NAG Library Routine Document

G03DCF

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

G03DCF allocates observations to groups according to selected rules. It is intended for use after G03DAF.

2   Specification

```
SUBROUTINE G03DCF (TYP, EQUAL, PRIORS, NVAR, NG, NIG, GMN, LDGMN, GC,      &
                   DET, NOBS, M, ISX, X, LDX, PRIOR, P, LDP, IAG, ATIQ,    &
                   ATI, WK, IFAIL)

INTEGER            NVAR, NG, NIG(NG), LDGMN, NOBS, M, ISX(M), LDX, LDP,    &
                   IAG(NOBS), IFAIL
REAL (KIND=nag_wp) GMN(LDGMN,NVAR), GC((NG+1)*NVAR*(NVAR+1)/2),            &
                   DET(NG), X(LDX,M), PRIOR(NG), P(LDP,NG),               &
                   ATI(LDP,*), WK(2*NVAR)
LOGICAL            ATIQ
CHARACTER(1)       TYP, EQUAL, PRIORS
```

3   Description

Discriminant analysis is concerned with the allocation of observations to groups using information from other observations whose group membership is known, X_t; these are called the training set. Consider p variables observed on n_g populations or groups. Let $\bar{x}_j$ be the sample mean and S_j the within-group variance-covariance matrix for the jth group; these are calculated from a training set of n observations with n_j observations in the jth group, and let x_k be the kth observation from the set of observations to be allocated to the n_g groups. The observation can be allocated to a group according to a selected rule. The allocation rule or discriminant function will be based on the distance of the observation from an estimate of the location of the groups, usually the group means. A measure of the distance of the observation from the jth group mean is given by the Mahalanobis distance, D_{kj}:

$$D_{kj}^2 = \left(x_k - \bar{x}_j\right)^{\mathrm{T}} S_j^{-1} \left(x_k - \bar{x}_j\right). \tag{1}$$

If the pooled estimate of the variance-covariance matrix S is used rather than the within-group variance-covariance matrices, then the distance is:

$$D_{kj}^2 = \left(x_k - \bar{x}_j\right)^{\mathrm{T}} S^{-1} \left(x_k - \bar{x}_j\right). \tag{2}$$

Instead of using the variance-covariance matrices S and S_j, G03DCF uses the upper triangular matrices R and R_j supplied by G03DAF such that $S = R^{\mathrm{T}}R$ and $S_j = R_j^{\mathrm{T}}R_j$. D_{kj}^2 can then be calculated as $z^{\mathrm{T}}z$ where $R^{\mathrm{T}}_j z = \left(x_k - x_j\right)$ or $R^{\mathrm{T}}z = \left(x_k - x\right)$ as appropriate.

In addition to the distances, a set of prior probabilities of group membership, π_j, for $j = 1, 2, \ldots, n_g$, may be used, with $\sum \pi_j = 1$. The prior probabilities reflect your view as to the likelihood of the observations coming from the different groups. Two common cases for prior probabilities are $\pi_1 = \pi_2 = \cdots = \pi_{n_g}$, that is, equal prior probabilities, and $\pi_j = n_j/n$, for $j = 1, 2, \ldots, n_g$, that is, prior probabilities proportional to the number of observations in the groups in the training set.

G03DCF uses one of four allocation rules. In all four rules the p variables are assumed to follow a multivariate Normal distribution with mean μ_j and variance-covariance matrix Σ_j if the observation comes from the jth group. The different rules depend on whether or not the within-group variance-covariance matrices are assumed equal, i.e., $\Sigma_1 = \Sigma_2 = \cdots = \Sigma_{n_g}$, and whether a predictive or estimative approach is used. If $p\left(x_k \mid \mu_j, \Sigma_j\right)$ is the probability of observing the observation x_k from

group j, then the posterior probability of belonging to group j is:

$$p(j \mid x_k, \mu_j, \Sigma_j) \propto p(x_k \mid \mu_j, \Sigma_j)\pi_j. \tag{3}$$

In the estimative approach, the arguments μ_j and Σ_j in (3) are replaced by their estimates calculated from X_t. In the predictive approach, a non-informative prior distribution is used for the arguments and a posterior distribution for the arguments, $p(\mu_j, \Sigma_j \mid X_t)$, is found. A predictive distribution is then obtained by integrating $p(j \mid x_k, \mu_j, \Sigma_j)p(\mu_j, \Sigma_j \mid X)$ over the argument space. This predictive distribution then replaces $p(x_k \mid \mu_j, \Sigma_j)$ in (3). See Aitchison and Dunsmore (1975), Aitchison *et al.* (1977) and Moran and Murphy (1979) for further details.

