# NAG Library Routine Document <br> g22ycf 

Note: please be advised that this routine is classed as 'experimental' and its interface may be developed further in the future. Please see Section 3.1.1 in How to Use the NAG Library and its Documentation for further information.

## 1 Purpose

g22ycf generates a design matrix from a data matrix and model description.

## 2 Specification

## Fortran Interface

```
Subroutine g22ycf (hform, hddesc, dat, lddat, sddat, hxdesc, x, ldx,
    sdx, mx, ifail)
Integer, Intent (In) :: lddat, sddat, ldx, sdx
Integer, Intent (Inout) :: ifail
Integer, Intent (Out) :: mx
Real (Kind=nag_wp), Intent (In) :: dat(lddat,sddat)
Real (Kind=nag_wp), Intent (Inout) : : x(ldx,sdx)
Type (c_ptr), Intent (In) :: hform, hddesc
Type (c_ptr), Intent (Inout) :: hxdesc
```


## 3 Description

g22ycf generates a design matrix from a data matrix and a model description. Design matrices encapsulate the observed values of the independent variables and the required model in a form that can be used by many of the model fitting routines available in the NAG Library, for example those in Chapter G02.

### 3.1 Notation

Let $D$ denote a data matrix with $n$ observations on $m_{d}$ independent variables, denoted by $V_{j}$, for $j=1,2, \ldots, m_{d}$. If $V_{j}$ is a categorical variable, let $L_{j}$ denote the number of levels associated with it. If $V_{j}$ is a binary, ordinal or continuous variable, let $L_{j}=1$.

Let $V_{j i}$ denote the $i$ th value of $V_{j}$.
Let $\mathcal{M}$ denote a model made up of one or more terms, denoted by $T_{i}$. Each term consists of either a main effect or an interaction and hence can be described using one or more variable names $V_{j}$ and the interaction operator ' $\because$ ' The operator ' + ' is used to denote the addition of a term to the model. Therefore, $\mathcal{M}=T_{1}+T_{2}+T_{3}=V_{1}+V_{2}+V_{1} \cdot V_{2}$ denotes a model with three terms, the first two terms being the main effects for variables $V_{1}$ and $V_{2}$ and the last term the interaction between them. For simplicity we reorder the terms of the model by the number of variables in them, so main effects come first, then two-way interactions, then three-way interactions etc. By default it is assumed that the model $\mathcal{M}$ contains a mean effect (or intercept term), if the mean effect is excluded, this will be denoted by ' -1 ', so $\mathcal{M}=T_{1}$ is a model with one term and a mean effect and $\mathcal{M}=T_{1}-1$ is the same model with the mean effect dropped.
g22ycf generates an $n$ by $m_{x}$ design matrix, $X$, from $D$ and $\mathcal{M}$.

### 3.2 Dummy Variables

When constructing a design matrix, we cannot work directly with categorical variables. Categorical variables must first be recoded into dummy variables. A categorical variable $V_{j}$ requires $L_{j}$ dummy variables. Let $\mathcal{D}^{j}$ denote an $n \times L_{j}$ matrix of dummy variables for $V_{j}$ defined as

$$
\mathcal{D}_{l i}^{j}= \begin{cases}1 ; & \text { if } V_{j i}=l \\ 0 ; & \text { otherwise }\end{cases}
$$

where $\mathcal{D}_{l}^{j}$ is the $l$ th column of $\mathcal{D}^{j}$ and $\mathcal{D}_{l i}^{j}$ is the $i$ th element of $\mathcal{D}_{l}^{j}$.
For a binary, ordinal or continuous variable, $\mathcal{D}_{1 i}^{j}=V_{j i}$.

