# Manual supplement for MLwiN Version 2.36 



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March 2016

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ISBN: 978-0-903024-98-3
Printed in the United Kingdom

First Printing September 2008.
Updated for University of Bristol, October 2009.
Updated for University of Bristol, September 2012.
Updated for University of Bristol, August 2014.

Updated for University of Bristol, March 2016.

## New Features

New features for version 2.1 include:

1. Improved model specification functionality
2. A new Customised predictions window for constructing and graphing model predictions
3. Basic surface plotting with rotation
4. Creation and export of model comparison tables
5. A new method for estimating autocorrelated errors in continuous time
6. Saving and retrieving of Minitab, Stata, SPSS and SAS data files
7. Saving and retrieving of MLwiN worksheets in a compressed (zipped) format
8. New data manipulation commands

## Acknowledgements

Thanks to Mike Kelly for converting this document from Word to $\mathrm{EA}_{\mathrm{E}} \mathrm{X}$.

## 1 Improved model specification functionality

When variables and interactions were created in previous versions, recoding main effects (centring, changing reference categories) did not result in automatic recoding of the same variables wherever they appeared in interactions. Interactions and main effects had to be removed, main effects recoded and then main effects and interactions re-entered. This can be a time consuming and error prone process. In the latest version, polynomials are created by specifying an optional order. If the polynomial order, reference category (for a categorical variable) or the type of centring used for a main effect are changed then all interactions involving that variable are updated.

### 1.1 Recoding: reference categories, centring, and polynomials

For example, the model below, which uses the tutorial dataset used in chapters 1-6 of the MLwiN User's Guide, contains main effects for the continuous variable standlrt and the categorical variable schgend (consisting of dummy variables mixedsch, boysch, and girlsch) and the interaction of standlrt and schgend.

| @. Equations $\quad$ - |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} \text { normexam }_{i j} \sim & \mathrm{~N}(X B, \Omega) \\ \text { normexam }_{i j}= & \beta_{0 i j} \text { cons }+\beta_{1} \text { standlrt }_{i j}+\beta_{2} \text { boysch }_{j}+\beta_{3} \text { girlsch }_{j}+ \\ & \beta_{4} \text { standlrt.boysch }_{i j}+\beta_{5} \text { standlrt.girlsch }_{i j} \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |
| $\beta_{0 i j}=\beta_{0}+u_{0 j}+e_{0 i j}$ |  |  |  |  |  |  |  |  |  |  |
| $\left[u_{0 j}\right] \sim \mathrm{N}\left(0, \Omega_{u}\right): \Omega_{u}=\left[\sigma_{u 0}^{2}\right]$ |  |  |  |  |  |  |  |  |  |  |
| $\left[e_{0 i j}\right] \sim \mathrm{N}\left(0, \Omega_{e}\right): \Omega_{e}=\left[\sigma_{e 0}^{2}\right]$ |  |  |  |  |  |  |  |  |  |  |
| 11 |  |  |  |  |  |  |  |  |  |  |
| Name | + | - | Add İerm | Estimates | Honlinear | Clear | Notation | Responses | Store | Help |

In previous versions, to change the reference category for schgend from mixedsch to boysch required:

- Click on term standlrt.boysch
- In the window that appears, click the delete Term button
- When asked if the term is to be deleted, select Yes
- Click on term schgend
- In the window that appears, click the delete Term button
- When asked if the term is to be deleted, select Yes
- Click on the Add Term button
- Select schgend in the variable drop-down list
- Select boysch in the drop-down list labelled reference category
- Click the Done button
- Click on the Add Term button
- Select 1 from the drop-down list labelled order
- Select standlrt in the first variable drop-down list
- Select schgend in the second variable drop-down list
- Select boysch in the drop-down list labelled reference category
- Click the Done button

In version 2.1 the same operation is achieved by:

- Click on the term boysch (or any term that involves schgend categories)
- In the window that appears click the Modify Term button
- Select boysch in the drop-down list labelled ref cat
- Click the Done button

Which produces:


The new form of the Specify term window for a continuous term can be seen if you:

- Click on the term standlrt
- In the window that appears click the Modify Term button

This produces the Specify term window:


If polynomial is ticked then a drop-down list appears for the degree of the polynomial. Continuous variables can be uncentred, centred around means of groups defined by codes contained in a specified column, centred around the grand mean (i.e. the overall mean) or centred around value. Thus,

- Click on the polynomial check box
- A drop-down list labelled poly degree will appear; select 3
- Click the Done button in the Specify term window
produces:


Note that changing standlrt to be a cubic polynomial also updates the interaction of standlrt and schgend to be cubic with respect to standlrt. If you want a cubic main effect for standlrt but interaction terms with schgend to be linear with respect to standlrt then click on any of the interaction terms and set the degree of polynomial for standlrt to be 1 .

### 1.2 Orthogonal Polynomials

### 1.2.1 Orthogonal Polynomials

Orthogonal polynomials are useful when fitting variables measured on an ordinal scale as predictors in models. An example would be Age with categories 21-30, 31-40, 41-50 and on. Instead of fitting the ordinal variable as a constant and a contrasted set of dummies (with one left out), we fit it as an orthogonal polynomial of degree at most one less than the number of categories. We thus have at most the same number of variables making up the orthogonal polynomial as we would have dummies if we fitted the ordinal variable using that specification. Unlike the dummies, the variables comprising the terms of the orthogonal polynomial are not $(0,1)$ variables. They contain values between -1 and 1 . For each term, there is a different value for each category of the ordinal variable. These values depend only on the number of categories the ordinal variable has. The values for ordinal variables with 3,4 and 6 categories are shown below. The values give the terms of the polynomial certain properties when the data are balanced:

- They are orthogonal. In mathematical terms this means that if you pick any two terms of the polynomial, and for each category multiply the value for that category for the first term by the value for that category for the second term, then add these products together, the result will be 0 : for example, picking the two terms of the polynomial for a 3 category variable, $-0.707 \times 0.408+0 \times-0.816+0.707 \times 0.408=0$. In statistical terms, this means that each pair of terms is uncorrelated, which turns out to be useful in modelling as we will see later: in particular estimates associated with these orthogonal variables are likely to be numerically stable.
- They each have the same mean and variance. The mean is always 0 but the variance depends on the number of categories in the ordinal variable. Again this will turn out to be useful in modelling
- Each term is a function of the appropriate power of some value. In other words, the linear term is always a linear function of some value, the quadratic term is a quadratic function of some value, the cubic term is a cubic function of some value and so on. Consequently, when an intercept and the full set of terms are included in the model, they can completely capture the effects of all the categories of the ordinal variable on the response, no matter what those effects are. Another consequence of this property is that in many cases we can achieve a more parsimonious model by using a subset of the terms, as we will see. The linear term captures the linear effect across categories of the ordinal variable, the quadratic term captures the quadratic effect, and so on. We cannot of course achieve this if we use an intercept plus a set
of contrasted dummies: to leave a dummy out means conflating that category with the reference category.

Note that the current implementation in MLwiN assumes that the categories of the ordinal variable are equally spaced.

Below are three examples of coding when 3, 4 and 6 categories of an ordered variable are included (it is presumed that the model contains a constant).

## Categorical Variables Codings for 3 categories

|  |  | Parameter coding |  |
| :--- | :--- | :--- | :--- |
|  | Linear | Quadratic |  |
| 3 groups | 1 | -.707 | .408 |
|  | 2 | .000 | -.816 |
|  | 3 | .707 | .408 |

## Categorical Variables Codings for 4 categories

|  |  | Parameter coding |  |  |
| :--- | :--- | :--- | :--- | :--- |
|  | Linear | Quadratic | Cubic |  |
| 4 groups | 1 | -.671 | .500 | -.224 |
|  | 2 | -.224 | -.500 | .671 |
|  | 3 | .224 | -.500 | -.671 |
|  | 4 | .671 | .500 | .224 |

## Categorical Variables Codings for 6 categories

|  |  | Parameter coding |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | Linear | Quadratic | Cubic | $4^{\text {th }}$ order | $5^{\text {th }}$ order |  |
| 6 groups | 1 | -.598 | .546 | -.373 | .189 | -.063 |
|  | 2 | -.359 | -.109 | .522 | -.567 | .315 |
|  | 3 | -.120 | -.436 | .298 | .378 | -.630 |
|  | 4 | .120 | -.436 | -.298 | .378 | .630 |
|  | 5 | .359 | -.109 | -.522 | -.567 | -.315 |
|  | 6 | .598 | .546 | .373 | .189 | .063 |

As an example we will work with the tutorial dataset and turn standlrt into 4 ordered categories: this requires 3 cut points; we use the nested means procedure explained in Section 2.1.4 to get our values. Note that we are making standlrt into an ordinal variable purely to show the operation of the orthogonal polynomial feature; if we were really performing some analysis
using a continuous variable like standlrt this would not be a recommended procedure. The nested means when rounded are $-0.81,0.00$, and 0.76 and we use these values to recode the data into 4 groups via the recode $\rightarrow$ by range option from the Data manipulation menu:


- In the Names window, change the name of $\mathbf{c 1 1}$ to be LRTgrps
- Click on Toggle categorical to change it from a continuous to an ordinal variable (note that the orthogonal polynomial facility can only be accessed when the variable has been predefined as categorical)

For purposes of comparison we begin with the 4 groups included in the model in the usual way for categorical variables i.e. as a constant and three contrasted dummies. We will then go on to see whether we can fit a more parsimonious model using orthogonal polynomials.

Start by setting up the model as follows:

| E. Equations $\quad$ - |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} & \operatorname{normexam}_{i j} \sim \mathrm{~N}(X B, \Omega) \\ & \text { normexam }_{i j}=\beta_{0 i j} \operatorname{cons} \\ & \beta_{0 i j}=-0.013(0.054)+u_{0 j}+e_{0 i j} \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| $\left[u_{0 j}\right] \sim \mathrm{N}\left(0, \Omega_{u}\right): \Omega_{u}=[0.169(0.032)]$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\left[e_{0 i j}\right] \sim \mathrm{N}\left(0, \Omega_{e}\right): \Omega_{e}=[0.848(0.019)]$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $-2 * \operatorname{loglikelihood}($ IGLS Deviance $)=11010.648(4059$ of 4059 cases in use) |  |  |  |  |  |  |  |  |  |  |  |  |
| Name | + | - | Add İerm | Estimates | Honlinear | Clear | Notation | Responses | Store | Help | Zoom 100 | $\square$ |

- Click on Add Term
- From the variable drop-down list select LRTgrps
- From the ref cat drop-down list select LRTgrps_1


We now fit a model with LRTgrps entered as an orthogonal polynomial instead of as three dummies. We start by including all three terms of the orthogonal polynomial. First, though, we need to change the tolerance used by MLwiN. The tolerance is set by default to a value which is most appropriate for the most commonly used kinds of estimation. However, using this value of the tolerance when working with orthogonal polynomials can lead to the wrong values being calculated for the terms of the polynomial, which in turn leads to incorrect estimates for the coefficients. This is particularly true when the categorical variable has a larger number of categories. To change the tolerance,

- From the Data Manipulation window, select Command interface
- In the Command interface window, type CTOL 10

The tolerance is now set to a value of $10^{10}$. This should be sufficient in most cases. The default tolerance that MLwiN normally uses is $10^{6}$ and the tolerance can be set back to this value by typing CTOL 6 in the Command interface window. This should be done after working with orthogonal polynomials as using a tolerance of $10^{10}$ can cause problems in other areas.

We can now proceed to set up the model

- Click on any of the three LRTgrps dummies
- Click on the Delete Term button
- Click Yes
- Click on the Add Term button
- Select LRTgrps from the variable drop-down list
- Tick the orthogonal polynomial box
- From the orthog poly degree drop-down list select 3 (note that the greatest degree that the software will allow you to specify is always one less than the number of categories)
- Click Done

| E. Equations $\quad$ - |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} \operatorname{normexam}_{i j} \sim & \mathrm{~N}(X B, \Omega) \\ \text { normexam }_{i j}= & \beta_{0 i j} \text { cons }+1.134(0.027) \operatorname{orthog}_{2} \text { LRTgrps }^{\wedge} 1_{i j}+ \\ & 0.041(0.025) \text { orthog_LRTgrps }^{\wedge} 2_{i j}+ \\ & 0.060(0.023) \text { orthog_LRTgrps }{ }^{\wedge} 3_{i j} \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| $\beta_{0 i j}=-0.017(0.043)+u_{0 j}+e_{0 i j}$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\left[u_{0 j}\right] \sim \mathrm{N}\left(0, \Omega_{u}\right): \Omega_{u}=[0.105(0.020)]$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\begin{aligned} & {\left[e_{0 i j}\right] \sim \mathrm{N}\left(0, \Omega_{e}\right): \Omega_{e}=[0.596(0.013)]} \\ & -2 * \text { loglikelihood(IGLS Deviance })=9571.227(4059 \text { of } 4059 \text { cases in use }) \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| Name | + | - | Add İerm | Estimates | Honlinear | Clear | Notation | Responses | Store | $\underline{H}$ elp | Zoom 100 |  |

Three new variables containing the appropriate values are automatically generated as appropriately named columns in the worksheet and added to the model:

| E. |  | Data |  |  |  |  | - $\square$ |  |  | x |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| goto lin | ne 1 | view | Help | Font |  | V Show value labels |  |  |  |  |
|  | standlit( 4059) | orthog | LRTgr |  | ortho | g_LRTgrps ${ }^{\wedge}$ | orthog_ | RTgrp |  |  |
| 1 | 0.619 | 0.224 |  |  | -0.50 |  | -0.671 |  |  |  |
| 2 | 0.206 | 0.224 |  |  | -0.50 |  | -0.671 |  |  |  |
| 3 | -1.365 | -0.671 |  |  | 0.500 |  | -0.224 |  |  |  |
| 4 | 0.206 | 0.224 |  |  | -0.50 |  | -0.671 |  |  |  |
| 5 | 0.371 | 0.224 |  |  | -0.50 |  | -0.671 |  |  |  |
| 6 | 2.189 | 0.671 |  |  | 0.500 |  | 0.224 |  |  |  |
| 7 | -1.117 | -0.671 |  |  | 0.500 |  | -0.224 |  |  |  |
|  | 1021 | n 671 |  |  | - 50 |  | 0221 |  |  |  |
| $<$ |  |  |  |  |  |  |  |  | > | $\checkmark$ |

At this point the model is equivalent to our first model with LRTgrps entered as dummies: it has the same deviance and the estimates for the random part are identical, although the coefficients are different because the terms of the polynomial are measured on a different scale to the dummies and the intercept now has a different value because it is the average value of the response when all three terms of the polynomial are 0 , not the average value of the response for the reference category of LRTgrps. We can see in the graph below that these two models give us the same results.

The important difference is that the four group model is not readily reducible whereas the orthogonal polynomial one is. The three terms all have the same mean and variance so their coefficients are directly comparable and so it is
clear from the estimates that the linear effect is markedly bigger than the quadratic and cubic, thereby suggesting that the model be simplified to have just a linear trend across all four ordered categories. We fit a model using just a linear effect:

- Click on any of the terms of the orthogonal polynomial
- Click Modify Term
- Select 1 from the orthog poly degree drop-down list
- Click Done

The graph shows that the linear trend model well captures the underlying trend in a parsimonious way. We have thus succeeded in simplifying our model without losing much information.


### 1.2.2 Using orthogonal polynomials with repeated measures data

Orthogonal polynomials are especially useful with repeated measures data and fitting a more parsimonious model is not the only reason to use them. Hedeker and Gibbons (2006)(3) give the following reasons to use orthogonal polynomials in their discussion of growth curves for longitudinal data where the predictor representing time is not a continuous variable but $1,2,3$ etc representing the first, second and third occasion on which the person has been measured:

- for balanced data, and compound symmetry structure (that is a vari-
ance components model), estimates of polynomial fixed effects (e.g. constant and linear) do not change when higher-order polynomial terms (e.g. quadratic and cubic) are added to the model
- using the original scale, it gets increasingly difficult to estimate higherdegree non-orthogonal polynomial terms
- using orthogonal polynomials avoids high correlation between estimates (which can cause estimation problems)
- using orthogonal polynomials provides comparison of the 'importance' of different polynomials, as the new terms are put on the same standardized (unit) scale. This holds exactly when the number of observations at each timepoint are equal, and approximately so when they are unequal.
- the intercept (and intercept-related parameters) represents the grand mean of the response, that is, the model intercept represents the mean of the response at the midpoint of time.

Another reason for using them is the orthogonality property: since each pair of terms in the polynomial are orthogonal, i.e. uncorrelated, the coefficients of the terms do not change according to which other terms are included. This means that if we decide that the linear and quadratic effects are the most important based on the model using all terms and go on to fit a model including just the linear and quadratic terms, we will not find for example that now the higher order terms have been removed, the quadratic effect is no longer important.

