

NAG Library Routine Document

G03ACF

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details.

1 Purpose

G03ACF performs a canonical variate (canonical discrimination) analysis.

2 Specification

```
SUBROUTINE G03ACF (WEIGHT, N, M, X, LDX, ISX, NX, ING, NG, WT, NIG, CVM,      &
                   LDCVM, E, LDE, NCV, CVX, LDCVX, TOL, IRANKX, WK, IWK,      &
                   IFAIL)
INTEGER              N, M, LDX, ISX(M), NX, ING(N), NG, NIG(NG), LDCVM,      &
                   LDE, NCV, LDCVX, IRANKX, IWK, IFAIL
REAL (KIND=nag_wp)  X(LDX,M), WT(*), CVM(LDCVM,NX), E(LDE,6),              &
                   CVX(LDCVX,NG-1), TOL, WK(IWK)
CHARACTER(1)        WEIGHT
```

3 Description

Let a sample of n observations on n_x variables in a data matrix come from n_g groups with n_1, n_2, \dots, n_{n_g} observations in each group, $\sum n_i = n$. Canonical variate analysis finds the linear combination of the n_x variables that maximizes the ratio of between-group to within-group variation. The variables formed, the canonical variates can then be used to discriminate between groups.

The canonical variates can be calculated from the eigenvectors of the within-group sums of squares and cross-products matrix. However, G03ACF calculates the canonical variates by means of a singular value decomposition (SVD) of a matrix V . Let the data matrix with variable (column) means subtracted be X , and let its rank be k ; then the k by $(n_g - 1)$ matrix V is given by:

$$V = Q_X^T Q_g,$$

where Q_g is an n by $(n_g - 1)$ orthogonal matrix that defines the groups and Q_X is the first k rows of the orthogonal matrix Q either from the QR decomposition of X :

$$X = QR$$

if X is of full column rank, i.e., $k = n_x$, else from the SVD of X :

$$X = QDP^T.$$

Let the SVD of V be:

$$V = U_x \Delta U_g^T$$

then the nonzero elements of the diagonal matrix Δ , δ_i , for $i = 1, 2, \dots, l$, are the l canonical correlations associated with the $l = \min(k, n_g - 1)$ canonical variates, where $l = \min(k, n_g)$.

The eigenvalues, λ_i^2 , of the within-group sums of squares matrix are given by:

$$\lambda_i^2 = \frac{\delta_i^2}{1 - \delta_i^2}$$

and the value of $\pi_i = \lambda_i^2 / \sum \lambda_i^2$ gives the proportion of variation explained by the i th canonical variate. The values of the π_i 's give an indication as to how many canonical variates are needed to adequately describe the data, i.e., the dimensionality of the problem.

To test for a significant dimensionality greater than i the χ^2 statistic:

$$(n - 1 - n_g - \frac{1}{2}(k - n_g)) \sum_{j=i+1}^l \log(1 + \lambda_j^2)$$

can be used. This is asymptotically distributed as a χ^2 -distribution with $(k - i)(n_g - 1 - i)$ degrees of freedom. If the test for $i = h$ is not significant, then the remaining tests for $i > h$ should be ignored.

The loadings for the canonical variates are calculated from the matrix U_x . This matrix is scaled so that the canonical variates have unit within-group variance.

In addition to the canonical variates loadings the means for each canonical variate are calculated for each group.

Weights can be used with the analysis, in which case the weighted means are subtracted from each column and then each row is scaled by an amount $\sqrt{w_i}$, where w_i is the weight for the i th observation (row).

4 References

- Chatfield C and Collins A J (1980) *Introduction to Multivariate Analysis* Chapman and Hall
- Gnanadesikan R (1977) *Methods for Statistical Data Analysis of Multivariate Observations* Wiley
- Hammarling S (1985) The singular value decomposition in multivariate statistics *SIGNUM Newsl.* **20**(3) 2–25
- Kendall M G and Stuart A (1969) *The Advanced Theory of Statistics (Volume 1)* (3rd Edition) Griffin

5 Arguments

- 1: WEIGHT – CHARACTER(1) *Input*
On entry: indicates if weights are to be used.
 WEIGHT = 'U'
 No weights are used.
 WEIGHT = 'W' or 'V'
 Weights are used and must be supplied in WT.
 If WEIGHT = 'W', the weights are treated as frequencies and the effective number of observations is the sum of the weights.
 If WEIGHT = 'V', the weights are treated as being inversely proportional to the variance of the observations and the effective number of observations is the number of observations with nonzero weights.
Constraint: WEIGHT = 'U', 'W' or 'V'.
- 2: N – INTEGER *Input*
On entry: n , the number of observations.
Constraint: $N \geq NX + NG$.
- 3: M – INTEGER *Input*
On entry: m , the total number of variables.
Constraint: $M \geq NX$.
- 4: X(LDX, M) – REAL (KIND=nag_wp) array *Input*
On entry: $X(i, j)$ must contain the i th observation for the j th variable, for $i = 1, 2, \dots, n$ and $j = 1, 2, \dots, m$.