### 3.3 Full Design Matrix

Given a model, $\mathcal{M}$, and the matrices of dummy variables constructing the full design matrix $X_{F}$ is trivial. Each term is processed in order and

1. If term $i$ is a main effect, that is $T_{i}=V_{j}$ for some $j, \mathcal{D}^{j}$ is copied into $X_{F}$.
2. If term $i$ is a two-way interaction, that is $T_{i}=V_{j} . V_{k}$, for some $j \neq k$, then
(i) Loop over $l_{j}=1,2, \ldots L_{j}$.
(ii) Loop over $l_{k}=1,2, \ldots L_{k}$.
(iii) Add a column to $X_{F}$ corresponding to the element-wise product of $\mathcal{D}_{l_{j}}^{j}$ and $\mathcal{D}_{l_{k}}^{k}$.
3. Higher interaction terms are handled in a similar manner as the two-way interactions by adding columns constructed from multiplying all combinations of the columns of the corresponding $\mathcal{D}$ s that correspond to the variables involved. In all cases, the variables towards the right hand side of a term are iterated over the quickest.

### 3.4 Contrasts

Using the full design matrix $X_{F}$ in an analysis can result in an overparameterized model. This is due to $X_{F}$ often not being of full rank as the sum of all the dummy variables for a particular variable is a vector of ones. This source of overparameterization can be alleviated by using a design matrix $X$ where (some) dummy variables are replaced by contrasts. For a categorical variable $V_{j}$ the contrasts are a set of $L_{j}-1$ functionally independent linear combinations of the dummy variables.
Whilst the choice of contrasts used in term $T_{i}$ will affect the individual model coefficients (parameters), it has no effect on the overall contribution of $T_{i}$.
For a given variable $V_{j}$, the contrasts can be represented by an $L_{j}$ by $L_{j}-1$ matrix, $C_{j}$. The rows of $C_{j}$ correspond to a particular value of $V_{j}$ and the columns correspond to the values to use in the design matrix.

Six types of contrast are available in g22ycf; two types of treatment contrasts, two types of sum contrasts, Helmert contrasts and polynomial contrasts. Unless specified otherwise, the contrasts used by $\mathbf{g 2 2} \mathbf{y c f}$ are treatment contrasts relative to the first level. See the description of the optional parameter Contrast in g22yaf for ways of changing the contrasts used.

### 3.4.1 Treatment Contrasts

Treatment contrasts are taken relative to either the first or last level of the variable. For example, if $L_{j}=4$,

$$
C_{j}=\left(\begin{array}{lll}
0 & 0 & 0 \\
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{array}\right)
$$

would be the contrast matrix for $V_{j}$ using treatment contrasts relative to the first level. The contrast matrix obtained when using treatment contrasts relative to the last level is similar, but the row of zeros appears at the bottom and all other rows are shifted up one.

Strictly speaking, the term contrast implies that each row in the contrast matrix sums to zero. That is not the case for treatment contrasts, however they are included as this coding is commonly used in practice.

### 3.4.2 Sum Contrasts

Sum contrasts are similar to treatment contrasts and again can be taken relative to the first or last level of the variable. Unlike treatment contrasts, sum contrasts effectively constrain the coefficients related to the variable to sum to zero. For example, if $L_{j}=4$,

$$
C_{j}=\left(\begin{array}{rrr}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
-1 & -1 & -1
\end{array}\right)
$$

would be the contrast matrix for $V_{j}$ using treatment contrasts relative to the last level. The contrast matrix obtained when using treatment contrasts relative to the first level is similar, but the row of -1 s appears at the top and all other rows are shifted down one.

### 3.4.3 Helmert Contrasts

With Helmert contrasts level $l$ of the variable is compared with the average effect of all previous levels. For example, if $L_{j}=4$,

$$
C_{j}=\left(\begin{array}{rrr}
-1 & -1 & -1 \\
1 & -1 & -1 \\
0 & 2 & -1 \\
0 & 0 & 3
\end{array}\right)
$$

would be the contrast matrix for $V_{j}$ using Helmert contrasts.

### 3.4.4 Polynomial Contrasts

With polynomial contrasts the entries in the columns of $C_{j}$ correspond in linear, quadratic, cubic, quartic, etc. terms to a hypothetical underlying numeric variable that takes equally spaced values at each level. For example, if $L_{j}=4$,

$$
C_{j}=\left(\begin{array}{rrr}
-0.67 & 0.50 & -0.22 \\
-0.22 & -0.50 & 0.67 \\
0.22 & -0.50 & -0.67 \\
0.67 & 0.50 & 0.22
\end{array}\right)
$$

would be the contrast matrix for $V_{j}$ using polynomial contrasts.