As an example of using orthogonal polynomials with repeated measures data, we will use the reading1 dataset which forms the basis for analysis in Chapter 13 of the User's Guide. We begin with the variance components model of page 184 (you will need to follow the instructions on pages 197 to 200 and 202 to get the data in the correct form to set this model up and create a constant column):

| E. Equations $\quad$ - |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} & \text { reading }_{i j} \sim \mathrm{~N}(X B, \Omega) \\ & \text { reading }_{i j}=\beta_{0 i j} \text { cons } \\ & \beta_{0 i j}=7.115(0.053)+u_{0 j}+e_{0 i j} \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\left[u_{0 j}\right] \sim \mathrm{N}\left(0, \Omega_{u}\right): \Omega_{u}=[0.078(0.083)]$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\begin{aligned} & {\left[e_{0 i j}\right] \sim \mathrm{N}\left(0, \Omega_{e}\right): \Omega_{e}=[4.561(0.172)]} \\ & -2 \text { *loglikelihood(IGLS Deviance })=7685.737(1758 \text { of } 2442 \text { cases in use }) \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| Name | + | - | Add İerm | Estimates | Honlinear | Clear | Notation | Responses | Store | Help | Zoom 100 |  |

We are going to pretend that we do not know the age at which the reading score was evaluated but only know that the reading was taken on 1st, 2nd,

3rd etc occasion. We can fit a linear trend by putting 'occasion' into the fixed part of the model:

- In the Names window, highlight occasion and click Toggle categorical
- Add occasion to the model


The estimate 3.235 gives the mean Reading score at occasion 0 (that is the occasion before the first measurement!) and the mean reading score improves by 1.19 for each subsequent occasion. We can now fit a similar model but replacing occasion by the linear orthogonal variable.

- Click on occasion
- Click Delete Term
- In the Names window, highlight occasion and click Toggle Categorical
- In the Equations window, click Add Term
- From the variable drop-down list select occasion
- Tick the orthogonal polynomial box
- From the orthog poly degree drop-down list select 1
- Click Done

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} & \text { reading }_{i j} \sim \mathrm{~N}(X B, \Omega) \\ & \text { reading }_{i j}=\beta_{0 i j} \text { cons }+4.977(0.049) \text { orthog_occasion } 1_{i j} \\ & \beta_{0 i j}=7.399(0.042)+u_{0 j}+e_{0 i j} \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |  |
| $\left[u_{0 j}\right] \sim \mathrm{N}\left(0, \Omega_{u}\right): \Omega_{u}=[0.552(0.049)]$ |  |  |  |  |  |  |  |  |  |  |  |  |  |
| $\begin{aligned} & {\left[e_{0 i j}\right] \sim \mathrm{N}\left(0, \Omega_{e}\right): \Omega_{e}=[0.539(0.021)]} \\ & -2 * \text { loglikelihood(IGLS Deviance })=4563.926(1758 \text { of } 2442 \text { cases in use }) \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Name | + | - | Add İerm | Estimates | Honlinear | Clear | Notation | Responses | Store | Help | Zoom |  | $\checkmark$ |

The deviance and the random part are the same (as is the Wald test for the growth term), but now the estimate of the intercept gives the grand mean at the mid-point of the occasions and the slope gives the improvement in reading with a unit change in the linear orthogonal polynomial. We now add the quadratic orthogonal polynomial into the model using the Modify Term option and should find that the linear term does not change (in fact it does a bit due to imbalance in the data). It is clear that the quadratic term is of much less 'importance' than the linear term.


Using the Predictions and Customised graphs windows we can see the quadratic growth curve which is characterized by a strong linear trend, with some slight curvature. We can now add in all the other polynomials (there is then a term for each occasion) and it is clear that there are 'diminishing returns' as each additional order is included

| Equations |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} \text { reading }_{i j} \sim & \mathrm{~N}(X B, \Omega) \\ \text { reading }_{i j}= & \beta_{0 i j} \text { cons }+5.139(0.038) \text { orthog_occasion^} 1_{i j}+ \\ & 0.951(0.036) \text { orthog_occasion^}{ }_{i j}+0.651(0.034) \text { orthog_occasion }{ }^{\wedge} 3_{i j}+ \\ & 0.322(0.032) \text { orthog_occasion^} \wedge_{i j}+0.097(0.031) \text { orthog_occasion } 5_{i j} \\ \beta_{0 i j}= & 7.442(0.041)+u_{0 j}+e_{0 i j} \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |
| $\left[u_{0 j}\right] \sim \mathrm{N}\left(0, \Omega_{u}\right): \Omega_{u}=[0.594(0.048)]$ |  |  |  |  |  |  |  |  |  |  |  |
| $\begin{aligned} & {\left[e_{0 i j}\right] \sim \mathrm{N}\left(0, \Omega_{e}\right): \Omega_{e}=[0.307(0.012)]} \\ & -2 * \text { loglikelihood(IGLS Deviance })=3786.824(1758 \text { of } 2442 \text { cases in use }) \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |
| Nam | + | Add Ierm | Estimates | Honlinear | Clear | Notation | Responses | store | Help | zoom | 100 |

but all terms have some effect: with even the 5th order term having a p value of 0.002

| E. Intervals and tests |  |  |  |  | - $\times$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | \#1 | \#2 | \#3 | \#4 | \#5 |
| fixed : cons | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| fixed : orthog_occasion^1 | 1.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| fixed : orthog_occasion ${ }^{\wedge} 2$ | 0.000 | 1.000 | 0.000 | 0.000 | 0.000 |
| fixed : orthog_occasion^3 | 0.000 | 0.000 | 1.000 | 0.000 | 0.000 |
| fixed : orthog_occasion^4 | 0.000 | 0.000 | 0.000 | 1.000 | 0.000 |
| fixed : orthog_occasion^5 | 0.000 | 0.000 | 0.000 | 0.000 | 1.000 |
| constant(k) | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 |
| function result(f) | 5.139 | 0.951 | 0.651 | 0.322 | 0.097 |
| f-k | 5.139 | 0.951 | 0.651 | 0.322 | 0.097 |
| chi sq, (f-k)=0. (1df) | 18742.505 | 716.205 | 370.086 | 100.650 | 9.691 |
| +/-95\% sep. | 0.074 | 0.070 | 0.066 | 0.063 | 0.061 |
| +/-95\% joint | 0.125 | 0.118 | 0.113 | 0.107 | 0.104 |
| joint chisq test(5df) $=19121.209$ |  |  |  |  |  |
| $C$ random fixed \# of functions 5 |  | Calc |  |  |  |

As in the example using the tutorial dataset, this model which fits an intercept and 5 growth terms is equivalent to fitting a separate parameter for each occasion; the graph below makes this clear. However we can readily leave out one or more terms of the orthogonal polynomial to achieve a more parsimonious model; the same is not true of the intercept and dummy variables specification.

## Two equivalent ways of entering Occasion


(Note that the way the response has been constructed will have a great effect on these results; see page 178 of the User's Guide)

The tolerance should now be set back to the default value before working further in MLwiN

- In the Command interface window, type CTOL 6


### 1.3 Commands

The ADDT command has been extended to allow specification of polynomial terms:

```
ADDT C <mode N}>\mathbf{C}<\mathrm{ mode N}
```

Create a main effect or interaction term from a series of one or more variables. Each variable can be categorical or continuous. Categorical variables can have a reference category specified, by setting the corresponding mode value to the number of the reference category. If no reference category is specified, then the lowest category number is taken as the reference category. If -1 is given as the reference category then no reference category is assumed and a full set of dummies are produced. Variables of appropriate names and data patterns are created and added as explanatory variables. If $N>10000$, then $N-10000$ is taken to be the polynomial degree that is required for the corresponding variable. If the corresponding variable is categorical then an orthogonal polynomial of degree $N-10000$ is fitted.

Examples:

```
ADDT 'standlrt' }10003\mathrm{ 'schgend'
```

adds an interaction between a cubic in standlrt and 2 dummies for schgend with reference category mixedsch.

```
ADDT 'standlrt' 'schgend' }1000
```

adds an interaction term between 'standlrt' and an orthogonal polynomial of degree 2 for schgend.

The SWAP command edits a main effect and updates all affected interactions

SWAP main effect $\mathbf{C}$ with $\mathbf{C}$ mode $\mathbf{N}$

Mode N has the same meaning as in the ADDT command.
Examples:

```
SWAP 'standlrt' 'standlrt' 10003
```

removes standlrt as a main effect and all interactions involving standlrt from the model and replaces them with a cubic polynomial in standlrt; note all interactions involving standlrt are also replaced.

Note that the SWAP command will not do anything if the variable you ask to swap is only present in an interaction term.

The CENT command controls centring for continuous explanatory variables

CENT mode 0: uncentred
CENT mode 1: around grand mean
CENT mode 2: around means of groups defined by codes in $\mathbf{C}$
CENT mode 3: around value $\mathbf{N}$

Examples:

- CENT 2 'school'
- ADDT 'standlrt'
adds the variable standlrt to the model centered around the group mean of standlrt, where groups are defined by the codes in the column 'school'

```
    CENT O
- ADDT 'standlrt'
```

adds standlrt to the model with no centring.
The default for CENT is no centring: if ADDT is used without CENT having been previously used, then the term is added with no centring. The kind of centring set up by use of the CENT command remains in place until the CENT command is used again to change it: it is not necessary to use the CENT command before every ADDT if the same kind of centring is required in each case.

## 2 Out of Sample predictions

### 2.1 Continuous responses

The current Predictions window generates a predicted value of the response for each level 1 unit in the dataset, using their values of the explanatory variables. Thus, predictions are only generated for the combinations of values of the explanatory variables occurring in the dataset. Often, however, we want to generate predictions for a specific set of explanatory variable values to best explore a multidimensional model predictions space.

We have added a Customised Predictions window, with an associated plot window, to aid this task by allowing predictions to be generated for any desired combinations of explanatory variable values, whether or not these combinations occur in the dataset. Given the model on the tutorial data

| Equations $\quad-\mathrm{a}$ x |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} & \text { normexam }_{i j} \sim \mathrm{~N}(X B, \Omega) \\ & \text { normexam }_{i j}=\beta_{0 i j} \text { cons }+\beta_{1 j} \text { standlrt }_{i j}+0.374(0.109) \text { avslrt }_{j}+ \\ & \quad 0.162(0.057) \text { standlrt.avslrt }_{i j} \\ & \beta_{0 i j}=-0.007(0.037)+u_{0 j}+e_{0 i j} \\ & \beta_{1 j}=0.558(0.019)+u_{1 j} \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\left[\begin{array}{l}u_{0 j} \\ u_{1 j}\end{array}\right] \sim \mathrm{N}\left(0, \Omega_{u}\right): \Omega_{u}=\left[\begin{array}{ll}0.074(0.015) & \\ 0.011(0.006) & 0.011(0.004)\end{array}\right]$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\begin{aligned} & {\left[e_{0 i j}\right] \sim \mathrm{N}\left(0, \Omega_{e}\right): \Omega_{e}=[0.554(0.012)]} \\ & -2 * \text { loglikelihood(IGLS Deviance })=9302.911(4059 \text { of } 4059 \text { cases in use }) \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| Name | + | - | Add İerm | Estimates | Honlinear | Clear | Notation | Responses | Store | Help | Zoom 100 |  |

where avslrt is the school mean for standlrt, we can use the old Predictions window to explore this relationship


This window applies the specified prediction function to every point in the dataset and produces a predicted value for each point. If we plot these
predictions, grouped by school, we get


This plot has one line for each school; the line for the $j$ th school is given by the prediction equation $\left(\hat{\beta}_{0}+\hat{\beta}_{2} \mathbf{a v s l r t}_{j}\right)+\left(\hat{\beta}_{1}+\hat{\beta}_{3}\right.$ avslrt $\left._{j}\right)$ standlrt $_{i j}$. However, it might be more revealing to plot lines for a small number of different values of avslrt, say $\{-0.5,0,0.5\}$

The Customised predictions window will now do this and other such prediction tasks automatically for us.

- Select Customised Predictions from the Model menu.

The following screen appears:


Main effects are listed in the setup pane. We can click on them and specify a set of values we want to make a prediction dataset for.

- Highlight standlrt
- Click Change Range

We see:


Currently the value is set to the mean of standlrt. We can specify a set of values for the predictor variables for which we want to make predictions.

We can do this for continuous variables as a set of Values, as a Range, as Percentiles, or Nested Means Here we use a range, postponing discussion of the other options until later.

Note that, whether we specify values as a set of values, as a range, as percentiles, or as nested means, we are setting values for the original predictor variable. If for example we have centred the variable using one of the options in the Specify Term window, or via the CENT and ADDT commands, then we specify values for the uncentred variable, not for the centred variable. The same applies for other transformations such as polynomials, as long as the transformation was carried out as part of entering the variable into the model, via the Specify Term window or the ADDT command. MLwiN will display the name of the original, untransformed variable in the Customised predictions and will apply the necessary transformation to produce transformed values to use in calculating the prediction. This behaviour makes it easier for the user to specify a range of values and also enables plotting predictions against the original rather than the transformed variable.

### 2.1.1 Setting values as a range

The output column is set by default to the next free column (c13 in this case)

- Click the Range tab and specify Upper Bound: 3, Lower: -3 , Increment: 1
- Click the Done button to close the Values to include window
- Using the same procedure, set the range for avslrt to be Upper Bound: 0.5, Lower: -0.5 , Increment: 0.5
- Click Fill Grid and Predict
- Select the Predictions tab

The Fill Grid button creates a mini dataset with all combinations of the explanatory variable values you have specified. The Predict button takes the estimates for the parameters of the current model and applies them to the mini dataset to create predicted values with confidence intervals.

| E9. |  | Customised predictions |  |  |  |  |  | - | - $\times$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Copy |  |  |  |  |  |  |  |  |  |
| Setup |  |  |  |  |  | Predictions |  |  |  |  |
| cons.pred |  | standirt.pred |  | avsirt.pred |  | mean.pred | mean.low.pre | mean.high.pr |  |  |
| 1.000 |  |  | -3.000 |  | -0.500 | -1.621 | -1.820 |  | -1.432 |  |
| 1.000 |  |  | -2.000 |  | -0.500 | -1.144 | -1.299 |  | -0.996 |  |
| 1.000 |  |  | -1.000 |  | -0.500 | -0.668 | -0.789 |  | -0.551 |  |
| 1.000 |  |  | 0.000 |  | -0.500 | -0.192 | -0.316 |  | -0.070 |  |
| 1.000 |  |  | 1.000 |  | -0.500 | 0.286 | 0.126 |  | 0.442 |  |
| 1.000 |  |  | 2.000 |  | -0.500 | 0.762 | 0.551 |  | 0.968 |  |
| 1.000 |  |  | 3.000 |  | -0.500 | 1.237 | 0.978 |  | 1.492 |  |
| 1.000 |  |  | -3.000 |  | 0.000 | -1.682 | -1.795 |  | -1.567 | $\checkmark$ |
| Fill Grid | Predict |  | Plot G |  |  |  |  |  |  |  |

The columns in this prediction grid have all been created as columns in the worksheet. The columns at the left (cons.pred, standlrt.pred, avslrt.pred) contain the values of the explanatory variables that we specified and requested predictions for; mean.pred contains the predicted value of the response for each combination of explanatory variable values, and mean.low.pred and mean.high.pred contain the lower and upper bounds respectively of the confidence intervals for the predictions.

We can plot these results :

## - Click Plot Grid



This screen has been designed to help construct plots from a multidimensional grid. Here we want

X: standlrt.pred
Y: mean.pred
Grouped by avslrt.pred
that is,


## - Click Apply



The settings for this plot are held in Display 1 of Customised graphs.
We can look at the differences (and the confidence intervals of the differences) from any reference group. For example if we wanted to look at the above plot as differences from avslrt.pred $=-0.5$, then we would

- Select the Customised predictions window
- Tick the Differences checkbox (click the Setup tab first if necessary)
- In the from variable drop-down list select avslrt
- In the box labelled Reference value type -0.5
- Click Predict

The graph will update automatically to look like this:


If we want to put confidence intervals around these differences then, in the Customised prediction plot window:

- Tick the Confidence interval check box

Options appear allowing the confidence intervals to be drawn as bars or lines, with lines as the default.

- Click Apply
- Click the OK button on the warning message which may appear
to produce:


We now discuss the other possibilities for specifying the values of the explanatory variables for which you want predictions.

### 2.1.2 Specification using the Values tab

- Return to the Customised Predictions window
- Highlight standlrt and click the Change Range button
- Click the Values tab
- In the top pane type - $\mathbf{2}$ and click the Add button
- Add the values $\mathbf{0}$ and $\mathbf{3}$ in the same way
- Click Done

Clicking Fill Grid and Predict in the Customised Predictions window will now produce predictions as before but this time taking $\{-2,0,3\}$ as the set of values for standlrt instead of $\{-3,-2,-1,0,1,2,3\}$. Notice that using the Values tab automatically cleared the values previously specified using the Range tab.

Note also that the software will automatically check whether the values you specify are within the range of the variable and an error message will appear if you try to specify a value outside of this range.

### 2.1.3 Specification using the Percentiles tab

- Highlight standlrt and click the Change Range button
- Click the Percentiles tab
- In the top pane type $\mathbf{1 0}$ and click the Add button
- Add the percentiles $\mathbf{5 0}$ and $\mathbf{9 0}$ in the same way
- Click Done

The set of values for standlrt that will be used if Fill Grid and Predict are pressed is now (to 2 d.p.) $\{-1.28,0.04,1.28\}$. These are the 10th, the 50th and the 90th percentile of standlrt respectively. Again, notice that the previously specified values have been automatically removed.