The observation is allocated to the group with the highest posterior probability. Denoting the posterior probabilities, $p(j \mid x_k, \mu_j, \Sigma_j)$, by q_j, the four allocation rules are:

(i)   Estimative with equal variance-covariance matrices – Linear Discrimination

$$\log q_j \propto -\tfrac{1}{2}D_{kj}^2 + \log \pi_j$$

(ii) Estimative with unequal variance-covariance matrices – Quadratic Discrimination

$$\log q_j \propto -\tfrac{1}{2}D_{kj}^2 + \log \pi_j - \tfrac{1}{2}\log |S_j|$$

(iii) Predictive with equal variance-covariance matrices

$$q_j^{-1} \propto ((n_j + 1)/n_j)^{p/2}\left\{1 + [n_j/((n - n_g)(n_j + 1))]D_{kj}^2\right\}^{(n+1-n_g)/2}$$

(iv) Predictive with unequal variance-covariance matrices

$$q_j^{-1} \propto C\left\{\left((n_j^2 - 1)/n_j\right)|S_j|\right\}^{p/2}\left\{1 + \left(n_j/\left(n_j^2 - 1\right)\right)D_{kj}^2\right\}^{n_j/2},$$

where

$$C = \frac{\Gamma\left(\tfrac{1}{2}(n_j - p)\right)}{\Gamma\left(\tfrac{1}{2}n_j\right)}.$$

In the above the appropriate value of D_{kj}^2 from (1) or (2) is used. The values of the q_j are standardized so that,

$$\sum_{j=1}^{n_g} q_j = 1.$$

Moran and Murphy (1979) show the similarity between the predictive methods and methods based upon likelihood ratio tests.

In addition to allocating the observation to a group, G03DCF computes an atypicality index, $I_j(x_k)$. The predictive atypicality index is returned, irrespective of the value of the parameter TYP. This represents the probability of obtaining an observation more typical of group j than the observed x_k (see Aitchison and Dunsmore (1975) and Aitchison *et al.* (1977)). The atypicality index is computed for unequal within-group variance-covariance matrices as:

$$I_j(x_k) = P\left(B \leq z : \tfrac{1}{2}p, \tfrac{1}{2}(n_j - p)\right)$$

where $P(B \leq \beta : a, b)$ is the lower tail probability from a beta distribution and

$$z = D_{kj}^2/\left(D_{kj}^2 + \left(n_j^2 - 1\right)/n_j\right),$$

and for equal within-group variance-covariance matrices as:

$$I_j(x_k) = P\left(B \leq z : \tfrac{1}{2}p, \tfrac{1}{2}(n - n_g - p + 1)\right),$$

with

$$z = D_{kj}^2/\left(D_{kj}^2 + (n - n_g)(n_j + 1)/n_j\right).$$

If $I_j(x_k)$ is close to 1 for all groups it indicates that the observation may come from a grouping not represented in the training set. Moran and Murphy (1979) provide a frequentist interpretation of $I_j(x_k)$.

4 References

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

Aitchison J, Habbema J D F and Kay J W (1977) A critical comparison of two methods of statistical discrimination *Appl. Statist.* **26** 15–25

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

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

Moran M A and Murphy B J (1979) A closer look at two alternative methods of statistical discrimination *Appl. Statist.* **28** 223–232

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

5 Arguments

1: TYP – CHARACTER(1) *Input*

On entry: whether the estimative or predictive approach is used.

TYP = 'E'
 The estimative approach is used.

TYP = 'P'
 The predictive approach is used.

Constraint: TYP = 'E' or 'P'.

2: EQUAL – CHARACTER(1) *Input*

On entry: indicates whether or not the within-group variance-covariance matrices are assumed to be equal and the pooled variance-covariance matrix used.

EQUAL = 'E'
 The within-group variance-covariance matrices are assumed equal and the matrix R stored in the first $p(p + 1)/2$ elements of GC is used.

EQUAL = 'U'
 The within-group variance-covariance matrices are assumed to be unequal and the matrices R_i, for $i = 1, 2, \ldots, n_g$, stored in the remainder of GC are used.