- 5: LDX – INTEGER Input
On entry: the first dimension of the array X as declared in the (sub)program from which G03ACF is called.
Constraint: $LDX \geq N$.
- 6: ISX(M) – INTEGER array Input
On entry: ISX(*j*) indicates whether or not the *j*th variable is to be included in the analysis.
 If ISX(*j*) > 0, the variables contained in the *j*th column of X is included in the canonical variate analysis, for $j = 1, 2, \dots, m$.
Constraint: ISX(*j*) > 0 for NX values of *j*.
- 7: NX – INTEGER Input
On entry: the number of variables in the analysis, n_x .
Constraint: $NX \geq 1$.
- 8: ING(N) – INTEGER array Input
On entry: ING(*i*) indicates which group the *i*th observation is in, for $i = 1, 2, \dots, n$. The effective number of groups is the number of groups with nonzero membership.
Constraint: $1 \leq \text{ING}(i) \leq \text{NG}$, for $i = 1, 2, \dots, n$.
- 9: NG – INTEGER Input
On entry: the number of groups, n_g .
Constraint: $\text{NG} \geq 2$.
- 10: WT(*) – REAL (KIND=nag_wp) array Input
Note: the dimension of the array WT must be at least N if WEIGHT = 'W' or 'V', and at least 1 otherwise.
On entry: if WEIGHT = 'W' or 'V', the first *n* elements of WT must contain the weights to be used in the analysis.
 If WT(*i*) = 0.0, the *i*th observation is not included in the analysis.
 If WEIGHT = 'U', WT is not referenced.
Constraints:

$$\text{WT}(i) \geq 0.0, \text{ for } i = 1, 2, \dots, n;$$

$$\sum_1^n \text{WT}(i) \geq \text{NX} + \text{effective number of groups}.$$
- 11: NIG(NG) – INTEGER array Output
On exit: NIG(*j*) gives the number of observations in group *j*, for $j = 1, 2, \dots, n_g$.
- 12: CVM(LDCVM, NX) – REAL (KIND=nag_wp) array Output
On exit: CVM(*i, j*) contains the mean of the *j*th canonical variate for the *i*th group, for $i = 1, 2, \dots, n_g$ and $j = 1, 2, \dots, l$; the remaining columns, if any, are used as workspace.
- 13: LDCVM – INTEGER Input
On entry: the first dimension of the array CVM as declared in the (sub)program from which G03ACF is called.
Constraint: $\text{LDCVM} \geq \text{NG}$.

- 14: E(LDE,6) – REAL (KIND=nag_wp) array *Output*
On exit: the statistics of the canonical variate analysis.
 E(*i*,1)
 The canonical correlations, δ_i , for $i = 1, 2, \dots, l$.
 E(*i*,2)
 The eigenvalues of the within-group sum of squares matrix, λ_i^2 , for $i = 1, 2, \dots, l$.
 E(*i*,3)
 The proportion of variation explained by the *i*th canonical variate, for $i = 1, 2, \dots, l$.
 E(*i*,4)
 The χ^2 statistic for the *i*th canonical variate, for $i = 1, 2, \dots, l$.
 E(*i*,5)
 The degrees of freedom for χ^2 statistic for the *i*th canonical variate, for $i = 1, 2, \dots, l$.
 E(*i*,6)
 The significance level for the χ^2 statistic for the *i*th canonical variate, for $i = 1, 2, \dots, l$.
- 15: LDE – INTEGER *Input*
On entry: the first dimension of the array E as declared in the (sub)program from which G03ACF is called.
Constraint: $LDE \geq \min(NX, NG - 1)$.
- 16: NCV – INTEGER *Output*
On exit: the number of canonical variates, l . This will be the minimum of $n_g - 1$ and the rank of X.
- 17: CVX(LDCVX, NG – 1) – REAL (KIND=nag_wp) array *Output*
On exit: the canonical variate loadings. CVX(*i*,*j*) contains the loading coefficient for the *i*th variable on the *j*th canonical variate, for $i = 1, 2, \dots, n_x$ and $j = 1, 2, \dots, l$; the remaining columns, if any, are used as workspace.
- 18: LDCVX – INTEGER *Input*
On entry: the first dimension of the array CVX as declared in the (sub)program from which G03ACF is called.
Constraint: $LDCVX \geq NX$.
- 19: TOL – REAL (KIND=nag_wp) *Input*
On entry: the value of TOL is used to decide if the variables are of full rank and, if not, what is the rank of the variables. The smaller the value of TOL the stricter the criterion for selecting the singular value decomposition. If a non-negative value of TOL less than **machine precision** is entered, the square root of **machine precision** is used instead.
Constraint: $TOL \geq 0.0$.
- 20: IRANKX – INTEGER *Output*
On exit: the rank of the dependent variables.
 If the variables are of full rank then $IRANKX = NX$.
 If the variables are not of full rank then IRANKX is an estimate of the rank of the dependent variables. IRANKX is calculated as the number of singular values greater than $TOL \times (\text{largest singular value})$.