### 3.4.5 When Contrasts Can Be Used

Depending on the specifics of the model, $\mathcal{M}$, it may not be possible to always replace the $L_{j}$ dummy variables with $L_{j}-1$ contrasts for all variables in all terms and retain the same model. A simple example of this is a data matrix, $D$, with four observations and two variables which have two and three levels respectively. This data matrix might look something like:

$$
D=\left(\begin{array}{ll}
1 & 1 \\
2 & 3 \\
1 & 2 \\
2 & 2
\end{array}\right)
$$

For the sake of argument, assume that our model contains the main effect for each variable, but does not contain a mean effect (or intercept term). So using the notation established earlier, $\mathcal{M}=V_{1}+V_{2}-1$. The full design matrix, $X_{F}$, for this data matrix and model would be

However, $X_{F}$ is not of full rank (and hence $\mathcal{M}$ is overparameterized) because the sum of the first two columns is a vector of ones as is the sum of the last three columns.

In order to alleviate this we might try constructing $X_{C}$ where the dummy variables have been replaced by contrasts. Assuming treatment contrasts, relative to the first level, we would have

$$
X_{C}=\left(\begin{array}{lll}
0 & 0 & 0 \\
1 & 0 & 1 \\
0 & 1 & 0 \\
1 & 1 & 0
\end{array}\right)
$$

However, using $X_{C}$ makes an implicit assumption that the expected value of the dependent variable (the quantity being modelled) is zero when $V_{1}=1$ and $V_{2}=1$. This assumption was not made when we used $X_{F}$ and hence the two design matrices are not equivalent. One solution would be to use dummy variables for $V_{1}$ and contrasts for $V_{2}$, which would result in a design matrix, $X$ of

$$
X=\left(\begin{array}{llll}
1 & 0 & & 0 \\
0 & 0 \\
0 & 1 & & 0 \\
1 \\
1 & 0 & & 1 \\
0 & 1 & & 0
\end{array}\right)
$$

Using $X$ would give an equivalent model to using $X_{F}$.
The algorithm used by g22ycf to decide which variables, in which terms, can be coded as contrasts and which need to be coded as dummy variables is described below.
Suppose $V_{j}$ is any variable that appears in term $T_{i}$, let $T_{i(j)}$ denote the term obtained by dropping $V_{j}$ from $T_{i}$. For example, if $T_{3}=V_{1} \cdot V_{2} \cdot V_{3}, T_{3(2)}=V_{1} \cdot V_{3}$. In this context, the empty term is taken to be the mean effect (or intercept term). We say that $T_{i(j)}$ appears in $\mathcal{M}$ if there exists a term $T_{k}, k<i$, that contains all of the variables appearing in $T_{i(j)}$. In most cases $T_{k}=T_{i(j)}$, but this is not required. Note, as stated earlier, the terms in $\mathcal{M}$ are ordered by the number of variables in them.
A variable, $V_{j}$ in term $T_{i}$ is coded by contrasts if $T_{i(j)}$ appears in $\mathcal{M}$ and by dummy variables otherwise. It is therefore possible for variable $V_{j}$ to be coded by contrasts in some terms and dummy variables in others within the same $X$.

The above rule assumes the presence of a mean effect. If no such effect is present in the model, the main effect of the first categorical variable is coded by dummy variables to compensate. If no main effects appear in the model, the warning ifail $=14$ is returned.

A longer description and informal proof that the resulting $X$ is a suitable design matrix for the model of interest can be found in chapter two of Chambers and Hastie (1992).

### 3.5 Mean Effect

The mean effect (or intercept term) is included in a design matrix by adding a column of ones as the first column of $X$. However, many model fitting routines in the NAG Library handle the mean effect as a special case and do not require it to be explicitly added to the design matrix. Therefore, by default, g22ycf does not explicitly add the mean effect to the design matrix. This behaviour can be changed via the optional parameter Explicit Mean in g22yaf.