Constraint: EQUAL = 'E' or 'U'.

3: PRIORS – CHARACTER(1) *Input*

On entry: indicates the form of the prior probabilities to be used.

PRIORS = 'E'
 Equal prior probabilities are used.

PRIORS = 'P'
 Prior probabilities proportional to the group sizes in the training set, n_j, are used.

PRIORS = 'I'
 The prior probabilities are input in PRIOR.

Constraint: PRIORS = 'E', 'I' or 'P'.

4: NVAR – INTEGER *Input*

On entry: p, the number of variables in the variance-covariance matrices.

Constraint: NVAR $\geq$ 1.

5: NG – INTEGER *Input*

   On entry: the number of groups, n_g.

   Constraint: $NG \geq 2$.

6: NIG(NG) – INTEGER array *Input*

   On entry: the number of observations in each group in the training set, n_j.

   Constraints:

   if $EQUAL = 'E'$, $NIG(j) > 0$ and $\sum_{j=1}^{n_g} NIG(j) > NG + NVAR$, for $j = 1, 2, \ldots, n_g$;

   if $EQUAL = 'U'$, $NIG(j) > NVAR$, for $j = 1, 2, \ldots, n_g$.

7: GMN(LDGMN, NVAR) – REAL (KIND=nag_wp) array *Input*

   On entry: the jth row of GMN contains the means of the p variables for the jth group, for $j = 1, 2, \ldots, n_j$. These are returned by G03DAF.

8: LDGMN – INTEGER *Input*

   On entry: the first dimension of the array GMN as declared in the (sub)program from which G03DCF is called.

   Constraint: $LDGMN \geq NG$.

9: GC$((NG + 1) \times NVAR \times (NVAR + 1)/2)$ – REAL (KIND=nag_wp) array *Input*

   On entry: the first $p(p+1)/2$ elements of GC should contain the upper triangular matrix R and the next n_g blocks of $p(p+1)/2$ elements should contain the upper triangular matrices R_j.

   All matrices must be stored packed by column. These matrices are returned by G03DAF. If $EQUAL = 'E'$ only the first $p(p+1)/2$ elements are referenced, if $EQUAL = 'U'$ only the elements $p(p+1)/2 + 1$ to $(n_g + 1)p(p+1)/2$ are referenced.

   Constraints:

   if $EQUAL = 'E'$, the diagonal elements of R must be $\neq 0.0$;
   if $EQUAL = 'U'$, the diagonal elements of the R_j must be $\neq 0.0$, for $j = 1, 2, \ldots, n_g$.

10: DET(NG) – REAL (KIND=nag_wp) array *Input*

   On entry: if $EQUAL = 'U'$. the logarithms of the determinants of the within-group variance-covariance matrices as returned by G03DAF. Otherwise DET is not referenced.

11: NOBS – INTEGER *Input*

   On entry: the number of observations in X which are to be allocated.

   Constraint: $NOBS \geq 1$.

12: M – INTEGER *Input*

   On entry: the number of variables in the data array X.

   Constraint: $M \geq NVAR$.

13: ISX(M) – INTEGER array *Input*

   On entry: $ISX(l)$ indicates if the lth variable in X is to be included in the distance calculations.

   If $ISX(l) > 0$, the lth variable is included, for $l = 1, 2, \ldots, M$; otherwise the lth variable is not referenced.

   Constraint: $ISX(l) > 0$ for NVAR values of l.

14: X(LDX, M) – REAL (KIND=nag_wp) array *Input*

On entry: X(k, l) must contain the kth observation for the lth variable, for $k = 1, 2, \ldots,$ NOBS and $l = 1, 2, \ldots,$ M.

15: LDX – INTEGER *Input*

On entry: the first dimension of the array X as declared in the (sub)program from which G03DCF is called.

Constraint: LDX $\geq$ NOBS.

16: PRIOR(NG) – REAL (KIND=nag_wp) array *Input/Output*

On entry: if PRIORS = 'I', the prior probabilities for the n_g groups.

Constraint: if PRIORS = 'I', PRIOR(j) > 0.0 and $\left| 1 - \sum_{j=1}^{n_g} \text{PRIOR}(j) \right| \leq 10 \times$ *machine precision*, for $j = 1, 2, \ldots, n_g$.

On exit: if PRIORS = 'P', the computed prior probabilities in proportion to group sizes for the n_g groups.