- 21: WK(IWK) – REAL (KIND=nag_wp) array Workspace
 22: IWK – INTEGER Input

On entry: the dimension of the array WK as declared in the (sub)program from which G03ACF is called.

Constraints:

if $NX \geq NG - 1$, $IWK \geq N \times NX + \max(5 \times (NX - 1) + (NX + 1) \times NX, N) + 1$;
 if $NX < NG - 1$, $IWK \geq N \times NX + \max(5 \times (NX - 1) + (NG - 1) \times NX, N) + 1$.

- 23: IFAIL – INTEGER Input/Output

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation for details.

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this argument, the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

On exit: IFAIL = 0 unless the routine detects an error or a warning has been flagged (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL = 0 or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL = 1

On entry, $NX < 1$,
 or $NG < 2$,
 or $M < NX$,
 or $N < NX + NG$,
 or $LDX < N$,
 or $LDCVX < NX$,
 or $LDCVM < NG$,
 or $LDE < \min(NX, NG - 1)$,
 or $NX \geq NG - 1$ and $IWK < N \times NX + \max(5 \times (NX - 1) + (NX + 1) \times NX, N)$,
 or $NX < NG - 1$ and $IWK < N \times NX + \max(5 \times (NX - 1) + (NG - 1) \times NX, N)$,
 or $WEIGHT \neq 'U', 'W'$ or $'V'$,
 or $TOL < 0.0$.

IFAIL = 2

On entry, $WEIGHT = 'W'$ or $'V'$ and a value of $WT < 0.0$.

IFAIL = 3

On entry, a value of $ING < 1$,
 or a value of $ING > NG$.

IFAIL = 4

On entry, the number of variables to be included in the analysis as indicated by ISX is not equal to NX.

IFAIL = 5

A singular value decomposition has failed to converge. This is an unlikely error exit.

IFAIL = 6

A canonical correlation is equal to 1. This will happen if the variables provide an exact indication as to which group every observation is allocated.

IFAIL = 7

On entry, less than two groups have nonzero membership, i.e., the effective number of groups is less than 2,
or the effective number of groups plus the number of variables, NX, is greater than the effective number of observations.

IFAIL = 8

The rank of the variables is 0. This will happen if all the variables are constants.

IFAIL = -99

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.9 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -399

Your licence key may have expired or may not have been installed correctly.

See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -999

Dynamic memory allocation failed.

See Section 3.7 in How to Use the NAG Library and its Documentation for further information.

7 Accuracy

As the computation involves the use of orthogonal matrices and a singular value decomposition rather than the traditional computing of a sum of squares matrix and the use of an eigenvalue decomposition, G03ACF should be less affected by ill-conditioned problems.

8 Parallelism and Performance

G03ACF is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

G03ACF 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 routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

None.

10 Example

This example uses a sample of nine observations, each consisting of three variables plus a group indicator. There are three groups. An unweighted canonical variate analysis is performed and the results printed.

