");
    exit(EXIT_FAILURE);
}
}

```

8.2. Program Data

```
g03dac Example Program Data
21 2 2 3 U
1.1314 2.4596 1
1.0986 0.2624 1
0.6419 -2.3026 1
1.3350 -3.2189 1
1.4110 0.0953 1
0.6419 -0.9163 1
2.1163 0.0000 2
1.3350 -1.6094 2
1.3610 -0.5108 2
2.0541 0.1823 2
2.2083 -0.5108 2
2.7344 1.2809 2
2.0412 0.4700 2
1.8718 -0.9163 2
1.7405 -0.9163 2
2.6101 0.4700 2
2.3224 1.8563 3
2.2192 2.0669 3
2.2618 1.1314 3
3.9853 0.9163 3
2.7600 2.0281 3
1 1
```

8.3. Program Results

```
g03dac Example Program Results

Group means
1.0433 -0.6034
2.0073 -0.2060
2.7097 1.5998

LOG of determinants
-0.8273 -3.0460 -2.2877

stat = 19.2410
df = 6.0000
sig = 0.0038
```

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