## 4 References

Chambers J M and Hastie T J (1992) Statistical Models in S Wadsworth and Brooks/Cole Computer Science Series

## 5 Arguments

1: hform - Type (c_ptr)
Input
On entry: a G22 handle to the internal data structure containing a description of the model $\mathcal{M}$ as returned in hform by g22yaf.

2: hddesc - Type (c_ptr)
Input
On entry: a G22 handle to the internal data structure containing a description of the data matrix, $D$ as returned in hddesc by $\mathbf{g 2 2 y b f}$.

3: dat(lddat, sddat) - Real (Kind=nag_wp) array
Input
On entry: the data matrix, $D$. By default $D_{i j}$, the $i$ th value for the $j$ th variable, for $i=1,2, \ldots, n$ and $j=1,2, \ldots, m_{d}$, should be supplied in $\operatorname{dat}(i, j)$.
If the optional parameter Storage Order, described in $\mathbf{g 2 2} \mathbf{y b f}$, is set to VAROBS, $D_{i j}$ should be supplied in $\operatorname{dat}(j, i)$.

4: Iddat - Integer
Input
On entry: the first dimension of the array dat as declared in the (sub)program from which g22ycf is called.
Constraints:
if the optional parameter Storage Order, described in g22ybf, is set to VAROBS, lddat $\geq m_{d}$;
otherwise lddat $\geq n$.
5: sddat - Integer Input
On entry: the second dimension of the array dat as declared in the (sub)program from which g22ycf is called.

Constraints:
if the optional parameter Storage Order, described in g22ybf, is set to VAROBS, sddat $\geq n$;
otherwise sddat $\geq m_{d}$.
6: hxdesc - Type (c_ptr)
Input/Output
On entry: must be set to c_null_ptr.
As an alternative an existing G22 handle may be supplied in which case this routine will destroy the supplied G22 handle as if g22zaf had been called.

On exit: holds a G22 handle to the internal data structure containing a description of the design matrix, $X$. You must not change the G22 handle other than through the routines in Chapter G22.

7: $\quad \mathbf{x}(\mathbf{l d x}, \mathbf{s d x})$ - Real (Kind=nag_wp) array
Output
On exit: the design matrix, $X$. By default $X_{i j}$, the $i$ th value for the $j$ th column, for $i=1,2, \ldots, n$ and $j=1,2, \ldots, m_{x}$, is returned in $\mathbf{x}(i, j)$
If the optional parameter Storage Order, described in g22yaf, is set to VAROBS, $X_{i j}$ is returned in $\mathbf{x}(j, i)$.
If ldx or sdx are too small to hold $\mathbf{x}$, the number of columns required to hold the design matrix is returned in $\mathbf{m x}$.

Under some conditions it is possible to use the data matrix in place of the design matrix. Specifically, if $D$ has no categorical variables, $\mathcal{M}$ has only main effects and either has no mean effect or the mean effect does not need to be explicitly added to the design matrix. If ldx or sdx
are too small under such circumstances, ifail $=71$ is returned and hxdese is set up in such a way as to allow dat to be used as the design matrix.

8: $\quad$ ldx - Integer
Input
On entry: the first dimension of the array $\mathbf{x}$ as declared in the (sub)program from which $\mathbf{g} 22 \mathbf{y c f}$ is called.

Constraints:
if the optional parameter Storage Order, described in g22yaf, is set to VAROBS, $\boldsymbol{l d x} \geq m_{x}$;
otherwise $\mathbf{l d x} \geq n$.
$9:$
sdx - Integer Input
On entry: the second dimension of the array $\mathbf{x}$ as declared in the (sub)program from which g22ycf is called.
Constraints:
if the optional parameter Storage Order, described in g22yaf, is set to VAROBS, $\mathbf{s d x} \geq n$; otherwise $\mathbf{s d x} \geq m_{x}$.