Percentiles are a useful way of specifying values when we would like, for example, a prediction for those with a 'low' value of standlrt, those with a 'mid' value of standlrt, and those with a 'high' value of standlrt because they provide a convenient way of deciding what counts as 'low', 'mid' and 'high', although there is still some subjectivity involved: in this case we could equally well have decided to use, for example, the 25th, 50 th and 75 th percentiles, which would give less extreme values for 'low' and 'high'.

We need not necessarily use three percentiles; we can specify as many as we like, though generally a small number of percentiles will be quite sufficient for what we want here.

### 2.1.4 Specification using the Nested Means tab

Nested means are another way of dividing a numerical variable into groups; again they provide a convenient means of choosing, for example, a 'low', a 'mid' and a 'high' value (if you use 4 groups). Simply put, a set of nested means which divides the values into 4 groups is doing the same thing as quartiles (i.e. the 25 th, 50 th and 75 th percentiles) but using the mean instead of the median. For quartiles, the 2 nd quartile (or 50 th percentile) is the median of the variable. The 1st quartile (or 25th percentile) is the median of the values between the minimum and the 2nd quartile, and the 3rd quartile (or 75 th percentile) is the median of the values between the 2 nd quartile and the maximum. In the same way, to get four groups using nested means we first calculate the mean of the variable and call this MidMean, then calculate the mean of the values between the minimum and MidMean and call this LowMean, and calculate the mean of the values between MidMean and the maximum and call this HighMean; LowMean, MidMean and HighMean are then the divisions between our four groups.

More generally, a frequency distribution is balanced about its mean, and this forms an obvious point of division to give two groups; each of these classes may be subdivided at its own mean; and so on, giving $2,4,8,16, \ldots$, classes.

Evans (1977)(1) claims this approach has desirable 'adaptive' properties
"Since means minimize second moments (sums of squared deviations), they are the balancing points of the part of the scale which they subdivide, with respect to both magnitude and frequency. Class intervals thus defined are narrow in the modal parts of a frequency distribution and broad in the tails. Extreme values are not allowed to dominate, but they do influence the positions of means of various orders so that the less closely spaced the values in a given magnitude range, the broader the classes. For a rectangular frequency distribution, nested means approximate the equal-interval or percentile solutions; for a normal one, they approximate a standard deviation basis; and for a J-shaped, a geometric progression. Hence nested means provide the most robust, generally applicable, replicable yet inflexible class interval system."

To specify values using the Nested Means tab,

- Highlight standlrt and click the Change Range button
- Click the Nested Means tab
- To get 4 groups, specify 1 level of nesting


## - Click Done

The three values that will be used for standlrt in predictions are now the cut points of the four groups: the overall mean, the mean of values between the minimum and the overall mean, and the mean of values between the overall mean and the maximum.

We could also have obtained 7 values (the cut points of 8 groups) by specifying 2 levels of nesting, or 15 values (the cut points of 16 groups) by specifying 3 levels of nesting, and so on.

### 2.1.5 Specifying values for categorical variables

Let's set up a model with categorical predictors. This can be done in the Equations window or via commands in the Command Interface window. First let us recode the variable girl:

- In the Names window, select girl and click the Edit name button
- Change the name of girl to 'gender'
- Click the Toggle Categorical button
- Click the View button in the categories section
- Change the names of the categories from gender_0 to 'boy' and from gender_1 to 'girl'
- Click OK to close the Set category names window

We will use as our predictors gender and vrband, which is a categorised prior ability measure on pupils (vb1 = high, vb2 = mid, vb3 = low). Type the commands in the left hand column of the table below in the Command interface window

| Command | Explanation |
| :--- | :--- |
| CLEAR | clear the current model |
| IDEN 1 'student' 2 'school' | declare multilevel structure |
| RESP 'normexam' | declare response variable |
| EXPL 1 <br> 'vrband' | spens' 'gender' |
| ADDT 'gender' 'vrband' | add interaction term |
| SETV 2 'cons ' | specify random intercept at level 2 |
| SETV 1 'cons' | specify constant variance at level 1 |
| STAR 1 | estimate model updating GUI |

Note that the command STAR 1 has the same effect as pressing the Start button at the top left of the screen. This will produce the following results in the Equations window


- Open the Customised predictions window

A message appears at the top of the window:
"Prediction is out of date, specification disabled until it is cleared"
This is because the current prediction grid refers to a previous model. Indeed looking at the list of explanatory variables in the Customised predictions window, you will see the variables standlrt and avslrt listed. When the main effects in a model are altered the prediction grid is flagged as being out of date. To proceed with a prediction for the new model we must clear the current prediction grid specification

- Press the Clear button in the Customised predictions window

This will clear any columns or graphs referred to by the prediction grid and set the prediction grid to refer to the current model. You will now see that the list of explanatory variables in the Customised predictions window is up to date. In the Customised predictions window:

- Highlight gender
- Click Change Range
- Select Category
- Select boy and girl in the Values to include list
- Click Done
- Highlight vrband in the Customised predictions window
- Click Change Range
- Click Category
- Select vb1, vb2 and vb3
- Click Done
- Click the Fill Grid and Predict buttons in the Customised predictions window
- Select the Predictions tab in the Customised predictions window

This shows us the predicted values and confidence intervals for the 6 combinations of gender and vrband


Note that, because simulation is used to calculate these values, these numbers may be slightly different every time.

Plotting this out using the Customised prediction plot window filled in as follows:

gives this:


This shows girls doing uniformly better than boys across all 3 levels of vrband. Recall that vrband is a categorised prior ability measure on pupils (vb1 $=$ high, vb2 $=$ mid, vb3 $=$ low). The default choice for displaying data against a categorical $x$ variable is to plot the data as bars. We can change this or other characteristics of the plots produced by the Customised prediction plot window by editing the Customised graph window for the appropriate graph display. For example, suppose we wanted to draw the above relationship using line + point instead of bars. Then

- Select Customised Graph(s) from the Graphs menu
- Select line + point from the drop-down list labelled plot type
- Click Apply

This produces:


Both these graphs show girls outperforming boys at all three levels of vrband. Looking at the graphs (and noting in which cases the error bars
overlap) it might appear that this gender difference is significant for vb3 children, but not for children in vb2 and vb1. However, care is needed here. The graphs are showing $95 \%$ confidence intervals around the predicted means for each of the 6 groups. If we are interested in making inferences about how the gender difference changes as a function of vrband, we must request confidence intervals for these differences:

- Select the Customised predictions window
- Tick the Differences checkbox
- In the from variable drop-down list select gender
- In the Reference value drop-down list select boy
- Click Predict

The graph will update

which shows that the $95 \%$ confidence intervals for the gender differences do not overlap zero for vb1, vb2 or vb3, and thus there is a significant gender difference for each of the three categories of vrband.

### 2.1.6 Commands for building customised predictions for Normal response models

PGDE : clears the current prediction grid - it should be used before constructing a new prediction grid

PGRI constructs a prediction grid:

```
PGRI \(\{\) Continuous \(\mathbf{C}\) contmode \(=\mathbf{N}\), contmode values \(\mathbf{N}\).. \(\mathbf{N}\) \}
\{categorical C catmode \(\mathbf{N}\), catmode \(\mathbf{N}\).. \(\mathbf{N}\) \} Outputcols \(\mathbf{C}\)..C
contmode \(\mathbf{N}\)
    \(=0\) list of values: \(\mathbf{N} . . \mathbf{N}\)
    \(=1\) range: upper bound \(\mathbf{N}\), lower \(\mathbf{N}\), increment \(\mathbf{N}\)
    \(=2\) centiles: \(\mathbf{N}\)..N
    \(=3\) nested means: level of nesting \(\mathbf{N}\)
catmode \(\mathbf{N}\)
    \(=1\) category numbers \(\mathbf{N} \ldots \mathbf{N}\)
    \(=2\) all categories
```

Example:

PGRId 'cons' 01 'standlrt' $13-31$ 'schgend' 2 C22 C23 C24

PREG calculates predictions for the prediction grid currently set up.
For Normal response models:

> PREG confidence interval $\mathbf{N}$ mean $\mathbf{C}$ lower $\mathbf{C}$ upper $\mathbf{C}$, differences $\mathbf{N}$ $($ differences for column $\mathbf{C}$, differences from category $\mathbf{N}$ ), multivariate $\mathbf{N}$ (respcol $\mathbf{C}$ ), coverages $\{$ level $\mathbf{N}$ coverage range $\mathbf{N}$ low $\mathbf{C}$ up $\mathbf{C}\} \ldots$

Examples:
(1)

PREG 95 mean c100 lower c101 upper c102, difference 0, multivariate 0

Given PGRID established as above, predicted mean +/- 95 percentile output to c100 c101 c102, no differences selected
(2)

```
PREG 95 mean c100 lower c101 upper c102, difference 0,
    multivariate 1 'normexam'
```

Given PGRID established for a multivariate response model, performs same task as example (1) above; predictions are for the response 'normexam'. (Note that we describe later how to make predictions for multivariate models using the customised predictions window).

```
- PREG 95 mean c100 lower c101 upper c102, difference 1
    'schgend' 1, multivariate 1 'normexam'
```

As (2) above but predictions are differenced from schgend category 1
(4)

PREG 95 mean c100 lower c101 upper c102, difference 1
'schgend' 1 , multivariate 1 'normexam' 299 c103 c104

As (3) above but also calculate $99 \%$ coverage for predictions based on level 2 variance; lower and upper coverage values to c103 and c104

### 2.1.7 Commands for plotting customised predictions

The PLTPrediction command is used for displaying predictions and performs the same task as the Customised prediction plot window; though it can also be used more generally to plot data other than predictions since it just plots one column against another, with confidence intervals if supplied, with the options to plot the data by groups and to split the plot into two separate graphs (horizontally or vertically), with data plotted on one graph or the other according to values of a supplied variable:

> PLTPrediction in graph display $\mathbf{N}$, dataset $(\mathrm{X}, \mathrm{Y})$, 0 (do nothing) or grouped by values in $\mathbf{C}$,
> 0 (do nothing) or split into separate graphs across rows of a trellis according to values in $\mathbf{C}$,
> 0 (do nothing) or split into separate graphs across columns of a trellis according to values in $\mathbf{C}$,
> \{confidence intervals: lower in $\mathbf{C}$, upper in $\mathbf{C}$, plot style $10=$ bar, $11=$ line $\}$

Note that if you do not already have the graph display window open then you will need to go to the Customised graph window and click Apply after entering the command.

Examples:

```
PLPT 2 c1 c2 0 0 0 c3 c4 11
```

Sets up graph display 2: $x=c 1 y=c 2$, lower and upper confidence intervals are in c3 and c4, plot confidence intervals as lines
(2)

```
PLPT 2 c1 c2 'social_class' 0 0
```

Sets up graph display 2: $x=c 1 y=c 2$, one line for each social class, don't display confidence intervals
(3)

```
PLPT 2 c1 c2 'social_class.pred' 'gender.pred' 0 c3 c4 11
```

Sets up graph display 2: $\mathrm{x}=\mathrm{c} 1 \mathrm{y}=\mathrm{c} 2$, one line for each social class, repeat plot in a $2 \times 1$ graph trellis for gender $=0$ in first pane and gender $=1$ in second pane (i.e. split into two plots arranged vertically, with the upper plot including data points for which gender $=0$ and the lower plot including data points for which gender $=1$ ), lower and upper confidence intervals are in c3 and c4, plot confidence intervals as lines

### 2.2 Binomial models

### 2.2.1 Predicting mean and median

To give ourselves a binary response variable so we can demonstrate prediction for binomial models, let's create a dichotomised variable from the Normalised response in the tutorial dataset. Responses with a value of greater than or equal to 1.5 we will set to 1 otherwise we will set the dichotomised variable to 0 . To do this, type in the Command interface window

- calc c11 = 'normexam' >= 1.5
- name c11 'pass'

Now set up the following multilevel binomial model and estimate the model with the non-linear options set to 2nd order PQL estimation :

| ®. Equations $\quad \begin{aligned} & \text { - } \\ & \text { a }\end{aligned}$ |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} & \operatorname{pass}_{i j} \sim \operatorname{Binomial}\left(\text { cons }_{i j} \pi_{i j}\right) \\ & \operatorname{logit}\left(\pi_{i j}\right)=\beta_{0 j} \text { cons } \\ & \beta_{0 j}=-3.183(0.189)+u_{0 j} \end{aligned}$ |  |  |  |  |  |  |  |  |  |
| $\left[u_{0 j}\right] \sim \mathrm{N}\left(0, \Omega_{u}\right): \Omega_{u}=[1.596(0.387)]$ |  |  |  |  |  |  |  |  |  |
| $\operatorname{var}\left(\operatorname{pass}_{i j} \mid \pi_{i j}\right)=\pi_{i j}\left(1-\pi_{i j}\right) / \operatorname{cons}_{i j}$ |  |  |  |  |  |  |  |  |  |
| (4059 of 4059 cases in use) |  |  |  |  |  |  |  |  |  |
| Name | + | - | Add Ierm | Estimates | Nonlinear | Clear | Notation | Responses | Store |

The Customised predictions window now looks like this:


The Customised predictions window for binomial response models looks similar to that for Normal response models. However there are a few changes. You can choose whether predictions should be made on the logit or probability scales and also you can ask for these predictions to be for the mean or
median value of the prediction distribution.
What does prediction distribution mean? This data is based on 65 schools. The level 2 variance of 1.596 on the logit scale is the between school variance, in the population from which our schools are sampled, of the school means (on the logit scale). Suppose we now ask the question of what the mean and median pass rates are on the probabilty scale, for pupils attending three schools (of identical size) with values of $u_{0 j}=\{-2,0,2\}$. This is a school from either end and the middle of the distribution of schools. We obtain $p_{k}$, the pass rate on the probability scale, for each school $k$ by taking the antilogit of the model equation $-3.18+u_{0 k}$ (putting in the appropriate value for $u_{0 k}$ )

$$
\begin{aligned}
p_{k} & =\{\operatorname{antilogit}(-3.18-2), \text { antilogit }(-3.18), \operatorname{antilogit}(-3.18+2)\} \\
& =\{0.006,0.040,0.234\} \\
\operatorname{mean}\left(p_{k}\right) & =0.093 \\
\operatorname{median}\left(p_{k}\right) & =0.040
\end{aligned}
$$

The thing to note is that if we take the antilogit of the mean of our three logit values, that is antilogit $(-3.18)=0.040$, this is equal to the median of our three probabilities but not the mean of the three probabilities (0.0918). This is because in this case before we take antilogits the mean of our three values equals the median, and the median of the antilogits of a set of values is always equal to the antilogit of the median of the set of values. The mean of the antilogits of a set of values on the other hand will in general not be equal to the antilogit of the mean of the set of values.

This comes about because of the non-linearity of the logit transformation as we can see from the graph below, which graphs $\operatorname{logit}(p)$ and places our three schools as the red points on the line.


When we fit a multilevel model and take the antilogit of a fixed part predictor
(i.e. a sum of fixed part coefficients multiplied by particular values of their associated explanatory variables), this gives us the median (not the mean) probability for the prediction case consisting of those values of the explanatory variables. Again, this is because before we take antilogits, median $=$ mean (since we are dealing with a normal distribution), and antilogit(median) $=$ median(antilogits). From the above multilevel model we get a prediction of -3.18 on the logit scale which corresponds to a median probability of passing of 0.040 . We may however want to know what the mean probability is of passing, not taking account of only three schools, but allowing for the whole distribution of schools. The mean cannot be directly calculated from the model in the same way that the median can; but we can estimate it using simulation. We know that the distribution of all schools on the logit scale is $\mathrm{N}\left(-3.183,1.596^{0.5}\right)$. Thus the following will give us an estimate of the mean pass rate

1. Simulate the value on the logit scale for a large number of schools, say 1000 , from the distribution $\mathrm{N}\left(-3.183,1.596^{0.5}\right)$. That is:

$$
Z_{j}=\mathrm{N}\left(-3.183,1.596^{0.5}\right), \quad j=1, \ldots, 1000
$$

2. Calculate the predicted probability for each of our 1000 schools and calculate their mean. That is, $\overline{\operatorname{antilogit}\left(Z_{j}\right)}$.

We can do this in MLwiN using the following commands (click the Output button on the Command interface window before typing them in order to properly see the output at the end)

| Command | Explanation |
| :--- | :--- |
| seed 8 | set random number seed (so we can <br> replicate our results) |
| nran $1000 \quad c 100$ | pick 1000 values from $\mathrm{N}(0,1)$ |
| calc <br> c100 $=c 100 * 1.596 \wedge 0.5-3.183$ | transform to $\mathrm{N}\left(-3.183,1.596^{0.5}\right)$ |
| calc $c 101=a \log (c 100)$ | generate 1000 probabilities |
| aver c101 | calculate their mean |

This produces an estimate of the mean pass rate as 0.072 . In this example our prediction case is very simple, it is simply the unconditional mean pass rate (i.e. the mean pass rate taking no explanatory variables into account); if we calculate that directly (by taking the mean of the variable pass) we get a value of 0.070 , so we can see our estimate is very good. In more complex conditional predictions, for example the mean pass rate for girls with intake scores of 1 in girls' schools, we may have very few (or in fact no) individuals exactly fitting our prediction case and a reasonable empirical estimate of the
mean for that prediction group is not available. However, the model based estimate is available.