10.1 Program Text

Program g03acfe

```
!      G03ACF Example Program Text
!
!      Mark 26 Release. NAG Copyright 2016.
!
!      .. Use Statements ..
!      Use nag_library, Only: g03acf, nag_wp, x04caf
!      .. Implicit None Statement ..
!      Implicit None
!      .. Parameters ..
!      Integer, Parameter          :: nin = 5, nout = 6
!      .. Local Scalars ..
!      Real (Kind=nag_wp)          :: tol
!      Integer                     :: i, ifail, irankx, iwk, ldcvm, ldcvx, &
!                                   lde, ldx, lwt, m, n, ncv, ng, nx
!      Character (1)               :: weight
!      .. Local Arrays ..
!      Real (Kind=nag_wp), Allocatable :: cvm(:,,:), cvx(:,,:), e(:,,:), wk(:), &
!                                   wt(:), x(:,,:)
!      Integer, Allocatable          :: ing(:), isx(:), nig(:)
!      .. Intrinsic Procedures ..
!      Intrinsic                     :: max, min
!      .. Executable Statements ..
!      Write (nout,*) 'G03ACF Example Program Results'
!      Write (nout,*)
!
!      Skip heading in data file
!      Read (nin,*)
!
!      Read in the problem size
!      Read (nin,*) n, m, nx, ng, weight
!
!      Select Case (weight)
!      Case ('W','w','V','v')
!         lwt = n
!      Case Default
!         lwt = 0
!      End Select
!      ldx = n
!      ldcvm = ng
!      lde = min(nx,ng-1)
!      ldcvx = nx
!      If (nx>=ng-1) Then
!         iwk = n*nx + max(5*(nx-1)+(nx+1)*nx,n) + 1
!      Else
!         iwk = n*nx + max(5*(nx-1)+(ng-1)*nx,n) + 1
!      End If
!      Allocate (x(ldx,m),isx(m),ing(n),wt(lwt),nig(ng),cvm(ldcvm,nx),e(lde,6), &
!               cvx(ldcvx,nx),wk(iwk))
!
!      Read in data
!      If (lwt>0) Then
!         Read (nin,*)(x(i,1:m),wt(i),ing(i),i=1,n)
!      Else
!         Read (nin,*)(x(i,1:m),ing(i),i=1,n)
!      End If
!
!      Read in variable inclusion flags
!      Read (nin,*) isx(1:m)
!
!      Use default tolerance
!      tol = 0.0E0_nag_wp
!
!      Perform canonical variate analysis
!      ifail = 0
!      Call g03acf(weight,n,m,x,ldx,isx,nx,ing,ng,wt,nig,cvm,ldcvm,e,lde,ncv, &
!               cvx,ldcvx,tol,irankx,wk,iwk,ifail)
```

```

!      Display results
      Write (nout,99999) 'Rank of X = ', irankx
      Write (nout,*)
      Write (nout,*)
      'Canonical      Eigenvalues Percentage      CHISQ      DF      SIG'
      Write (nout,*) 'Correlations      Variation'
      Write (nout,99998)(e(i,1:6),i=1,ncv)
      Write (nout,*)
      Flush (nout)
      ifail = 0
      Call x04caf('General',' ',nx,ncv,cvx,ldcvx,
      'Canonical Coefficients for X',ifail)
      Write (nout,*)
      Flush (nout)
      ifail = 0
      Call x04caf('General',' ',ng,ncv,cvm,ldcvm,'Canonical variate means',
      ifail)

99999 Format (1X,A,I0)
99998 Format (1X,2F12.4,F11.4,F10.4,F8.1,F8.4)
      End Program g03acfe

```

10.2 Program Data

G03ACF Example Program Data

```

9 3 3 3 'U'
13.3 10.6 21.2 1
13.6 10.2 21.0 2
14.2 10.7 21.1 3
13.4 9.4 21.0 1
13.2 9.6 20.1 2
13.9 10.4 19.8 3
12.9 10.0 20.5 1
12.2 9.9 20.7 2
13.9 11.0 19.1 3
1 1 1

```

10.3 Program Results

G03ACF Example Program Results

Rank of X = 3

Canonical	Eigenvalues	Percentage	CHISQ	DF	SIG
Correlations		Variation			
0.8826	3.5238	0.9795	7.9032	6.0	0.2453
0.2623	0.0739	0.0205	0.3564	2.0	0.8368

Canonical Coefficients for X

	1	2
1	-1.7070	0.7277
2	-1.3481	0.3138
3	0.9327	1.2199

Canonical variate means

	1	2
1	0.9841	0.2797
2	1.1805	-0.2632
3	-2.1646	-0.0164