10: $\quad \mathbf{m x}$ - Integer
Output
On exit: the minimum number of columns required to hold the design matrix.
In most cases $\mathbf{m x}=m_{x}$. The one exception is when ifail $=71$, that is the size of $\mathbf{x}$ was too small but the data matrix given in dat can be used as the design matrix. In this case $\mathbf{m x}$ holds the number of columns that would be required if only the relevant parts of dat were copied into a new array.

11: 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 $\mathbf{x 0 4 a a f}$ ).

Errors or warnings detected by the routine:
ifail $=11$
hform has not been initialized or is corrupt.
ifail $=12$
hform is not a G22 handle as generated by g22yaf.

## ifail $=13$

A variable name used when creating hform is not present in hddesc. Variable name: $\langle$ value $\rangle$.

## ifail $=14$

The model contains categorical variables, but no intercept or main effects terms have been requested. Please check the design matrix returned matches the model you require.

## $\mathbf{i f a i l}=21$

hddesc has not been initialized or is corrupt.
ifail $=22$
hddese is not a G22 handle as generated by g22ybf.

## ifail $=31$

On entry, column $j$ of the data matrix, $D$, is not consistent with information supplied in hddesc, $j=\langle$ value $\rangle$.

## ifail $=41$

On entry, $n=\langle$ value $\rangle$ and Iddat $=\langle$ value $\rangle$.
Constraint: lddat $\geq n$.

## ifail $=42$

On entry, $m_{d}=\langle$ value $\rangle$ and lddat $=\langle$ value $\rangle$.
Constraint: lddat $\geq m_{d}$.

## $\mathbf{i f a i l}=51$

On entry, $m_{d}=\langle$ value $\rangle$ and sddat $=\langle$ value $\rangle$.
Constraint: sddat $\geq m_{d}$.
ifail $=52$
On entry, $n=\langle$ value $\rangle$ and sddat $=\langle$ value $\rangle$.
Constraint: sddat $\geq n$.
$\mathbf{i f a i l}=61$
On entry, hxdesc is not c_null_ptr or a recognised G22 handle.
$\mathbf{i f a i l}=71$
On entry, the size of $\mathbf{x}$ is too small to hold the design matrix. dat can be used instead.
$\mathbf{i f a i l}=81$
On entry, $n=\langle$ value $\rangle$ and $\mathbf{l d x}=\langle$ value $\rangle$.
Constraint: $\mathbf{l d} \mathbf{x} \geq n$.
ifail $=82$
On entry, $m_{x}=\langle$ value $\rangle$ and $\mathbf{l d x}=\langle$ value $\rangle$.
Constraint: $\boldsymbol{l d x} \geq m_{x}$.
ifail $=91$
On entry, $m_{x}=\langle$ value $\rangle$ and $\mathbf{s d x}=\langle$ value $\rangle$.
Constraint: $\mathbf{s d x} \geq m_{x}$.

$$
\text { ifail }=92
$$

On entry, $n=\langle$ value $\rangle$ and $\mathbf{s d x}=\langle$ value $\rangle$.
Constraint: $\mathbf{s d x} \geq n$.
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.

$$
\text { ifail }=-399
$$

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.

$$
\text { ifail }=-999
$$

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

## 7 Accuracy

Not applicable.

## 8 Parallelism and Performance

g22ycf is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.
g22ycf 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

g22ydf can be used to obtain labels for the columns of the design matrix $X$.
Many of the analysis routines that require a design matrix to be supplied allow submodels to be defined through the use of a vector of ones or zeros indicating whether a column of $X$ should be included or excluded from the analyses (see for example isx in g02daf or g02gaf). This allows nested models to be fit without having to reconstruct the design matrix for each analysis. g22ydf offers a mechanism for constructing these vectors using submodels specified using g22yaf.

## 10 Example

This example creates and outputs two design matrices for a simple linear regression model. The first design matrix uses sum contrasts for all variables and the second uses a combination of polynomial and Helmert contrasts. Column labels are generated using g22ydf.
See also the examples for g22yaf, g22ybf and g22ydf.