If PRIORS = 'I', the input prior probabilities will be unchanged.

If PRIORS = 'E', PRIOR is not set.

17: P(LDP, NG) – REAL (KIND=nag_wp) array *Output*

On exit: P(k, j) contains the posterior probability p_{kj} for allocating the kth observation to the jth group, for $k = 1, 2, \ldots,$ NOBS and $j = 1, 2, \ldots, n_g$.

18: LDP – INTEGER *Input*

On entry: the first dimension of the arrays P and ATI as declared in the (sub)program from which G03DCF is called.

Constraint: LDP $\geq$ NOBS.

19: IAG(NOBS) – INTEGER array *Output*

On exit: the groups to which the observations have been allocated.

20: ATIQ – LOGICAL *Input*

On entry: ATIQ must be .TRUE. if atypicality indices are required. If ATIQ is .FALSE. the array ATI is not set.

21: ATI(LDP, $*$) – REAL (KIND=nag_wp) array *Output*

Note: the second dimension of the array ATI must be at least NG if ATIQ = .TRUE., and at least 1 otherwise.

On exit: if ATIQ is .TRUE., ATI(k, j) will contain the predictive atypicality index for the kth observation with respect to the jth group, for $k = 1, 2, \ldots,$ NOBS and $j = 1, 2, \ldots, n_g$.

If ATIQ is .FALSE., ATI is not set.

22: WK($2 \times$ NVAR) – REAL (KIND=nag_wp) array *Workspace*

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, NVAR < 1,
or   NG < 2,
or   NOBS < 1,
or   M $<$ NVAR,
or   LDGMN $<$ NG,
or   LDX $<$ NOBS,
or   LDP $<$ NOBS,
or   TYP $\neq$ 'E' or 'P',
or   EQUAL $\neq$ 'E' or 'U',
or   PRIORS $\neq$ 'E', 'I' or 'P'.

IFAIL $= 2$

On entry, the number of variables indicated by ISX is not equal to NVAR,
or   EQUAL $=$ 'E' and NIG$(j) \leq 0$, for some j,

or   EQUAL $=$ 'E' and $\displaystyle\sum_{j=1}^{n_g}NIG(j) \leq$ NG $+$ NVAR,

or   EQUAL $=$ 'U' and NIG$(j) \leq$ NVAR for some j.

IFAIL $= 3$

On entry, PRIORS $=$ 'I' and PRIOR$(j) \leq 0.0$ for some j,

or   PRIORS $=$ 'I' and $\displaystyle\sum_{j=1}^{n_g}$PRIOR$(j)$ is not within $10 \times$ ***machine precision*** of 1.

IFAIL $= 4$

On entry, EQUAL $=$ 'E' and a diagonal element of R is zero,
or   EQUAL $=$ 'U' and a diagonal element of R_j for some j is zero.

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

The accuracy of the returned posterior probabilities will depend on the accuracy of the input R or R_j matrices. The atypicality index should be accurate to four significant places.

8   Parallelism and Performance

G03DCF 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

The distances D_{kj}^2 can be computed using G03DBF if other forms of discrimination are required.

10   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 group means and R matrices are computed by G03DAF. A further six observations of unknown type are input and allocations made using the predictive approach and under the assumption that the within-group covariance matrices are not equal. The posterior probabilities of group membership, q_j, and the atypicality index are printed along with the allocated group. The atypicality index shows that observations 5 and 6 do not seem to be typical of the three types present in the initial 21 observations.