All the predictions and confidence intervals calculated with the out of sample predictions window are derived by simulation, in a similar fashion to the example we just typed in the commands for. The detailed simulation algorithms for a range of model types are given in Appendix 1 of this document.

These median and mean predictions are often referred to as cluster specific and population average predictions respectively. Instead of typing in the above commands, we can obtain these simply using the Customised predictions window:

- Select Probabilities
- Check boxes to request predicted Medians and Means
- Click Fill Grid
- Click Predict
- Select the Predictions tab

| E. | Customised predictions |  |  |  |  |  |  | - - x |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Copy |  |  |  |  |  |  |  |
| Setup |  |  |  |  |  | Predictions |  |  |
| cons.pred | median.pred |  | median.low.p |  | median.high.\| | mean.pred | mean.low.prt | mean.high.pr |
| 1.000 |  | 0.040 |  | 0.027 | 0.056 | 0.072 | 0.052 | 0.095 |
| Fill Grid | Predict | Plot Grid |  |  |  |  |  |  |

We see that the median ('median.pred') and mean ('mean.pred') predictions are as expected. Note that these results are from simulation algorithms where we have drawn a particular number of simulated values.

If you click on the Setup panel in the Customised predictions window you will see
\# predicted cases: 1
\# draws from $\operatorname{cov}$ (Beta) 2000
\# nested draws from $\operatorname{cov}(\mathrm{u}) 1000$
\# simulations 2000000
The number of predicted cases is 1 because we are predicting for the unconditional mean only. When we typed in commands to estimate the mean probability and generated 1000 draws from $\mathrm{N}\left(-3.183,1.596^{0.5}\right)$, we always used the same value for $\hat{\beta}_{0}$ of -3.183 . In fact, s.e. $\left(\hat{\beta}_{0}\right)=0.189$ and the full simulation procedure as implemented by the Customised predictions window is as follows

1. Simulate $K=2000$ values of

$$
\beta_{0 k} \sim \mathrm{~N}\left(-3.183,0.189^{0.5}\right), \quad k=1: K
$$

2. For each value of $\beta_{0 k}$ simulate $j=1000$ values of $\beta_{0 k j} \sim \mathrm{~N}\left(\beta_{0 k}, 0.189^{0.5}\right), \quad j=1: J$
3. Then let $p_{k j}=\operatorname{antilogit}\left(\beta_{0 k j}\right)$ and for each value of $k$ calculate $p_{k}=$ $\frac{1}{J} \sum_{j=1}^{J} p_{k j}$
4. Finally we calculate the mean probability as $p=\frac{1}{K} \sum_{k=1}^{K} p_{k}$

This actually involves $K \times J=2000000$ simulation draws and the results in this case are identical to the simplified procedure where we typed in commands and assumed a fixed value for $\hat{\beta}_{0}$.

### 2.2.2 Predictions for more complex Binomial response models

Let's fit a model where the probability of passing is a function of pupil intake score (standlrt), peer group ability (avslrt) and an interaction of pupil intake score and peer group ability. Note the interaction effect between avslrt and standlrt is not significant; we leave it in the model for the purposes of demonstrating the graphing of interactions, particularly for log odds ratios in the next section.

| Equations |  |  |  |  |  |  |  |  | 可 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |
| $\operatorname{var}\left(\operatorname{pass}_{i j} \mid \pi_{i j}\right)=\pi_{i j}\left(1-\pi_{i j}\right) /$ cons $_{\text {ij }}$ |  |  |  |  |  |  |  |  |  |
| (4059 of 4059 cases in use) |  |  |  |  |  |  |  |  |  |
| name | + | Add Ierm | Estimates | Nonlinear | Clear | Motation | Responses |  | tore |

In the Customised predictions window, set

- standlrt $=$ range $\{3,-3,0.25\}$ (note we will use this notation from now on for convenience; it means 'define the values of standlrt using the Range tab; set Upper Bound $=3$, Lower $=-3$, Increment $=$ 0.25 ')
- avslrt $=$ values $\{0.5,-0.5\}$
- Select Median predictions
- Select predictions for Probabilities
- Click Fill grid
- Click Predict
- Click Plot grid

In the Customised prediction plot window

- Select Y: median.pred
- Select X: standlrt.pred
- Select Grouped by: avslrt.pred
- Click Apply

Which produces:


The graph shows how the probability of passing increases as pupil intake ability increases, with the increase being stronger for those in high ability peer groups. We now explore the differences between low and high ability peer groups as functions of standlrt and assess if and where those differences are significant. In the Customised predictions window

- Select Differences; from variable: avslrt Reference value: -0.5
- Press the Predict button

In the Customised prediction plots window

- Select Confidence interval:
- Click Apply


We can see that after standlrt scores become greater than around -0.5 , the probability of passing for those in the high ability group becomes significantly different from the low ability group.

### 2.2.3 Log Odds ratios

Return to the Customised predictions window

- Select logit
- Click Predict


The variable standlrt.pred contains the requested values range $\{-3,3$, $0.25\}$. The graph plots

$$
\left.\begin{array}{c}
\log \left(\frac{\text { odds passing } \mid \text { avslrt.pred }=0.5, \text { standlrt.pred }}{i} \text { odds passing } \mid \text { avslrt.pred }=-0.5, \text { standlrt.pred }_{i}\right.
\end{array}\right),
$$

that is, the log odds ratio of passing for high versus low peer groups as a function of pupil intake score. We may want to view the graph as odds ratios, rather than log odds ratios. Looking at the Names window we see that the log odds ratio and its upper and lower bounds are in the columns named median.pred, median.low.pred and median.high.pred, that is c18-c20. To create a graph of odds ratios type the command

- expo 'median.pred' 'median.low.pred' 'median.high.pred' 'median.pred' 'median.low.pred' 'median.high.pred'

A message will appear asking if you want to clear the prediction grid; click "No".


### 2.2.4 Customised prediction commands for discrete response models

```
PREG confidence interval N,
predict mean values N (mean values output set C lower C upper C),
predict median values N (median C lower C upper C)
prediction scale N,
differences \mathbf{N}\mathrm{ (diffcol C, diff reference C)}
multivariate N (respcol C)
coverages {level N coverage range N low C up C} ..
```

This is an extension of the PREG command for Normal responses. The differences are

```
predict mean values N=
0: no mean value output set to follow
1: mean value output set required
(mean value output set: mean to C, lower confidence interval for mean
to C, upper confidence interval for mean to C)
predict median values }\mathbf{N}
0: no median value output set to follow
1: median value output set required
(median value output set: median to C, lower confidence intervals for
median, upper confidence intervals for median)
```

Prediction scale $\mathbf{N}=$
0 : for raw response scale
2: for link function attached to model
Note raw response scale is probability (binomial, multinomial models) or counts (negative binomial, Poisson models)

Examples
(1)

```
PREG 95 0 1 c100 c101 c102 0 0 0
```

If we have a binary response model set up, then the above command evaluates the current PGRID, calculating median (i.e. cluster specific) predictions on the probability scale, and writes the predicted medians and their lower and upper $95 \%$ confidence intervals to c100, c101, c102
(2)

- PREG 9501 c100 c101 c102 1 'schgend' 100

As (1) above but predictions are differenced from schgend category 1

### 2.3 Multinomial models

### 2.3.1 Unordered Multinomial Models

We will take the contraception dataset used in Chapter 10 of the User's Guide:

- Open bang.ws
- Select the variable use4 in the Names window
- Click the View button in the categories section

Set the 4 categories to be :


Let's use the Command interface window to set up a multinomial model, where the log odds of using different types of contraception compared with no contraception are allowed to vary as a function of age.

| Command | Explanation |
| :--- | :--- |
| MNOM 0 'use4' c13 c14 4 | the reference category is 4- none |
| NAME c13 'resp' c14 <br> 'resp_cat' |  |
| IDEN 1 'resp_cat' 2 'woman' <br> 3 <br> 'district' | specify level IDs |
| ADDT 'cons ' | add 3 intercepts - one for each log <br> odds ratio |
| ADDT 'age' | add 3 age coefficients - one for each <br> log odds ratio |
| SETV 3 'cons.ster' <br> 'cons.mod' 'cons.trad' | specify random intercepts across dis- <br> tricts |
| DOFFs 1 'cons' | specify denominator |
| LINEarise 1 2 | select PQL order 2 |

Running this model gives:

$$
\begin{aligned}
& \text { Q. Equations - - } x \\
& \operatorname{resp}_{i j k} \sim \text { Multinomial }\left(\text { cons }_{j k}, \pi_{i j k}\right. \text { ) } \\
& \log \left(\pi_{1 j k} / \pi_{4 j k}\right)=\beta_{0 k} \text { cons.ster }_{i j k}+0.058(0.007) \text { age.ster }{ }_{i j k} \\
& \beta_{0 k}=-2.045(0.119)+v_{0 k} \\
& \log \left(\pi_{2 j k} / \pi_{4 j k}\right)=\beta_{1 k} \text { cons.mod }{ }_{i j k}+-0.023(0.006) \text { age.mod }_{i j k} \\
& \beta_{1 k}=-1.378(0.099)+v_{1 k} \\
& \log \left(\pi_{3 j k} / \pi_{4 j k}\right)=\beta_{2 k} \text { cons.trad }{ }_{i j k}+0.029(0.007) \text { age.trad }_{i j k} \\
& \beta_{2 k}=-1.914(0.101)+v_{2 k} \\
& {\left[\begin{array}{l}
v_{0 k} \\
v_{1 k} \\
v_{2 k}
\end{array}\right] \sim \mathrm{N}\left(0, \Omega_{v}\right): \Omega_{v}=\left[\begin{array}{lll}
0.470(0.141) & & \\
0.281(0.093) & 0.374(0.103) & \\
0.200(0.090) & 0.123(0.075) & 0.298(0.105)
\end{array}\right]} \\
& \operatorname{cov}\left(y_{\mathrm{sjk}} y_{\mathrm{tjk}}\right)=-\pi_{\mathrm{s} j k} \pi_{\mathrm{rj} k} / \operatorname{cons}_{j k}: \mathrm{s} \neq \mathrm{r} ; \quad \pi_{\mathrm{s} j k}\left(1-\pi_{\mathrm{rjk}}\right) / \operatorname{cons}_{j j k}: \mathrm{s}=\mathrm{r} ; \\
& \text { ( } 8601 \text { of } 8601 \text { cases in use) } \\
& \begin{array}{|l|l|l|l|l|l|l|l|l|l|l|l|}
\underline{\text { Name }} & + & - & \text { Add Ierm } & \underline{E s t i m a t e s} & \text { Nonlinear } & \text { Clear } & \text { Notation } & \text { Responses } & \text { Store } & \underline{H e l p} & \text { Zoom } \\
\hline
\end{array}
\end{aligned}
$$

In the Customised predictions window :

- Set age to range $\{19,-14,1\}$
- Select Probabilities
- Select Medians
- Click the Fill grid, Predict and Plot Grid buttons

In the Customised prediction plot window

- Select Y: median.pred, X: age.pred, Grouped by: use4.pred
- Click Apply
which produces

or with error lines


Let's elaborate the model adding number of children (lc) and an lc*age interaction:

- ADDT 'lc'
- ADDT 'lc' 'age'

Running this model produces:

```
E.
                Equations
                    - - x
\mp@subsup{\operatorname{resp}}{ijk}{~ Multinomial(cons (ck}
log}(\mp@subsup{\pi}{1jk}{}/\mp@subsup{\pi}{4jk}{})=\mp@subsup{\beta}{0k}{}\mp@subsup{c}{0}{cons.ster ijkk
    2.297(0.359)lc2.ster 
    -0.022(0.039)lc2.age.ster ijjk}+-0.105(0.036)lc3plus.age.ster ijjk
\beta 0k}=-3.811(0.348)+\mp@subsup{v}{0k}{
log( }\mp@subsup{\pi}{2jk}{}/\mp@subsup{\pi}{4jk}{})=\mp@subsup{\beta}{1k}{}\mathrm{ cons.mod
        1.041(0.233)lc2.mod
        -0.027(0.028)lc2.age.mod
\beta
log}(\mp@subsup{\pi}{3jk}{}/\mp@subsup{\pi}{4jk}{})=\mp@subsup{\beta}{2k}{}\mp@subsup{c}{cons.trad}{ijk
    1.087(0.287)lc2.trad ijk}+1.227(0.278)lc3plus.trad ijjk +0.005(0.037)lc1.age.trad ijjk 
    0.004(0.033)lc2.age.trad}\mp@subsup{|}{ijk}{}+-0.021(0.028)lc3plus.age.trad ijj
\beta}\mp@subsup{\beta}{2k}{}=-2.669(0.257)+\mp@subsup{v}{2k}{
[l}\mp@subsup{v}{0k}{0
\operatorname{cov}(\mp@subsup{y}{\textrm{s}jk}{}\mp@subsup{y}{\textrm{f}jk}{})=- \mp@subsup{\pi}{\textrm{s}jk}{}\mp@subsup{\pi}{\textrm{rj}/k}{}/\mp@subsup{\operatorname{cons}}{jkk}{}:\textrm{s}\not=\textrm{r};\quad\mp@subsup{\pi}{\textrm{s}jk}{}(1-\mp@subsup{\pi}{\textrm{r}jk}{})/\mp@subsup{\operatorname{cons}}{jkk}{}:\textrm{s}=\textrm{r};
(8601 of 8601 cases in use)
Name + - Add Ierm Estimates Nonlinear Clear 
```

Let's now set up a prediction to explore the interactions between age (old and young mothers), number of children and the probabilities of using different methods of contraception. In the Customised predictions window make the following specifications:

- use4: all categories
- age: Values $(10,-10)$ (note you will have to remove the mean value of -0.3278697 )
- lc: select all categories
- Select Probabilities
- Select Medians
- Click the Fill grid, Predict and Plot Grid buttons
and then set plot up as follows
- Select Y: median.pred, X: lc.pred,
- Select Grouped by: use4.pred
- Select Trellis X: age.pred
- Select Confidence intervals
- Select Error bars


## - Click Apply

This produces:


This graph shows that across ages (top graph panel = young, bottom graph panel $=$ old) and parities (that is, number of children) the most prevelent contraceptive behaviour is to use no contraception at all. However, some interesting trends can be observed - for example, the probability of using no contaception is highest for women with no children. For both young and old women once they have had one child the probability of using some form of active contraception increases. For young women the pattern is more striking and the preferred method of active contraception for young women is modern contraception. Active contraceptive use is strongest for young women with 3 or more children.

We may wish to explore whether differences from a particular reference group are statistically significant. For example, we may wish to choose women with no children as a reference group and evaluate:
$p($ usage $=$ ster $\mid \mathbf{l c}=\mathbf{l c} \mathbf{1}$, age $=-10)-p($ usage $=$ ster $\mid \mathbf{l c}=\mathbf{l c} \mathbf{0}$, age $=-10)$
$p($ usage $=$ ster $\mid \mathbf{l c}=\mathbf{l c} 3$, age $=-10)-p($ usage $=$ ster $\mid \mathbf{l c}=\mathbf{l c} 0$, age $=-10)$

That is, see how the difference from women with no children changes as a function of age, usage type and number of children. In the Customised predictions window:

- Select Differences; from variable: lc; Reference value: lc0
- Click the Predict button

The graph display will update to:


Remember each bar represents the difference of a probability of usage for a specified method, age and number of children from the same method and age with number of children $=0$. So all the bars corresponding to number of children $=0$ disappear since we are subtracting a probability of usage for a particular combination of explanatory values from itself.

Let's look at the 4 bars for the 4 usage types at number of kids $=1$, age $=-10$. That is, young women with one child. This is the leftmost cluster of bars in the top graph panel which corresponds to prediction cases 5-8 in the Predictions tab of the Customised predictions window.


We see from row 8 of the above table (under median.pred) that

$$
\begin{aligned}
& p(\operatorname{method}=\text { none } \mid \mathbf{l c}=\mathbf{l c} \mathbf{c}, \text { age }=-10) \\
&-p(\boldsymbol{\operatorname { m e t h }}=\mathbf{n o d} \mid \mathbf{l c}=\mathbf{l c} \mathbf{0}, \text { age }=-10)=-0.162
\end{aligned}
$$

That is, the probability that young women with one child used no contraception is 0.162 less than young women with no children. Once young women have had a child they are more likely to use some active form of contraception. We can see which form of contraception these young women switch to by looking at rows $5-7$ of the prediction table. We thus discover that $0.162=0.034($ ster $)+0.097(\bmod )+0.033(\operatorname{trad})$. Note that there is a tiny discrepancy in this equality due to rounding error.

We can carry out the same prediction on the logit scale and get log odds ratios. In the Customised predictions window

- Select logit
- Click Predict


Now the leftmost blue bar in the upper graph panel represents the log odds ratio
$\log \left[\frac{p(\text { usage }=\text { ster } \mid \text { age }=-10, \mathbf{l c}=\mathbf{l c} \mathbf{1}) / p(\text { usage }=\text { none } \mid \text { age }=-10, \mathbf{l c}=\mathbf{l c} \mathbf{1})}{p(\text { usage }=\text { ster } \mid \text { age }=-10, \mathbf{l c}=\mathbf{l c} \mathbf{0}) / p(\text { usage }=\text { none|age }=-10, \mathbf{l c}=\mathbf{l c} \mathbf{0})}\right]$

We get a log odds ratio (as opposed to a logit) because in our prediction we asked for logits to be differenced from lc $=\mathrm{lc} 0$.