### 10.1 Program Text

```
G22YCF Example Program Text
Mark 26.1 Release. NAG Copyright 2017.
Module g22ycfe_mod
        G22YCF Example Program Module:
                        Parameters and User-defined Routines
    .. Use Statements ..
    Use nag_library, Only: nag_wp
    .. Implicit None Statement ..
    Implicit None
    .. Accessibility Statements ..
    Private
    Public :: print_x, read_line
    .. Parameters ..
    Integer, Parameter, Public :: nin = 5, nout = 6
```

    Contains
    Subroutine read_line(ierr,v1,v2)
        Read in a line from NIN, remove any comments and optionally
        split out the first word
        .. Scalar Arguments ..
        Integer, Intent (Out) :: ierr
        Character (*), Intent (Out) :: v1
        Character (*), Intent (Out), Optional :: v2
        .. Local Scalars ..
        Integer : : pend
        .. Intrinsic Procedures ..
        Intrinsic :: adjustl, index, present
        .. Executable Statements ..
        Continue
        Read (nin,'(A200)',Iostat=ierr) v1
        If (ierr==0) Then
            pend = index(v1,': :')
            If (pend/=0) Then
                \(\mathrm{v} 1=\mathrm{v} 1(1:\) pend-1)
            End If
            v1 = adjustl(v1)
            If (present(v2)) Then
                split the first word from the line
                    pend = index(v1,' ')
                If (pend/=0) Then
                        v2 = adjustl(v1(pend:))
                        \(\mathrm{v} 1=\operatorname{adjustl(v1(1:pend))}\)
                Else
                        v2 = ' '
                End If
            End If
        End If
        Return
    End Subroutine read_line
    Subroutine print_x(intcpt,plab, nobs,mx,x,text)
        Print the transpose of the first 10 rows of the design matrix
        .. Parameters ..
        Integer, Parameter :: max_rows = 10
        . . Scalar Arguments ..
        Integer, Intent (In) :: mx, nobs
        Character (*), Intent (In) : intcpt, text
        .. Array Arguments ..
        Real (Kind=nag_wp), Intent (In) :: x(:,:)
        Character (*), Intent (In) :: plab(:)
        Integer Scalars .. : i, pnobs, si
        .. Intrinsic Procedures ..
        Intrinsic :: min, repeat, trim
    ```
! .. Executable Statements ..
    Continue
    PLAB holds the labels for the model parameters, so includes a label
    for the mean effect, if one is present. As the mean effect is not
    being explicitly included in the design matrix, we may need to skip
    the first element of PLAB (which will always be the label for the
    mean effect if one is present)
    If (intcpt=='M') Then
        si = 1
    Else
        si = 0
    End If
    Printing the first MAX_ROWS rows of the design matrix
    pnobs = min(max_rows,nobs)
    Display the design matrix
    Write (nout,99998) 'Transpose of First ', pnobs, ' Rows of the ',
        text, ' Design Matrix (X)'
    Write (nout,99997) 'Column Name', (i,i=1,pnobs)
    Write (nout,99996) repeat('_',15+pnobs*5)
    Do i = 1, mx
        Write (nout,99999) plab(i+si), x(1:pnobs,i)
    End Do
    Write (nout,*) 'Intercept flag = ', trim(intcpt)
    Return
99999 Format (1X,A15,100(1X,F4.1))
9 9 9 9 8 ~ F o r m a t ~ ( 1 X , A , I O , A , A , A )
99997 Format (1X,A,3X,100(3X,I2))
99996 Format (1X,A)
    End Subroutine print_x
    End Module g22ycfe_mod
    Program g22ycfe
        G22YCF Example Program Text
    Mark 25 Release. NAG Copyright 2015.
    .. Use Statements ..
    Use g22ycfe_mod, Only: nin, nout, print_x, read_line
    Use, Intrinsic :: iso_c_binding, Only: c_null_ptr, &
    c_ptr
    Use nag_library, Only: g22yaf, g22ybf, g22ycf, g22ydf, g22zaf, g22zmf
    Use nag_precisions, Only: wp
! .. Implicit None Statement ..
    Implicit None
! .. Local Scalars ..
    Type (c_ptr) :: hddesc, hform, hxdesc
    Integer :: i, ierr, ifail, ip, lddat, ldx, &
    lisx, lplab, lvinfo, lvnames, mx, &
    nobs, nvar, sddat, sdx
    Character (200)
:: formula, intcpt, line, tcontrast, &
    tvname
! .. Local Arrays ..
    Real (Kind=wp), Allocatable :: dat(:,:), x(:,:)
    Real (Kind=wp) : : tx (0,0)
    Integer, Allocatable :: isx(:), levels(:), vinfo(:)
    Character (50), Allocatable :: plab(:), vnames(:)
    .. Intrinsic Procedures ..
    Intrinsic :: trim
.. Executable Statements ..
    Write (nout,*) 'G22YCF Example Program Results'
    Write (nout,*)
    hform = c_null_ptr
    hddesc = c__null__ptr
    hxdesc = c_null_ptr
! Skip heading in data file
```