10.1 Program Text

```
    Program g03dcfe

!     G03DCF Example Program Text

!     Mark 26 Release. NAG Copyright 2016.

!     .. Use Statements ..
      Use nag_library, Only: g03daf, g03dcf, nag_wp
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter                :: nin = 5, nout = 6
!     .. Local Scalars ..
      Real (Kind=nag_wp)                :: df, sig, stat
      Integer                           :: i, ifail, ldgmn, ldox, ldp, ldx,    &
                                           lgc, lwk, lwt, m, n, ng, nobs, nvar, &
                                           tdati
      Logical                           :: atiq
      Character (1)                     :: equal, priors, typ, weight
      Character (80)                    :: fmt
!     .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable   :: ati(:,:), det(:), gc(:), gmn(:,:),   &
                                           ox(:,:), p(:,:), prior(:), wk(:),    &
                                           wt(:), x(:,:)
      Integer, Allocatable              :: iag(:), ing(:), isx(:), iwk(:),      &
```

```
                                                        nig(:)
!     .. Intrinsic Procedures ..
      Intrinsic                           :: count, max
!     .. Executable Statements ..
      Write (nout,*) 'G03DCF Example Program Results'
      Write (nout,*)

!     Skip headings in data file
      Read (nin,*)

!     Read in the problem size
      Read (nin,*) n, m, ng, weight

      If (weight=='W' .Or. weight=='w') Then
        lwt = n
      Else
        lwt = 0
      End If
      ldox = n
      Allocate (ox(ldox,m),ing(n),wt(lwt),isx(m))

!     Read in data
      If (lwt>0) Then
        Read (nin,*)(ox(i,1:m),ing(i),wt(i),i=1,n)
      Else
        Read (nin,*)(ox(i,1:m),ing(i),i=1,n)
      End If

!     Read in variable inclusion flags
      Read (nin,*) isx(1:m)

!     Calculate NVAR
      nvar = count(isx(1:m)==1)

      lwk = max(n*(nvar+1),2*nvar)
      ldgmn = ng
      lgc = (ng+1)*nvar*(nvar+1)/2
      Allocate (nig(ng),gmn(ldgmn,nvar),det(ng),gc(lgc),wk(lwk),iwk(ng))

!     Compute covariance matrix
      ifail = 0
      Call g03daf(weight,n,m,ox,ldox,isx,nvar,ing,ng,wt,nig,gmn,ldgmn,det,gc,  &
        stat,df,sig,wk,iwk,ifail)

!     Read in parameters controlling grouping
      Read (nin,*) typ, equal, priors, nobs, atiq

      If (atiq) Then
        tdati = ng
      Else
        tdati = 1
      End If
      ldx = nobs
      ldp = nobs
      Allocate (x(ldx,m),prior(ng),p(ldp,ng),iag(nobs),ati(ldp,tdati))

!     Read in data to group
      Read (nin,*)(x(i,1:m),i=1,nobs)

!     Read in priors
      If (priors=='I' .Or. priors=='i') Then
        Read (nin,*) prior(1:ng)
      End If

!     Allocate observations to groups
      ifail = 0
      Call g03dcf(typ,equal,priors,nvar,ng,nig,gmn,ldgmn,gc,det,nobs,m,isx,x,  &
        ldx,prior,p,ldp,iag,atiq,ati,wk,ifail)

!     Display results
      If (atiq) Then
```

```
        Write (fmt,99999) '(2(I6,5X,', ng, 'F6.3))'
        Write (nout,*) '   Obs        Posterior       Allocated',        &
          '     Atypicality'
        Write (nout,*) '                probabilities   to group      index'
        Write (nout,*)
        Write (nout,fmt)(i,p(i,1:ng),iag(i),ati(i,1:ng),i=1,nobs)
      Else
        Write (fmt,99999) '(I6,5X,', ng, 'F6.3,I6))'
        Write (nout,*) '   Obs        Posterior       Allocated'
        Write (nout,*) '                probabilities   to group '
        Write (nout,*)
        Write (nout,fmt)(i,p(i,1:ng),iag(i),i=1,nobs)
      End If

99999 Format (A,I0,A)
      End Program g03dcfe
```

10.2 Program Data

```
G03DCF Example Program Data
  21 2 3 'U'                : N,M,NG,WEIGHT
  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  : End of X,ING (G03DAF)
   1        1          : ISX
   'P' 'U' 'E' 6 T       : TYP,EQUAL,PRIORS,NOBS,ATIQ
  1.6292   -0.9163
  2.5572    1.6094
  2.5649   -0.2231
  0.9555   -2.3026
  3.4012   -2.3026
  3.0204   -0.2231        : End of X
```

10.3 Program Results

```
 G03DCF Example Program Results


    Obs        Posterior       Allocated     Atypicality
               probabilities   to group      index


     1      0.094 0.905 0.002     2      0.596 0.254 0.975
     2      0.005 0.168 0.827     3      0.952 0.836 0.018
     3      0.019 0.920 0.062     2      0.954 0.797 0.912
     4      0.697 0.303 0.000     1      0.207 0.860 0.993
     5      0.317 0.013 0.670     3      0.991 1.000 0.984
     6      0.032 0.366 0.601     3      0.981 0.978 0.887
```