### 2.3.2 Ordered Multinomial

We will take the A-level dataset used in Chapter 11 of the User's Guide:

- Retrieve alevchem.ws

Let's set up a basic model using the following commands:

| Command | Explanation |
| :--- | :--- |
| MNOM 1 'a-point'c10 c11 6 | note the reference category is $6,<=\mathrm{A}$ |
| NAME c10 'resp'c11 <br> 'respcat' |  |
| IDEN 1 <br> 3 'estab' | specat' 2 'pupil' <br> add a different intercept for each re- <br> sponse category |
| ADDT 'CONS' | specify that future added terms have <br> same coefficient for each multinomial <br> category |
| RPAT 1 1 1 1 1 | add a common intercept for categories <br> $1-5$ |
| ADDT 'cons' | allow common intercept to vary across <br> establishments |
| SETV 3 'cons.12345' | remove common intercept from fixed <br> part of the model so it is no longer <br> overparameterized |
| FPAR 0 'cons.12345' | specify denominator |
| DOFFs 1 'cons' | select PQL order 2 |
| LINEarise 1 2 |  |

$$
\begin{aligned}
& \text { E. Equations } \quad \begin{array}{ll|l|}
\hline-\mathbf{a} \\
\hline
\end{array} \\
& \operatorname{resp}_{i j k} \sim \text { Ordered Multinomial }\left(\text { cons }_{j k k}, \pi_{i j k}\right) \\
& \gamma_{1 j k}=\pi_{1 / k} ; \gamma_{2 j k}=\pi_{1 j k}+\pi_{2 j k} ; \gamma_{3 j k}=\pi_{1 j k}+\pi_{2 j k}+\pi_{3 j k} ; \\
& \gamma_{4 j k}=\pi_{1 j k}+\pi_{2 j k}+\pi_{3 j k}+\pi_{4 j k} ; \\
& \gamma_{5 j k}=\pi_{1 j k}+\pi_{2 j / k}+\pi_{3 j k}+\pi_{4 j / k}+\pi_{5 j k} ; \gamma_{6 j / k}=1 \\
& \operatorname{logit}\left(\gamma_{i j k}\right)=-1.375(0.102) \text { cons. }(<=\mathrm{F})_{i j k}+h_{j k} \\
& \operatorname{logit}\left(\gamma_{2 j k}\right)=-0.492(0.097) \text { cons. }(<=\mathrm{E})_{i j k}+h_{j k} \\
& \operatorname{logit}\left(\gamma_{3 j k}\right)=0.278(0.097) \text { cons. }(<=\mathrm{D})_{i j k}+h_{j k} \\
& \operatorname{logit}\left(\gamma_{4 j k}\right)=1.152(0.099) \text { cons. }(<=\mathrm{C})_{i j k}+h_{j k} \\
& \operatorname{logit}\left(\gamma_{j j k}\right)=2.370(0.109) \text { cons. }(<=\mathrm{B})_{i j k}+h_{j k} \\
& h_{j k}=v_{5 k} \text { cons. } 12345 \\
& {\left[v_{5 k}\right] \sim \mathrm{N}\left(0, \Omega_{v}\right): \Omega_{v}=[1.281(0.174)]} \\
& \operatorname{cov}\left(y_{\mathrm{sjk}} y_{\mathrm{tjk}}\right)=\gamma_{\mathrm{sjk}}\left(1-\gamma_{\mathrm{j} j k}\right) / \operatorname{cons}_{j k} \quad \mathrm{~s}<=\mathrm{r} \\
& \text { ( } 10830 \text { of } 10830 \text { cases in use) }
\end{aligned}
$$

In the Customised predictions window:

- Set a-point to all categories apart from the reference category A
- Select Probabilities
- Select Medians
- Click the Fill grid and Predict buttons
- Select the Predictions tab

This prediction gives the cumulative probabilities of passing across the grade categories

| E9. | Customised predictions |  |  |  |  | - | - $\times$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Copy |  |  |  |  |  |  |
| Setup |  |  |  |  | Predictions |  |  |
| a-point.pred |  | cons.pred |  | median.pred | median.low.p | median.high.\| |  |
|  | F |  | 1.000 | 0.202 | 0.173 |  | 0.237 |
|  | E |  | 1.000 | 0.380 | 0.338 |  | 0.427 |
|  | D |  | 1.000 | 0.570 | 0.526 |  | 0.617 |
|  | C |  | 1.000 | 0.761 | 0.725 |  | 0.793 |
|  | B |  | 1.000 | 0.915 | 0.897 |  | 0.930 |
| Fill Grid | Predict |  | Plot Grid |  |  |  |  |

The Differences from functionality, in the Customised predictions window, is not currently implemented for ordered multinomial models.

### 2.4 Poisson models

We will work with the skin cancer dataset used in Chapter 12 of the User's Guide.

- Open the worksheet mmmec.ws

Let's model malignant melanoma county level death rates as a function of UVBI exposure, allowing for between region and country variation:

| Command | Explanation |
| :--- | :--- |
| resp 'obs' |  |
| iden 1 'county' 2 'region' <br> 3 'nation' |  |
| expl 1 'cons' 'uvbi' |  |
| rdist 1 1 | set response to be Poisson |
| lfun 3 | specify log link function |
| doffs 1 'exp' | offsets in 'exp' |
| loge 'exp' 'exp' | 51 |
| setv 2 'cons' |  |
| setv 3 'cons' |  |


| Equations |  |  |  |  |  |  |  | - - ${ }^{\text {x }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| obs $_{i j k} \sim \operatorname{Poisson}\left(\pi_{i j k}\right)$ |  |  |  |  |  |  |  |  |
| $\begin{aligned} & \log \left(\pi_{i j k}\right)=\exp _{i j k}+\beta_{0 j k} \operatorname{cons}+-0.028(0.011) \mathrm{uvb}_{i j k} \\ & \beta_{0 j k}=-0.081(0.133)+v_{0 k}+u_{0 j k} \end{aligned}$ |  |  |  |  |  |  |  |  |
| $\left[v_{0 k}\right] \sim \mathrm{N}\left(0, \Omega_{v}\right): \Omega_{v}=[0.136(0.072)]$ |  |  |  |  |  |  |  |  |
| $\left[u_{0 j k}\right] \sim \mathrm{N}\left(0, \Omega_{u}\right): \Omega_{u}=[0.048(0.011)]$ |  |  |  |  |  |  |  |  |
| $\operatorname{var}\left(\mathrm{obs}_{i j k} \mid \pi_{i j k}\right)=\pi_{i j k}$ |  |  |  |  |  |  |  |  |
| (354 of 354 cases in use) |  |  |  |  |  |  |  |  |
| Name | + | Add Ierm\| | Estimates | Nonlinear | Clear | Motation | Responses | store |

In the Customised predictions window

- Set uvbi to range $\{13,-8,1\}$
- Select Medians and Means
- Click the Fill Grid and Predict buttons
- Using the Customised graphs window from the Graphs menu, plot the median and the mean predictions (median.pred and mean.pred) against UBVI exposure (uvbi.pred)


We see that the mean is uniformly higher than the median. This is due to the shape of the link function. This difference that we see emphasises the need to consider the shape of the distribution when reporting results
or making inferences: for example, just as we saw for binomial models, the mean probability cannot be obtained by taking the exponential of the mean $X B$; and confidence intervals must be found before, not after, transforming to probabilities via the exponential. This also explains why we won't expect the predicted value of, for example, the unconditional mean to exactly match our observed value.

### 2.5 Multivariate models

The Customised predictions window can deal with only one response at a time when a multivariate model is set up. To demonstrate this, let's create a binary variable from the exam scores in the tutorial data. We then fit a multilevel bivariate response model with the original continuous score as the first response and the dichotomised variable as the second response. Open the tutorial worksheet and type the following commands

```
- calc c11 = c3 > 1.5
- name c11 'pass'
- mvar 1 c3 c11
- expl 1 'cons' 'standlrt'
- iden 2 'student' 3 'school'
- setv 3 'cons.normexam' 'cons.pass'
- setv 2 'cons.normexam'
- linea }1
- rdist 2 0
- doffs 2 'cons'
```

|  |  |  |  | tion |  |  |  | - $\times$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |
| $\left[\begin{array}{l} v_{0 k} \\ v_{1 k} \end{array}\right] \sim \mathrm{N}\left(0, \Omega_{v}\right): \Omega_{v}=\left[\begin{array}{ll} 0.090(0.018) \\ 0.298(0.061) & 1.009(0.241) \end{array}\right]$ |  |  |  |  |  |  |  |  |
| $\begin{aligned} & \operatorname{cov}\left[\begin{array}{l} u_{0 j k} \\ \text { resp }_{2 j k} \mid \pi_{2 j k} \end{array}\right]=\left[\begin{array}{l} 0.570(0.013) \\ 0.280(0.011) \sigma_{u 0} g\left(\pi_{2 j k}\right)^{0.5} g\left(\pi_{2 j k}\right) \end{array}\right] \\ & g(\pi)=\pi(1-\pi) / n \\ & (8118 \text { of } 8118 \text { cases in use }) \end{aligned}$ |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |

In the Customised prediction window notice in the top right hand corner the name of the response we are working with, normexam. This means that any prediction we specify will be applied to the continuous response normexam only.

- Set standlrt to range $\{3,-3,1\}$
- Click Fill Grid, Predict and Plot Grid
- Set X: standlrt.pred, Y: mean.pred
- Click Apply

Now let's make a prediction for the binomial response. In the Customised predictions window

- Change normexam to pass in the drop-down list on the top right of the window
- Click Predict and Plot Grid
- Set Y: median.pred and Click Apply



## 3 3D Graphics

We have implemented some preliminary 3D graphics in the software. These are currently implemented as 3 commands:

SURF 3d graph number $\mathbf{N}, \mathbf{X}, \mathbf{Y}, \mathbf{Z}$

SCATt 3d graph number $\mathbf{N}, \mathbf{X}, \mathbf{Y}, \mathbf{Z}$, [group column]

## SHOW 3d graph number $\mathbf{N}$

Let's start by constructing a surface with the Customised predictions window and then plotting it.

Return to the model

| E. Equations - - - |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} \text { normexam }_{i j} \sim & \mathrm{~N}(X B, \Omega) \\ \text { normexam }_{i j}= & \beta_{0 i j} \text { cons }+\beta_{1 j} \text { standlrt }_{i j}+0.374(0.109) \text { avslrt }_{j}+ \\ & 0.162(0.057) \text { standlrt.avslrt }_{i j} \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\begin{aligned} & \beta_{0 i j}=-0.007(0.037)+u_{0 j}+e_{0 i j} \\ & \beta_{1 j}=0.558(0.019)+u_{1 j} \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\left[\begin{array}{l}u_{0 j} \\ u_{1 j}\end{array}\right] \sim \mathrm{N}\left(0, \Omega_{u}\right): \Omega_{u}=\left[\begin{array}{ll}0.074(0.015) & \\ 0.011(0.006) & 0.011(0.004)\end{array}\right]$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\begin{aligned} & {\left[e_{0 i j}\right] \sim \mathrm{N}\left(0, \Omega_{e}\right): \Omega_{e}=[0.554(0.012)]} \\ & -2 * \text { loglikelihood(IGLS Deviance })=9302.911(4059 \text { of } 4059 \text { cases in use }) \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| Name | + | - | Add Ierm | Estimates | Honlinear | Clear | Notation | Responses | Store | Help | Zoom 100 |  |

In the Customised Predictions window

- Set the range for standlrt to be Upper Bound: 3, Lower: -3 , Increment: 1
- Set the range for avslrt to be Upper Bound: 0.5, Lower: -0.5, Increment: 0.1
- Click Fill Grid and Predict

Set up the plot using

which produces:


To plot this as a surface, in the Command interface window type
surf 1 'standlrt.pred' 'avslrt.pred' 'mean.pred'

- show 1
which produces (after rotating the view using the horizontal slider to 80.0 see top left of window for current view angle):


Right clicking on the graph and selecting
$<$ Plotting Method $><$ Surface with Contouring $>$ produces


The SURF plot requires a rectangular data grid of $\mathrm{X}, \mathrm{Y}$ values with a Z value in each cell of the grid. So to plot the function $z=2 x^{3}+3 y$ for $x=\{1,2,3\}$, $y=\{4,5,6,7\}$ we need to first construct

| x | y |
| :---: | :---: |
| 1 | 4 |
| 1 | 5 |
| 1 | 6 |
| 1 | 7 |
| $\vdots$ | $\vdots$ |
| 3 | 4 |
| 3 | 5 |
| 3 | 6 |
| 3 | 7 |

then create $z$ from these two columns. This can be done by typing the following commands into the Command interface window (close the 3d
graph display window first)

- gene 131 c100
- gene 471 c101
- ucom c100 c101 c102 c103
- name c102 'x' c103 'y' c104 'z'
- calc 'z'=2*'x'~3+3*'y'
- surf $1{ }^{\prime} x^{\prime} \quad y^{\prime} \quad z^{\prime}$
show 1
which produces (after right clicking on the graph and selecting <Plotting Method><Wire Frame>):


Going back to the model we have just fitted:

the intercept and slopes are distributed

$$
\theta=\left[\begin{array}{l}
u_{0 j} \\
u_{1 j}
\end{array}\right] \sim N\left(0, \Omega_{u}\right), \quad \Omega_{u}=\left[\begin{array}{ll}
0.074 & \\
0.011 & 0.011
\end{array}\right]
$$

The probability density function for this bivariate Normal model where the means of the two variables are 0 is

$$
p(\theta)=\frac{1}{(2 \pi)}\left|\Omega_{u}\right|^{-1 / 2} \exp \left(-\frac{1}{2}\left(\theta^{T} \Omega_{u}^{-1} \theta\right)\right.
$$

To calculate and plot this bivariate distribution, close the graph then type:

| Command | Explanation |
| :---: | :---: |
| erase 'z' |  |
| join 0.0740 .0110 .011 c100 | create $\Omega_{u}$ |
| calc c101 $=$ sym(c100) | fill in (1,2) value of $\Omega_{u}$ (omitted in notation because $\Omega_{u}$ a symmetric matrix) |
| gene -0.8 0.800 .05 c 102 | generate values for $u_{0 j}$ |
| gene -0.40 .40 .05 c103 | generate values for $u_{1 j}$ |
| ucom c102 c103 c104 c105 | create all combinations of ( $u_{0 j}, u_{1 j}$ ) |
| $\begin{aligned} & \hline \text { name c104 'u0' c105 'u1' } \\ & \text { c107 'z' } \end{aligned}$ |  |
| count 'u1' b1 |  |
| join 'u0' 'u1' c106 |  |
| matr c106 b1 2 | turn this grid into a $b 1$ by 2 matrix |
| $\begin{aligned} & \text { calc } ' z^{\prime}=1 /(2 * 3.1416) \\ & * \operatorname{det}(c 101)^{\wedge}(-0.5)^{*} \\ & \operatorname{expo}(-0.5 * \operatorname{diag}(c 106 \\ & \left.\left.* . \operatorname{inv}(c 101)^{*}(\sim c 106)\right)\right) \end{aligned}$ | Apply the Normal PDF to all values of of $\left(u_{0 j}, u_{1 j}\right)$ in c106 |
| surf 1 'u0' 'u1' 'z' |  |
| show 1 |  |

Selecting <plotting method><surface with contouring> on the graph that appears produces


The SCATter command can produce 3D scatters. For example,

- Close the 3d graph window
- In the Command interface window type:
- SCAT 1 'avslrt' 'normexam' 'standlrt'
- Show 1


We can group the plot by vrband:

- Close the 3D graph window
- In the Command interface window type:
- SCAT 1 'avslrt' 'normexam' 'standlrt' 'vrband'
- show 1



## 4 Model Comparison Tables

MLwiN now has a mechanism for storing the results of a series of models and displaying them in a single table. This has two main uses. Firstly, it is useful when conducting an analysis as it enables the user to easily see the results of a series of models. Secondly, often when writing papers, results from a series of models are presented in a single table; constructing these tables manually can be a time consuming and error prone process. To a large extent MLwiN now automates this process.