```
Read (nin,*)
Read in the formula for the first specification of the model,
remove comments and parse it
Call read_line(ierr,formula)
ifail = 0
Call g22yaf(hform,formula,ifail)
Read in the contrast to use for all parameters, remove comments and
set the contrast optional parameter
Call read_line(ierr,tcontrast)
line = 'Contrast=' // trim(tcontrast)
ifail = 0
Call g22zmf(hform,line,ifail)
! Read in size of the data matrix and number of variable labels supplied
Read (nin,*) nobs, nvar, lvnames
! Read in number of levels and names for the variables
    Allocate (levels(nvar),vnames(lvnames))
    Read (nin,*) levels(1:nvar)
    If (lvnames>0) Then
    Read (nin,*) vnames(1:lvnames)
    End If
! Create a description of the data matrix
    ifail = 0
    Call g22ybf(hddesc,nobs,nvar,levels,lvnames,vnames,ifail)
! Read in the data matrix and response variable
    lddat = nobs
    sddat = nvar
    Allocate (dat(lddat,sddat))
    Read (nin,*)(dat(i,1:nvar),i=1,nobs)
! Calculate the size of the design matrix
    ldx = 0
    sdx = 0
    ifail = 1
    Call g22ycf(hform,hddesc,dat,lddat,sddat,hxdesc,tx,ldx,sdx,mx,ifail)
    If (ifail/=91) Then
    redisplay any error messages, other than IFAIL = 91
    ifail = 0
    Call g22ycf(hform,hddesc,dat,lddat,sddat,hxdesc,tx,ldx,sdx,mx,ifail)
    End If
! Generate the design matrix, X
    ldx = nobs
    sdx = mx
    Allocate (x(ldx,sdx))
    ifail = 0
    Call g22ycf(hform,hddesc,dat,lddat,sddat,hxdesc,x,ldx,sdx,mx,ifail)
! Generate labels for the columns of X
    lplab = mx + 1
    lvinfo = 0
    lisx = 0
    Allocate (isx(lisx),vinfo(lvinfo),plab(lplab))
    ifail = 0
    Call g22ydf(hform,hxdesc,intcpt,ip,lisx,isx,lplab,plab,lvinfo,vinfo, &
    ifail)
    Display the design matrix
    Call print_x(intcpt,plab,nobs,mx,x,'First')
c_lp: Do
! Read in the name of the variable whose contrasts need to be changed,
    the value to change them to, remove comments and set the contrast
    optional argument for the specified variable
    Call read_line(ierr,tvname,tcontrast)
    If (ierr/=0) Then
```

```
            Exit c_lp
            End If
            line = 'Contrast:' // trim(tvname) // '=' // trim(tcontrast)
            ifail = 0
            Call g22zmf(hform,line,ifail)
    End Do c_lp
    Regenerate the design matrix using the new contrasts
    (the size of X should be the same as previously)
    ifail = 0
    call g22ycf(hform,hddesc,dat,lddat,sddat,hxdesc,x,ldx,sdx,mx,ifail)
! Generate labels for the columns of X
    ifail = 0
    Call g22ydf(hform,hxdesc,intcpt,ip,lisx,isx,lplab,plab,lvinfo,vinfo, &
        ifail)
! Display the design matrix
    Write (nout,*)
    Call print_x(intcpt,plab,nobs,mx,x,'Second')
    Clean-up the G22 handles
    ifail = 0
    Call g22zaf(hform,ifail)
    Call g22zaf(hddesc,ifail)
    Call g22zaf(hxdesc,ifail)
    Deallocate (dat,x)
    Deallocate (isx,levels,vinfo)
    Deallocate (plab,vnames)
End Program g22ycfe
```


### 10.2 Program Data

```
G22YCF Example Program Data
F1*F2*Con - F1.F2.Con :: FORMULA
Sum First :: contrast to use
25 3 :: NOBS,NVAR,LVNAMES
3 1 :: LEVELS
F1 F2 Con :: VNAMES
3 1 -2.4
3 3 0.2
1 3 -1.4
2 1 -5.4
3 0.2
3 2 1.4
126.8
126.7
1 5.3
3-1.3
2 -3.6
2 -0.7
1 5.7
3 2.3
2 3.3
3-0.5
1 -2.6
2 3.7
2 0.9
    1 -1.1
    2 . 1
34.6
34.6
2 5.1
1 3 0.9 :: DAT
F1 Helmert
F2 Polynomial :: new contrasts to use
```


### 10.3 Program Results



## 11 Optional Parameters

As well as the optional parameters common to all G22 handles described in $\mathbf{g 2 2 z m f}$ and $\mathbf{g 2 2 z n f}$, a number of additional optional parameters can be specified for a G22 handle holding the description of a design matrix as returned by g22ycf in hxdesc.
The value of an optional parameter can be queried using g22znf.
The remainder of this section can be skipped if you wish to use the default values for all optional parameters.
The following is a list of the optional parameters available. A full description of each optional parameter is provided in Section 11.1.

## Formula

Min Number of Columns
Number of Columns
Number of Observations

## Storage Order

### 11.1 Description of the Optional Parameters

For each option, we give a summary line, a description of the optional parameter and details of constraints.

The summary line contains:
a parameter value, where the letters $a, i$ and $r$ denote options that take character, integer and real values respectively;

Keywords and character values are case and white space insensitive.

## Formula

## $a$

Read Only
This optional parameter returns a verbose formula string describing the model, $\mathcal{M}$, used to create the design matrix. This formula will only contain variable names, the operators ' + ' and '.' and any contrast identifiers present.

Min Number of Columns
$i$
Read Only
This optional parameter returns the minimum number of columns required to hold the design matrix, $X$. In most cases Min Number of Columns = Number of Columns. The one exception is when ifail $=71$, that is the size of $\mathbf{x}$ was too small but the data matrix given in dat can be used as the design matrix. In this case, Number of Columns $=m_{x}=m_{d}$ and Min Number of Columns holds the number of columns that would be required if only the relevant parts of dat were copied into a new array.

## Number of Columns

## $i$

Read Only
This optional parameter returns $m_{x}$, the number of columns in the design matrix.

## Number of Observations

 $i$Read Only
This optional parameter returns $n$, the number of observations in the design matrix.

## Storage Order

 $a$Read Only
This optional parameter returns how the design matrix, $X$, is stored in $\mathbf{x}$.
If Storage Order $=$ OBSVAR, $X_{i j}$, the value for the $j$ th variable of the $i$ th observation of the design matrix is stored in $\mathbf{x}(i, j)$.
If Storage Order $=$ VAROBS, $X_{i j}$, the value for the $j$ th variable of the $i$ th observation of the design matrix is stored in $\mathbf{x}(j, i)$.
It should be noted that Storage Order is not writeable. If you wish to change the storage order of the design matrix you need to change Storage Order in hform as described in Section 11 in g22yaf prior to calling g22ycf.