Let's set up a variance components model on the tutorial dataset

- Open the tutorial worksheet
- In the Equations window click on $\mathbf{y}$
- In the $y$ variable window select:
y: Normexam
N levels: 2
level 2(j): school
level 1(i): student
- Click done
- Click on $\beta_{0} x_{0}$
- Select cons from the drop-down list in the $\mathbf{X}$ variable window
- Tick j(school), i(student)
- Click Done

Running the model gives:

| Equations $\quad-\mathbf{- a}$ |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\begin{aligned} & \operatorname{normexam}_{i j} \sim \mathrm{~N}(X B, \Omega) \\ & \text { normexam }_{i j}=\beta_{0 i j} \text { cons } \\ & \beta_{0 i j}=-0.013(0.054)+u_{0 j}+e_{0 i j} \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\left[u_{0 j}\right] \sim \mathrm{N}\left(0, \Omega_{u}\right): \Omega_{u}=[0.169(0.032)]$ |  |  |  |  |  |  |  |  |  |  |  |  |
| $\begin{aligned} & {\left[e_{0 i j}\right] \sim \mathrm{N}\left(0, \Omega_{e}\right): \Omega_{e}=[0.848(0.019)]} \\ & -2 * \log \text { likelihood(IGLS Deviance) }=11010.648(4059 \text { of } 4059 \text { cases in use }) \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |  |  |
| Name | + | - | Add İerm | Estimates | Monlinear | Clear | Notation | Responses | store | Help | Zoom 100 | $\square$ |

We can add this model to the stored sequence of models under the name 'Model 1' by clicking on the Store button at the bottom of the Equations window and typing a name for the model in the window which appears, in this case Model 1. We can view the sequence of stored models (so far only one model) by selecting Compare stored models from the Model menu. This produces:

| E. | Results Table |  | - $\quad$ - |
| :---: | :---: | :---: | :---: |
| Copy |  |  |  |
|  | Model 1 | S.E. | Corr |
| Response | normexam |  |  |
| Fixed Part |  |  |  |
| cons | -0.013 | 0.054 |  |
| Random Pan |  |  |  |
| Level: schor |  |  |  |
| cons/cons | 0.169 | 0.032 | 1.000 |
| Level: stude |  |  |  |
| cons/cons 0.848 0.019 |  |  |  |
|  |  |  |  |
| vglikelihood: | 11010.648 |  |  |
| DIC: |  |  |  |
| pD: |  |  |  |
| Units: schoc | 65 |  |  |
| Units: studel | 4059 |  |  |

Clicking the Copy button will paste a tab-delimited text file into the clipboard.

- Click the Copy button

In Microsoft Word:

- Paste the text into a document
- Highlight the pasted text in Microsoft Word
- Select the <Table><Insert><Table. . > menu item

This produces:

|  | Model 1 | S.E. | Model 2 | S.E. | Model 3 | S.E. |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Response | normexam |  | normexam |  | normexam |  |
|  |  |  |  |  |  |  |
| Fixed Part |  |  |  |  |  |  |
| cons | -0.013 | 0.054 | 0.002 | 0.040 | -0.012 | 0.040 |
| standlrt |  |  | 0.563 | 0.012 | 0.557 | 0.020 |
|  |  |  |  |  |  |  |
| Random Part |  |  |  |  |  |  |
| Level: school |  |  |  |  |  |  |
| cons/cons | 0.169 | 0.032 | 0.092 | 0.018 | 0.090 | 0.018 |
| standlıt/cons |  |  |  |  | 0.018 | 0.007 |
| standlrt/standlrt |  |  |  |  | 0.015 | 0.004 |
| Level: student |  |  |  |  |  |  |
| cons/cons | 0.848 | 0.019 | 0.566 | 0.013 | 0.554 | 0.012 |
|  |  |  |  |  |  |  |
| $-2^{*}$ loglikelihood: | 11010.648 |  | 9357.242 |  | 9316.870 |  |
| DIC: |  |  |  |  |  |  |
| pD: |  |  |  |  |  |  |
| Units: school | 65 |  | 65 |  | 65 |  |
| Units: student | 4059 |  | 4059 |  | 4059 |  |

We can see a list of all models currently stored by selecting Manage stored models from the Model menu (shown here after storing several more models).


This allows us to select just some of the models to view in a results table, rather than having to display all of them as we would if we selected Compare stored models; to delete any or all stored models; or to rename any stored model. Note that there is no way to bring any of the stored models up again in the Equations window - if you wish to be able to easily return to working with a certain model after moving on to another one, you should save the worksheet (probably under a different name), and then you can return to that model by returning to that saved worksheet.

The tick-boxes control how much information is displayed in the Results Table for each of the models. These are:
S.E. - Standard Error Correlation - Correlation between random parameters C.I. - Upper and Lower 95p-value - p-value for (R)IGLS models, Bayesian p-value for MCMC models z-score - Z-score for (R)IGLS models Median - Median of parameter chain for MCMC models ESS - Effective sample size for paramter chain for MCMC models

All of this information is recorded regardless of which boxes are ticked when
the model is stored

Note that neither the Results Table nor the list of stored models will not refresh automatically when a new model is stored. You will need to close them and once again select Compare stored models or Manage stored models from the Model menu for the new model to be included.

Storing and retrieving of model results can also be done using commands. The formats of the model table commands are

## MSTO $<\mathbf{S}>$ : store model results as $\mathbf{S}$

for example, entering the command

```
MSTOre 'modela'
```

appends the current model to the table of models and names the model 'modela'

MPRI : print stored model results to Output window
MCOM $<\mathbf{S}>\ldots<\mathbf{S}>$ : compare the listed models; compare all if no parameters
for example, entering the command

```
MCOM 'Model 1' 'modela' 'Model 4'
```

would create a model table comparing Model 1, modela and Model 4
MERA $<\mathbf{S}>$ : erase stored model results for listed models
for example:

```
MERA 'modela'
```

erases modela
MWIPe : erase all stored models
Let's create a macro to run a sequence of models and store each one in a model comparison table

| Command | Explanation |
| :---: | :---: |
| clear | clear any current model |
| mwipe | clear model comparison table |
| resp 'normexam' | set response |
| iden 1 'student' 2 'school' | set level IDs |
| addt 'cons' | intercept |
| setv 2 |  |
| setv 1 | set variance components |
| expa 3 | expand terms in Equations window |
| estm 2 | show estimates in Equations window |
| maxi 1000 | set maximum iterations to 1000 |
| batc 1 | do not pause in between iterations |
| star 1 | run the variance components model |


| msto 'Model 1' | store the results |
| :--- | :--- |
| addt 'standlrt' | add a slope to the model |
| next 1 | run the new model |
| msto 'Model 2' | store the fixed slope variance compo- <br> nents model |
| setv 2 | add a random slope |
| next 1 | run the random slopes model |
| msto 'Model 3' | store the random slopes model |

Note the START and NEXT commands when called from a macro with parameter 1 will cause the Equations window to be updated after each modelling iteration. Sometimes this can result in the software spending too much time updating the screen and not enough time doing sums. In this case you may prefer to use the START and NEXT commands with no added parameter, in which case screens are not updated during macro file execution. You can however place a PAUSE 1 command at any point in a macro script which will cause all displayed windows to update themselves.

- From the File menu select New Macro
- Type or paste the above command sequence into the macro window
- Make sure the Equations window is open and visible
- Click the Execute button at the bottom of the macro window

You should now see the sequence of requested models being executed in the Equations window. To view the model comparison table, type
in the Command interface window or select Compare stored models from the Model menu. This produces:

| E. | Results Table |  |  |  |  |  |  |  | - - ${ }^{\text {x }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Copy |  |  |  |  |  |  |  |  |  |
|  | Model 1 | S.E. | Corr | Model 2 | S.E. | Corr | Model 3 | S.E. | Corr |
| Response | normexam |  |  | normexam |  |  | normexam |  |  |
| Fixed Part |  |  |  |  |  |  |  |  |  |
| cons | -0.013 | 0.054 |  | 0.002 | 0.040 |  | -0.012 | 0.040 |  |
| standrit |  |  |  | 0.563 | 0.012 |  | 0.557 | 0.020 |  |
|  |  |  |  |  |  |  |  |  |  |
| Random Pal |  |  |  |  |  |  |  |  |  |
| Level: schor |  |  |  |  |  |  |  |  |  |
| cons/cons | 0.169 | 0.032 | 1.000 | 0.092 | 0.018 | 1.000 | 0.090 | 0.018 | 1.000 |
| standirt/con |  |  |  |  |  |  | 0.018 | 0.007 | 0.498 |
| standirt/star |  |  |  |  |  |  | 0.015 | 0.004 | 1.000 |
| Level: stude |  |  |  |  |  |  |  |  |  |
| cons/cons | 0.848 | 0.019 |  | 0.566 | 0.013 |  | 0.554 | 0.012 |  |
|  |  |  |  |  |  |  |  |  |  |
| 2glikelihood: | 11010.648 |  |  | 9357.242 |  |  | 9316.870 |  |  |
| DIC: |  |  |  |  |  |  |  |  |  |
| pD: |  |  |  |  |  |  |  |  |  |
| Units: schoc | 65 |  |  | 65 |  |  | 65 |  |  |
| Units: studel | 4059 |  |  | 4059 |  |  | 4059 |  |  |

Suppose we decided to recode a variable, e.g., turning standlrt into a binary variable. We can recode the variable and reanalyse and the model comparison table will get reformed.

- In the Command interface window, type
- calc 'standlrt' = 'standlrt' > 0
- Rerun the analysis macro file
- In the Command interface window, type

```
mcomp
```

which then produces the updated results table:

| E | Results Table |  |  |  |  |  |  |  | - - $\times$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Copy |  |  |  |  |  |  |  |  |  |
|  | Model 1 | S.E. | Corr | Model 2 | S.E. | Corr | Model 3 | S.E. | Corr |
| Response | normexam |  |  | normexam |  |  | normexam |  |  |
|  |  |  |  |  |  |  |  |  |  |
| Fixed Part |  |  |  |  |  |  |  |  |  |
| cons | -0.013 | 0.054 |  | -0.453 | 0.047 |  | -0.462 | 0.043 |  |
| standlit |  |  |  | 0.875 | 0.027 |  | 0.878 | 0.044 |  |
|  |  |  |  |  |  |  |  |  |  |
| Random Pai |  |  |  |  |  |  |  |  |  |
| Level: schor |  |  |  |  |  |  |  |  |  |
| cons/cons | 0.169 | 0.032 | 1.000 | 0.120 | 0.023 | 1.000 | 0.095 | 0.021 | 1.000 |
| standirt/con |  |  |  |  |  |  | 0.002 | 0.015 | 0.023 |
| standirt/star |  |  |  |  |  |  | 0.073 | 0.021 | 1.000 |
| Level: stude |  |  |  |  |  |  |  |  |  |
| cons/cons | 0.848 | 0.019 |  | 0.670 | 0.015 |  | 0.655 | 0.015 |  |
|  |  |  |  |  |  |  |  |  |  |
| gglikelihood: | 11010.648 |  |  | 10050.762 |  |  | 10007.835 |  |  |
|  |  |  |  |  |  |  |  |  |  |
| pD: |  |  |  |  |  |  |  |  |  |
| Units: schoc | 65 |  |  | 65 |  |  | 65 |  |  |
| Units: studel | 4059 |  |  | 4059 |  |  | 4059 |  |  |

## 5 A new method for estimating autocorrelated errors in continuous time

Previous versions of MLwiN implemented in a set of macro files the algorithms in Goldstein et al. (1994) to estimate models with autocorrelated errors at level 1. The macros were rather unstable and we removed them in version 2.02 of MLwiN. We introduce here a simpler method of estimating these models.

A common use of these models is where we have repeated measures data and the measurement occasions are close together in time.


The above graph shows a linear time trend fitted to repeated measurements on one individual. We can see that the residuals around the graph are not independent. Residuals close together in time show positive correlations; this correlation decreases as the time distance between measurements increases. In a multilevel analysis we will have many such lines, one for each individual in the dataset. In the multilevel case too, the residuals around each person's line may show a pattern of non-independence which is a violation of our model assumptions and could potentially lead to incorrect estimates of parameters. The covariance between two measurements taken at occasions $i_{1}$ and $i_{2}$ on individual $j$ cannot be assumed to be 0 . That is

$$
\operatorname{cov}\left(e_{i_{1} j}, e_{i_{2} j}\right) \neq 0
$$

We expect this covariance to decrease as the time interval between the measurements increases. Let $t_{i j}$ denote the time of the $i$ th measurement on the $j$ th individual. A natural model for the covariance is

$$
\operatorname{cov}\left(e_{i_{1} j}, e_{i_{2} j}\right)=\alpha \frac{1}{\left|t_{i_{1} j}-t_{i_{2} j}\right|}
$$

The autocorrelation is then

$$
\begin{equation*}
\operatorname{cor}\left(e_{i_{1} j}, e_{i_{2} j}\right)=\frac{\alpha \frac{1}{\mid \overline{t_{i_{1}}-t_{i_{2} j} \mid}}}{\sigma_{e}^{2}} \tag{1}
\end{equation*}
$$

We will use the Oxford boys dataset to illustrate how to fit multilevel time series models with autocorrelated errors modelled as (1). The Oxford boys
dataset contains height measurements on 26 boys each measured on nine occasions between the ages of 11 and 13 .

First we set up a repeated measures model on the oxboys data with no autocorrelation structure. The data is in the worksheet oxboys.ws. The following model should already be set up in the Equations window:

$$
\begin{aligned}
& -2 * \log \text { likelihood(IGLS Deviance) }=625.366(234 \text { of } 234 \text { cases in use })
\end{aligned}
$$

To add the term (1) to the model we first construct

$$
\delta_{\left(i_{1}, i_{2}\right) j}=\left|t_{i_{1} j}-t_{i_{2} j}\right|
$$

In this dataset we have 26 individuals each with 9 measurements so $\delta$ is a list of 26 symmetric matrices of dimension $9 x 9$. That is

$$
\begin{aligned}
& {\left[\begin{array}{cccc}
t_{1,1}-t_{1,1} & & & \\
t_{2,1}-t_{1,1} & 0 & & \\
\vdots & \vdots & \ddots & \\
t_{9,1}-t_{1,1} & t_{9,1}-t_{2,1} & \cdots & t_{9,1}-t_{9,1}
\end{array}\right]} \\
& {\left[\begin{array}{cccc}
t_{1,26}-t_{1,26} & & & \\
t_{2,26}-t_{1,26} & 0 & & \\
\vdots & \vdots & \ddots & \\
t_{9,26}-t_{1,26} & t_{9,26}-t_{2,26} & \cdots & t_{9,26}-t_{9,26}
\end{array}\right]}
\end{aligned}
$$

The SUBS command can set up such difference matrices (see 'command SUBS' in MLwiN Help for details on how to use this command). In the Command interface window type

```
subs c1 -1 c2 c2 c10
```

In this format the command calculates the required 26 symmetric matrices and stacks them in c10. These matrices can be viewed with the MVIEw command:

```
MVIE 'ID' c10
```

which produces, after clicking the Output button in the Command interface window:


Now we form $\frac{1}{\left|t_{i_{1} j} t_{i_{2} j}\right|}$

| Command | Explanation |
| :--- | :--- |
| chan $0 \quad$ c10 -1 c10 | avoid zero divide |
| calc $\quad$ 11=1/c10 |  |
| chan $-1 \quad$ c11 0 c11 | set diagonal back to 0 |

C10 now contains the required structure to be added to the covariance matrix automatically specified by the multilevel model

$$
\operatorname{cov}\left(e_{i_{1} j}, e_{i_{2} j}\right)=\alpha \frac{1}{\left|t_{i_{1} j}-t_{i_{2} j}\right|}
$$

where $\frac{1}{\left|t_{i_{1} j} j t_{i_{2} j}\right|}$ are known and stored in c11, and $\alpha$ is to be estimated. The command

## SETDesign 2 C11

adds the design matrix held in C11 to the model at level 2. It may seem odd that this design matrix is applied at level 2 even though we are modelling autocorrelation between level 1 errors. This is because MLwiN thinks of any design matrices modelling non-independence between level 1 units as a higher level phenomenon.

At the moment the Equations window does not show the matrices specified via SETD and their associated parameter estimates. We have to revert to the Command interface to see them. In the Command interface window type

| Command | Explanation |
| :--- | :--- |
| batc 1 | don't pause in between iterations |
| maxi 50 | set maximum no. of iterations to 50 |
| star | run model |
| fixed | print out fixed parameters |
| random | print out random parameters |
| like | print out log likelihood |

which updates the text Output window:


The estimate of $\alpha$ is 0.01625 . The range of $t_{i_{1} j}-t_{i_{2 j} j}$ is from 0.16 to 2 years. So we can generate the autocorrelation function by

| Command | Explanation |
| :--- | :--- |
| gene 0.1620 .01 c 100 | generate $t_{i_{1} j}-t_{i_{2} j}$ |
| calc c101 $=$ | calculate $\alpha \frac{1}{\left\|t_{i_{1} j}-t_{i_{2} j}\right\|}$ |
| $0.01625 *(1 / \mathrm{c} 100)$ |  |
| calc c101 $=c 101 / 0.275$ |  |

Then plotting c101 against c100 gives:


The drop in the likelihood from adding the autocorrelation parameter to this model is only 2 . So in this case the extra term is not required.

## 6 Saving and retrieving of Minitab, Stata and SPSS work files

MLwiN now provides the following additional data file types on the Save / Open worksheet dialogue boxes:

Stata (*.dta files, versions 5-12)
SPSS (*.sav files, up to version 14)
Minitab (*.mtw, versions 12 and 13)
SAS transport (*.xpt)
Data, missing data values, variable names and category names are transferred.

Commands:

| Command | Function |
| :--- | :--- |
| RSTAta filename | -open a Stata file |
| SSTAta filename | -save as a Stata file |
| RSPSs filename | -open an SPSS file |
| SSPSs filename | -save as an SPSS file |
| RMTW filename | -open a Minitab file |
| SMTW filename | -save as a Minitab file |
| RSAS filename | -open a SAS transport file |
| SSAS filename | -save as a SAS transport file |

## 7 Zipped MLwiN worksheets

MLwiN can now save and open zipped versions of MLwiN worksheets (*.wsz). This format can reduce disc space usage by between $95 \%$ and $99 \%$. Saving as a zipped version is the default option when selecting Save from the File menu; there are also commands which will save and open zipped versions of worksheets.

Commands:

| Command | Function |
| :--- | :--- |
| ZRETr filename | -open a zipped worksheet |
| ZSAVe filename | -save worksheet in zipped form |

## 8 Other new features

### 8.1 Window tabs

There is now a series of tabs shown at the bottom of MLwiN, with one for each window open. Clicking on these provides an easy way to bring up the required window.


When there are too many windows open for all the tabs to be able to be shown at once, a pair of arrow buttons are shown which allow the user to scroll through the tabs:

Customised prediction plot $\mid$ Command interface $|$| Names | \| |
| :---: | :---: |

### 8.2 The Names window

The new Names window has some extra features for ease of usage. The new Names window looks like this:


### 8.2.1 Column buttons

The Name button under Column allows the name of the highlighted column to be changed.

You can now add descriptions for each variable in the worksheet by selecting a column in the Names window and pressing the Description button.

See section 8.2.3 for documentation of the Toggle Categorical button.

### 8.2.2 Data buttons

You can now highlight variables in the Names window and view the corresponding data directly by pressing the View button under Data. For example (using the tutorial dataset),

- Highlight columns $8-10$ (avslrt, schav, vrband) in the Names window (use ctrl + click to select multiple columns)
- Click View under Data

This produces:

| E. |  | Data |  |  | - | $\mathbf{x}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| goto li | ne 1 | view | Help | $\nabla$ Show value labels |  |  |
|  | avsitt( 4059) | schav( 4059) |  | vrband (4059) |  | $\wedge$ |
| 1 | 0.166 | mid |  | vb1 |  |  |
| 2 | 0.166 | mid |  | vb2 |  |  |
| 3 | 0.166 | mid |  | vb3 |  |  |
| 4 | 0.166 | mid |  | vb2 |  |  |
| < |  |  |  |  | > | $\checkmark$ |

The Copy and Paste buttons under Data can be used to copy and paste variables from column to column in the worksheet, from one MLwiN worksheet to another, or to/from other applications such as Excel spreadsheets. To copy, highlight a column or columns (which need not be consecutive) and click Copy under Data. The column name is also copied and placed into the first row of the relevant column (the data the column contains being shifted down to row 2 onwards). To paste, first the destination columns must be highlighted. You can highlight the required number of columns, which need not be consecutive; in this case any data already present in these columns will be overwritten. Alternatively, you can highlight just one column; in this case the first column of data will be pasted into this column, whether it contains data or not, and the remaining columns will be pasted into the next free columns in the worksheet after this one. After highlighting, click Paste under Data. See section 8.2.3 for more details on copying and pasting categorical variables. If the first row of the pasted data contains a non-numerical string, this will be used as the column name; otherwise the column keeps the name it already has. This means that if copying and pasting from column to column within a worksheet, you will get an error message when you paste warning you that a column with the name you are trying to assign to the column you are pasting into already exists "duplicate name(PAST)". Simply click ok, and the column will retain the name it had before you pasted into it. You can then change this name if you wish to something else (that is not already used as a name by another column in the worksheet).

The Delete button will erase all the data in the highlighted column(s) and
rename them as $\mathrm{c}<$ column number $>$.

### 8.2.3 Categorical variables

There is now a column in the Names window that indicates whether a variable is categorical or not. The Toggle Categorical button will toggle the categorical status of a variable. When converting a non-categorical variable to categorical using this button, category names are automatically generated. These will be of the form < variable name>_<category number>, e.g. ethnicity_1. The category labels can be viewed and edited using the View under Categories, as we will see shortly. (Note that from v2.10 to v2.17, this function was performed by the Categories button).

Beware unexpected behaviour for categorical variables. When the underlying data in a column defined as categorical changes MLwiN does not update the list of category names associated with that column. To illustrate this:

- Select the schav variable in the Names window
- Click the View button in the categories section

This shows schav is a 3 category variable


- Click the OK button

Let's now overwrite the data in this column with a set of uniform random numbers:

- In the Command interface window type:

```
uran 4059 'schav'
```

- Now click the Data button in the Names window

This shows the following odd mixture of numbers and category names for column 9


What has happened is that the category information for column 9 has persisted and where any numbers in column 9 , rounded to the nearest integer, correspond to a category number the name for that category is displayed. You can verify this by deselecting the Show value labels tick box in the Data window.

Whenever the underlying data for a categorical variable changes in such a way that the categories present in the data change, you need to update the category information. Changes to the underlying data could happen through a recoding (such as we just carried out), or when selecting or omitting certain cases, for example omitting all cases belonging to a certain category. Updating the category information would mean toggling the categorical status variable off if the variable has become continuous. If instead the variable remains categorical, you can Toggle categorical off, Toggle categorical on and then, if non-default category names are required, use View under Categories to re-enter the category names.

A shortcut when some of the categories remain the same is the Regenerate button. This retains category names for numbers which are still present in that variable, discards the category names for any numbers which are no longer present in the variable, and adds automatically generated category names for any numbers which did not already have category names assigned but are now present in the variable. These automatically generated names (if any) can then if desired be edited as described above using the View button under Categories. Take care when using the Regenerate button after recoding the underlying numerical values to be sure that any retained category names apply to the appropriate category numbers (since the numbers the names should apply to may change when you recode).

The Regenerate button may also be useful after importing data to MLwiN from other programs such as SPSS or Stata which allow several different categories of MISSING. On importing, MLwiN will recode all these values to its MISSING value but the labels remain assigned to their original codes, causing extra unwanted dummies or equations to appear when entering the variable into a model as an explanatory or response variable. Highlighting each variable in turn and pressing the Regenerate button will remove the
unneeded category labels.
Category labels can be copied from a variable by highlighting this variable and pressing Copy under Categories. These can then be pasted onto another column by highlighting that column and pressing Paste under Categories. The column pasted to need not already be categorical; if it is not then it will become categorical when the categories are pasted into it. (Note that there is no undo button for this paste operation). Category labels can also be pasted into a program such as Word Pad, Excel, or Word, edited here if desired, then copied from these programs and pasted back into MLwiN.

Copying a categorical variable (not just its labels) to another column in the same worksheet or to a different worksheet and preserving its category labels is a two step task. First the data must be copied, by highlighting the variable, pressing Copy under Data, highlighting the destination column, and pressing Paste under Data. This will copy the numerical values of the variable, but the variable will not be declared as categorical, and if Toggle Categorical is pressed it will not have the original category labels but instead automatically generated ones. To preserve the labels, the second step is, after pasting, to highlight the original variable again, press Copy under Categories, highlight the new variable, and press Paste under Categories.

### 8.2.4 New commands

We document here new commands in v2.1* and v2.2* which carry out the same functions as the buttons in the Names window.

```
DESC C 'description'
```

assigns a description to a column
e.g.

DESC c10 'This variable was collected from...'

COPY Mode N C..C
$\mathbf{N}=0 / 1$ exclude/include column headings
copies listed variables into the clipboard with tab delimited format

```
PASTe C..C
```

pastes clipboard data into listed columns. If there are fewer columns provided in the command than columns of data on the clipboard then writing of data continues from the last column number supplied (note that in this case, the data is not only pasted into free columns: the writing of data continues into consecutive columns whether or not they already contain data).

## CCAT C

copies the category labels from the specified column

## PCAT C

pastes the category labels on the clipboard to the specified column

## RCAT C

regenerates the category labels for the specified column

### 8.3 New data manipulation windows and commands

### 8.3.1 Combining categorical columns

The COMBine command combines 2 or more columns containing categorical data. The categories of the output column will consist of a category for each possible different combination of the input codes with the names of these categories formed from the concatenation of the input category names. For example, given we have variables schav ( $1=$ low, $2=\mathrm{mid}, 3=$ high $)$ and vrband ( $1=\mathrm{vb} 1,2=\mathrm{vb} 2,3=\mathrm{vb} 3$ )

- If you carried out the demonstration in 8.1.2 showing how category names persist after changing the data in the schav column, then close the worksheet without saving and re-open it so you will have the correct data for schav
- In the Command interface window type:

```
- comb 'schav' 'vrband' c11
```

- Select C11 in the Names window
- Click the View button in the categories section of the Names window

This will produce:

| E Set categ... |  | - | $\square$ | X |
| :---: | :---: | :---: | :---: | :---: |
| Edit | OK |  |  |  |
| Name |  | Cod |  |  |
| mid\&vb1 |  | 0 |  |  |
| mid\&vb2 |  | 1 |  |  |
| mid\&vb3 |  | 2 |  |  |
| high\&vb2 |  | 3 |  |  |
| high\&vb1 |  | 4 |  |  |
| high\&vb3 |  | 5 |  |  |
| low\&vb2 |  | 6 |  |  |
| low\&vb3 |  | 7 |  |  |
| low\&vb1 |  | 8 |  |  |

### 8.3.2 Finding unique codes

The UNIQue command will find each different value that occurs in the input column and place it just once in the output column (regardless of how many times it appears in the input column). For example, typing the command

## UNIQue 'normexam' c12

and then looking at the Names window shows that c12 contains 71 unique values in the range $(-3.66,3.66)$. This will have come about because our "continuous" variable Normexam was originally formed by applying a normal score transformation to a discrete scale with data on 71 points.

### 8.3.3 Creating numeric grids

It is sometimes useful to create a set of output columns containing all combinations of values occurring in a set of input columns. The UCOM command does this. For example,

- join 123 c100
- join 456 c101
- UCOM c100 c101 c102 c103
would create

| E. |  | Data |  |  |  | - $\square$ | x |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| goto lin | 1 | view | Help | Font $\bar{\square}$ | Show value labels |  |  |
|  | c100(3) | c101 |  | c102(9) | c103( 9) |  | $\Delta$ |
| 1 | 1.000 | 4.000 |  | 1.000 | 4.000 |  |  |
| 2 | 2.000 | 5.000 |  | 2.000 | 4.000 |  |  |
| 3 | 3.000 | 6.000 |  | 3.000 | 4.000 |  |  |
| 4 | - | - |  | 1.000 | 5.000 |  |  |
| 5 | - | - |  | 2.000 | 5.000 |  |  |
| 6 | - | - |  | 3.000 | 5.000 |  |  |
| 7 | - | - |  | 1.000 | 6.000 |  |  |
| 8 | - | - |  | 2.000 | 6.000 |  |  |
| 9 | - | - |  | 3.000 | 6.000 |  |  |
| 10 | - | - |  | - | - |  | - |

### 8.3.4 Recoding variables with short sequences of codes

The existing Recode window is convenient for discretising continuous variables according to a set of ranges. When we have variables with a small number of values an interface which lists each unique value and allows a new value to be specified is more helpful for recoding or merging short sequences of codes. Both these options are now available on the Recode sub-menu of the Data Manipulation menu.

Note that when you recode a categorical variable the category code information is not updated. So if you recode a variable so as to collapse 4 categories into 3 , the variable will still be considered to have 4 categories (though one will have zero observations); or if you recode all observations in category 3 to have the value 10 and you do not already have a category with code 10 , then category 3 will still have code 3 (and will have no observations) and observations with code 10 will not be considered to belong to any category. In order to update the category information after recoding you will need to highlight the variate in the Names window and press Toggle Categorical twice. This switches the variable to continuous and back to categorical, and when it is switched back to categorical the category names are re-created (if you have specific names you want to give the categories you will need to re-enter these by clicking on Categories).

### 8.3.5 Unvectorising data

For repeated measures analyis MLwiN requires the data to be structured one row per occasion, and for multivariate response modelling MLwiN automatically structures the data with one row per response variable. Sometimes it useful to take MLwiN data with one row per multivariate response or one row per occasion and unvectorise it, that is, turn it back so that it has one row per individual. This can be done with the UNVEctorise command:

UNVEctorise $\mathbf{N}$ stacked variables, stacked variable indicators in $\mathbf{C}$, repeated individual codes in $\mathbf{C}$, stacked data values in $\mathbf{C}$, unique individual codes to $\mathbf{C}$, unstacked data to $\mathbf{C} . . \mathbf{C}$

Which is a bit of a mouthful. An example will help. Given the stacked data

| Individual ID | Indicator | Value |
| :--- | :--- | :--- |
| C 1 | C 2 | C 3 |
| 1 | 1 | 11 |
| 1 | 2 | 12 |
| 1 | 3 | 14 |
| 2 | 1 | 16 |
| 2 | 3 | 18 |

```
UNVEct 3 c2 c1 c3 c4 c5 c6 c7
```

will produce

| C4 | C5 | C6 | C7 |
| :--- | :--- | :--- | :--- |
| 1 | 11 | 12 | 14 |
| 2 | 16 | MISSING | 18 |

The Unsplit Records menu item on the Data Manipulation menu provides a window to help specify the UNVEct command. It also makes it possible to unstack several variables at once, which cannot be done with the UNVEct command (to unstack multiple variables you have to use the command repeatedly). To demonstrate how to use the window:

- Open the reading1.ws worksheet
- Split the data as shown on pages 179-182 of the MLwiN User's Guide.
- Delete columns c1-c13
- Choose Unsplit Records from the Data Manipulation menu
- Set up the Unsplit records window as follows:

- Click Unstack
- Select No when the box appears asking if you want to save the worksheet.
- Ignore the warning message that appears.
c1-c13 will now contain the data as it was when you opened the worksheet.


### 8.4 Macro Programming

### 8.4.1 Executing models from macros

You can run models from macros using the STARt and NEXT commands. By default the Equations window is not updated. Let's set up and run a couple of basic binary response models on the Bangladeshi fertility data from a macro. Open the worksheet bang.ws, then type or copy and paste the sequence of commands in the left column of the table below into an MLwiN macro

| Command | Explanation |
| :--- | :--- |
| mwipe | clear model comparison table |
| wset 15 1 | show the Equations window |
| resp 'use' | declare response |
| rdist 1 0 | set distribution for first (and only) re- <br> sponse to be binomial |
| lfun 0 | set link function to logit |
| linea 1 2 | set linearisation to 2nd order PQL |
| doffs 1 'cons' | set denominator to column of 1's |
| iden 1 'woman' 2 'district' | declare level ids |
| addt 'cons' | add intercept |
| setv 2 'cons' | declare random intercepts |
| maxi 50 | set maximum iteration $=50$ |
| batc 1 | don't pause in between iterations |
| star | run model |
| msto 'model 1' |  |
| addt 'age' | add age |
| next |  |
| msto 'model 2' |  |
| mcomp |  |

If you execute this macro, the screen will not be updated until macro execution has been completed. You will then see the final model in the Equations window and both models in the model comparison table (click the Estimates button on the Equations window to see the results). (Note that the estimates in the Equations window always appear in blue when you run models from a macro, rather than in green, but this does not mean they have not converged).


You may want to see the results after each model has been completed. In which case we place a PAUSe 1 command after the first STARt command in the macro. Even finer grained updating of the Equations (and other windows) is possible when running models from a macro. If you use the
commands STARt and NEXT commands with the optional parameter 1, then windows are updated after each model estimation iteration.

It is sometimes useful to control the Equations window display from a macro. The following commands are useful for this
notation N: $0 ; 1=$ Simple; General

EXPAnd N: $0 ; 1 ; 2 ; 3=$ Show $\beta$ s only; show $\beta \mathbf{s}$ and $u_{j} \mathrm{~s} ;$ show $\beta \mathrm{s}, u_{j} \mathrm{~S}$ and $\Omega_{u}$; show $\beta \mathrm{s}, u_{j} \mathrm{~s}, \Omega_{u}$ and priors (if MCMC)

NMVA $\mathbf{N}: 0 ; 1=$ display observed variables as symbols; display observed variables as names

INDExing $\mathbf{N}: 0 ; 1=$ multiple subscript; single subscript

ESTMates N: 0; 1; $2=$ symbols all black; symbols + convergence indication (blue, green); numbers + convergence indication

Other useful commands for specifying discrete response models in macros:

RDISTribution for response $\mathbf{N}$, distribution type $\mathbf{M}$
$\mathbf{N}$ is in range 1 to Number of responses, $\mathbf{M}=0$ binomial, 1 Poisson, 2 negative binomial, 3 Normal, 4 multinomial, 5 ordered multinomial

LFUN $\mathbf{N}: 0,1,2=\operatorname{logit}$, probit, cloglog, $\log$
If response distribution is Normal LFUN setting is ignored and identity link is used.

LINEarise $\mathbf{N} \mathbf{M}: \mathbf{N}$ is $0,1=\mathrm{MQL}, \mathrm{PQL} ; \mathbf{M}$ is $1,2=$ order 1 , order 2
Taylor expansion

> DOFFs for response $\mathbf{N}$ is in $\mathbf{C}$ : set denominator or offset column to $\mathbf{C}$
> $\mathbf{N}$ is in range 1 to Number of responses. If the response variable has a binomial or multinomial distribution the column is taken to contain denominators. If the response variable has a Poisson or Negative Binomial distribution, the column is taken to be the natural $\log$ of the required offset value.

### 8.4.2 Other New Commands

The following commands have been added / extended, which may be useful when programming in macros.

```
SJOIn S 'text' B N...S : string concatenation. For example:
```

- sjoin 'There are' s1
- set b1 7
- sjoin s1 ' ' b1 ' deadly sins' s2
- say s2
produces (in the Output window): There are 7 deadly sins NMSTr C S : create a string consisting of the name of a column for example:
- NAME c1 'hello'
- NMSTR c1 s1
- SAY s1

The following commands have been updated to work with string variables:

```
All worksheet save and retrieve commands
PREf
POSTf
DESCription
SAY
WMSG
LOGOn
```

```
MSTOre
```

MPRInt
MDELete

For example,

```
SAVE c:\test.ws
```

is equivalent to

- SJOIN 'c:\test.ws' s1
- SAVE s1


### 8.5 Invoking MLwiN from a command line (or other packages)

MLwiN can be invoked from a command line with a number of potentially useful switches. Probably the main purpose of this is if MLwiN is to be called from an external scripting engine.

```
mlwin <switches> <worksheet name>
Switches:
/help show list of switch options
/run an mlwin macro file
/load an mlwin macro into mlwin's macro file editor
/sheetsize worksheet size in k cells
/levels number of levels to allow in analysis
/columns number of worksheet columns
/min start MLwiN minimized
/nogui hide MLwiN graphical interface
/reset reset MLwiN settings to defaults
/nowarn suppress warning messages
```


## A Algorithm used for producing predicted means and intervals

Simulation techniques, for predicting means, intervals and coverage (from higher level variances), are used for all models even when there is an analytical solution (eg for Normal response models and cluster specific predictions from discrete repsonse models). This is not always computationally most efficient, but allows the same code for all model types.

## A. 1 Normal response models

$$
\begin{aligned}
y_{i j} & =(X \beta)_{i j}+Z_{i j} u_{j}^{T}+e_{i j} \\
u_{j} & \sim \mathrm{~N}\left(0, \Omega_{u}\right) \\
e_{i j} & \sim \mathrm{~N}\left(0, \sigma_{e}^{2}\right)
\end{aligned}
$$

Suppose the user wants to make predictions for a user specified set of values of explanatory variables. We have $x^{(c)}$, the set of user specified explanatory variable values for the $c$ th prediction case and $z^{(c)}$, the set of user defined explanatory variables with random coefficients at level 2 (note that the code generalises to any number of hierarchical levels).

For case $c$ we pick

$$
\mathrm{B}_{k} \sim \mathrm{~N}(\hat{\beta}, \operatorname{cov}(\hat{\beta})), \quad k=1, \ldots, K
$$

and form

$$
\hat{y}_{c k}=x_{c} \mathrm{~B}_{k}
$$

Thus for case $c$ we have $K$ predictions from which we derive required statistics eg mean, upper and lower confidence intervals eg

$$
\hat{y}_{c}=\frac{1}{K} \sum_{k=1}^{K} \hat{y}_{c k}
$$

If coverage intervals, from higher level variances, are required we pick $M$ values of $u$ from $\mathrm{N}\left(0, \hat{\Omega}_{u}\right)$. We then construct

$$
\hat{y}_{c m}=x_{c} \hat{\beta}+Z_{c} u_{m}^{T}
$$

from which we can derive coverage statistics for case $c$

## A.1.1 Predictions and confidence intervals for differences

We often want predictions and confidence intervals not for means but for differences. For example given a model:

$$
\begin{aligned}
y_{i j} & =\beta_{0} x_{0}+\beta_{1} x_{1 i j}+\beta_{2} x_{2 i j}+\beta_{3} x_{1 i j} x_{2 i j}+u_{j}+e_{i j} \\
u_{j} & \sim \mathrm{~N}\left(0, \sigma_{u}^{2}\right) \\
e_{i j} & \sim \mathrm{~N}\left(0, \sigma_{e}^{2}\right)
\end{aligned}
$$

we may want the difference curve with confidence intervals for $x_{2 i j}=a$ and $x_{2 i j}=b$, i.e. the curve giving the difference in $y_{i j}$ for two different values of $x_{2 i j}, a$ and $b$, across a range of values of $x_{1 i j}$. In the Normal case this can be derived analytically: the difference curve is given by the formula $\beta_{2} x_{2 \mathrm{~d} i j}+\beta_{3} x_{1 i j} x_{2 \mathrm{~d} i j}$, where $x_{2 \mathrm{~d} i j}=a-b$; however the software uses simulation. For example if the user asks for the difference curve for $x_{2 i j}=$ 0 and $x_{2 i j}=1$ for $x_{1 i j}=\{-3,0,3\}$, by asking for predictions for values $\left\{x_{1 i j}=\{-3,0,3\} ; x_{2 i j}=\{0,1\}\right\}$ and setting differences from $x_{2 i j}=0$, the software follows this procedure:

1. Simulate $\mathrm{B}_{k} \sim \mathrm{~N}(\hat{\beta}, \operatorname{cov}(\hat{\beta})), \quad k=1: K$
2. For each $k$, calculate $x_{c} \mathrm{~B}_{k}$ for each combination $x_{c}$ of values of the other explanatory variables (in this case, just $x_{1 i j}$ ), for both $x_{2 i j}=0$ (call this $\hat{y}_{0 c k}$ ) and $x_{2 i j}=1$ (call this $\hat{y}_{1 c k}$ ). So in this example, for each k calculate

| $c$ | $x_{1 i j}$ | $\hat{\hat{0} c k}$ | $\hat{y} \hat{1 c k}$ |
| :---: | :---: | :---: | :---: |
| 1 | -3 | $\beta_{k 0}-3 \beta_{k 1}$ | $\beta_{k 0}-e \beta_{k 1}+\beta_{k 2}-3 \beta_{k 3}$ |
| 2 | 0 | $\beta_{k 0}$ | $\beta_{k 0}+\beta_{k 2}$ |
| 3 | 3 | $\beta_{k 0}+3 \beta_{k 1}$ | $\beta_{k 0}+3 \beta_{k 1}+\beta_{k 2}+3 \beta_{k 3}$ |

3. Now for each $c$ calculate

$$
d_{c k}=\hat{y}_{0 c k}-\hat{y}_{1 c k}
$$

and then

$$
d_{c}=\frac{1}{K} \sum_{k=1}^{K} d_{c k}
$$

is the difference for prediction case $c$, so the set $\left\{d_{c}\right\}$ is the set of values requested by the user. The software uses the same simulation process to calculate confidence intervals for differences, finding for each $c$ the range of values between which $d_{c k}$ lies for $95 \%$ of the $B_{k}$.

If coverage intervals are required, then in step 1 the software simulates M values of $u$ from $\mathrm{N}\left(0, \hat{\Omega}_{u}\right)$. In step 2 the software calculates $x_{c} \hat{\beta}+Z_{c} u_{m}^{T}$ for
each $c$, for $x_{2 i j}=a\left(\right.$ call this $\left.\hat{y}_{a c m}\right)$ and $x_{2 i j}=b$ (call this $\hat{y}_{b c m}$ ), and then the difference between these, $\hat{d}_{c m}=\hat{y}_{a c m}-\hat{y}_{b c m}$.
$\hat{d}_{c}=\frac{1}{M} \sum_{m=1}^{M} \hat{d}_{c m}$ now gives the required coverage intervals.

## A. 2 Binomial models

As an example let's take a 2 level binomial model

$$
\begin{aligned}
y_{i j} & \sim \operatorname{Binomial}\left(n_{i j}, \pi_{i j}\right) \\
f\left(\pi_{i j}\right) & =(X \beta)_{i j}+Z_{i j} u_{j}^{T} \\
u_{j} & \sim \mathrm{~N}\left(0, \Omega_{u}\right)
\end{aligned}
$$

Now we can get predictions on the raw (probabilities) or transformed (logit) scales and predictions can be for the median or mean

## A.2.1 Median (Cluster specific)

As with Normal models we form

$$
\mathrm{B}_{k} \sim \mathrm{~N}(\hat{\beta}, \operatorname{cov}(\hat{\beta})), \quad k=1: K
$$

Now for each $k$ and each $c$, the median (cluster specific) predicted probability is

$$
\hat{p}_{c k}=\operatorname{antilogit}\left(x_{c} \mathrm{~B}_{k}\right)
$$

and the median predicted probability from the cluster specific predictions is

$$
\hat{p}_{c}=\operatorname{median}\left(\hat{p}_{c k}\right) \text { across } k
$$

Again percentiles are derived from the set $\hat{p}_{c k}$.
Predictions and confidence intervals on the logit scale we derive from

$$
\hat{y}_{c k}=x_{c} \mathrm{~B}_{k}
$$

Required summary statistics for differences are calculated from the following:

$$
\begin{gathered}
\hat{d}_{c k}^{(y)}=x_{c} \mathrm{~B}_{k}-\left(x_{c_{r}} \mathrm{~B}_{k}\right) \\
\hat{d}_{c k}^{(p)}=\operatorname{antilogit}\left(x_{c} \mathrm{~B}_{k}\right)-\operatorname{antilogit}\left(x_{c_{r}} \mathrm{~B}_{k}\right)
\end{gathered}
$$

For coverage intervals from higher level variances, we pick $M$ values of $u$ from $\mathrm{N}\left(0, \Omega_{u}\right)$. We then construct

$$
\hat{p}_{c m}=\operatorname{antilogit}\left(x_{c} \hat{\beta}+z_{c} u_{m}^{T}\right)
$$

and required coverage intervals can be calculated from the $\hat{p}_{c m}$ chain and likewise for logit predictions. Coverage intervals for differences:

$$
\begin{gathered}
\hat{d}_{c m}^{(y)}=x_{c} \hat{\beta}+z_{c} u_{m}^{T}-\left(x_{c_{r}} \hat{\beta}+z_{c_{r}} u_{m}^{T}\right) \\
\hat{d}_{c, m}^{(p)}=\operatorname{antilogit}\left(x_{c} \hat{\beta}+z_{c} u_{m}^{T}\right)-\operatorname{antilogit}\left(x_{c_{r}} \hat{\beta}+z_{c_{r}} u_{m}^{T}\right)
\end{gathered}
$$

## A.2.2 Mean (Population average)

We pick $M$ values of $u$ from $\mathrm{N}\left(0, \Omega_{u}\right)$; these $M$ values are applied to each combination of $x_{c}$ and $B_{k}$. So now

$$
\begin{gathered}
\hat{p}_{c k}=\frac{1}{M} \sum_{m} \operatorname{antilogit}\left(x_{c} \mathrm{~B}_{k}+z_{c} u_{m}^{T}\right) \\
\hat{p}_{c}=\frac{1}{K} \sum_{k}^{\hat{p}_{c k}}
\end{gathered}
$$

Again upper and lower intervals can be calculated from the $\hat{p}_{c}$ chain. On the population average logit scale we work with:

$$
\hat{y}_{c k}=\operatorname{logit}\left(\hat{p}_{c k}\right)
$$

and

$$
\hat{y}_{c}=\frac{1}{K} \sum_{k} \hat{y}_{c k}
$$

Coverage intervals from level 2 variance do not apply in population average models

Differences on the probability scale are given by

$$
\hat{d}_{c k}^{(p)}=\frac{1}{k} \sum_{k}\left(\hat{p}_{c k}-\hat{p}_{c_{r k}}\right)
$$

and on the logit scale are given by

$$
\hat{d}_{c k}^{(y)}=\frac{1}{K} \sum_{k}\left(\operatorname{logit}\left(p_{c k}\right)-\operatorname{logit}\left(p_{c_{r k}}\right)\right)
$$

## A. 3 Unordered Multinomial

With $A$ categories and the $A$ th category as the base

$$
\begin{aligned}
f\left(p_{c}^{(s)}\right) & =\log \left(p_{c}^{(s)} / p_{c}^{(A)}\right) \\
p_{c}^{(s)}=f^{\prime}(\beta, s, c) & =\left\{\begin{array}{cl}
\frac{\exp \left(\left(x_{c} \beta\right)^{(s)}\right)}{1+\sum_{a=1}^{A-1} \exp \left(\left(x_{c} \beta\right)^{(a)}\right)} & a \neq A \\
1-\sum_{a=1}^{A} p_{c}^{(a)} & \text { otherwise }
\end{array}\right.
\end{aligned}
$$

where $s$ and $a$ both index the categories of the multinomial response

$$
\mathrm{B}_{k} \sim \mathrm{~N}(\hat{\beta}, \operatorname{cov}(\hat{\beta})), \quad k=1: K
$$

Now

$$
\hat{p}_{c k}^{(s)}=f^{\prime}\left(\mathrm{B}^{(k)}, s, c\right)
$$

and the median predicted probability from the cluster specific predictions is

$$
\hat{p}_{c}^{(s)}=\frac{1}{K} \sum_{k} \hat{p}_{c k}^{(s)}
$$

The simulation method gives us confidence intervals for all categories including the reference category $A$.

For cluster specific logits:

$$
\hat{y}_{c k}^{(s)}=\left\{\begin{array}{cc}
0 & s=A \\
\left(x_{c} \beta_{k}\right)^{(s)} & \text { otherwise }
\end{array}\right.
$$

and

$$
\hat{y}_{c}^{(s)}=\frac{1}{K} \sum_{k} \hat{y}_{c k}^{(s)}
$$

Required summary statistics for differences are calculated from the following chains:

$$
\begin{gathered}
\hat{d}_{c k}^{(y)(s)}=\left\{\begin{array}{cc}
0 & s=A \\
\left(x_{c} \mathrm{~B}_{k}\right)^{(s)}-\left(x_{r_{c}} \mathrm{~B}_{k}\right)^{(s)} & \text { otherwise }
\end{array}\right. \\
\hat{d}_{c k}^{(p)(s)}=f^{\prime}\left(\mathrm{B}^{(k)}, s, c\right)-f^{\prime}\left(\mathrm{B}^{(k)}, s, c_{r}\right)
\end{gathered}
$$

For coverage intervals from higher level variances, we pick $M$ values of $u$ from $\mathrm{N}\left(0, \Omega_{2}\right)$. We then construct

$$
\hat{p}_{c m}^{(s)}=f^{\prime}(\beta, s, c, m)= \begin{cases}1-\sum_{a=1}^{A-1} p_{c}^{(a)} & s=A \\ \frac{\exp \left(\left(x_{c} \beta\right)^{(s)}+\left(z_{c} u_{m}^{T}\right)^{(s)}\right)}{1+\sum_{a=1}^{A-1} \exp \left(\left(x_{c} \beta\right)^{(a)}+\left(z_{c} u_{m}^{T}\right)^{(a)}\right)} & \text { otherwise }\end{cases}
$$

and required coverage intervals can be calculated from the $\hat{p}_{c m}^{(s)}$ chain and likewise for logit predictions. Coverage intervals for differences:

$$
\begin{gathered}
\hat{d}_{c m}^{(y)(s)}= \begin{cases}0 & s=A \\
\left(\left(x_{c} \hat{\beta}\right)^{(s)}+\left(z_{c} u_{m}^{T}\right)^{(s)}\right)-\left(\left(x_{r_{c}} \hat{\beta}\right)^{(s)}+\left(z_{r_{c}} u_{m}^{T}\right)^{(s)}\right) & \begin{array}{l}
\text { otherwise }
\end{array} \\
\hat{d}_{c m}^{(p)(s)}=f^{\prime}(\hat{\beta}, s, c, m)-f \prime(\hat{\beta}, s, c, m)\end{cases}
\end{gathered}
$$

## A.3.1 Population average

We pick $M$ values of $u$ from $\mathrm{N}\left(0, \Omega_{u}\right)$, these $M$ values are applied to each combination of $c$ and $k$. So now

$$
\begin{gathered}
\hat{p}_{c k}^{(s)}=\frac{1}{M} \sum_{m} f^{\prime}\left(\beta_{k}, s, c, m\right) \\
\hat{p}_{c}^{(s)}=\frac{1}{K} \sum_{k} \hat{p}_{c k}^{(s)}
\end{gathered}
$$

Again upper and lower intervals can be calculated from the $\hat{p}_{c}$ chain. On the population average logit scale we work with:

$$
\hat{y}_{c k}^{(s)}=\log \left(\hat{p}_{c k}^{(s)} / \hat{p}_{c k}^{(A)}\right)
$$

and

$$
\hat{y}_{c}^{(s)}=\frac{1}{K} \sum_{k} \hat{y}_{c k}
$$

Coverage intervals from level 2 variance do not apply in population average models

Differences on the probability scale are given by

$$
\hat{d}_{c k}^{(p)(s)}=\frac{1}{K} \sum_{k}\left(\hat{p}_{c k}^{(s)}-\hat{p}_{c_{r k}}^{(s)}\right)
$$

and on the logit scale are given by

$$
\hat{d}_{c k}^{(y)(s)}=\frac{1}{K} \sum_{k}\left(\log \left(\hat{p}_{c k}^{(s)} / \hat{p}_{c k}^{(A)}\right)-\log \left(\hat{p}_{c r k}^{(s)} / \hat{p}_{c_{r k}}^{(A)}\right)\right)
$$

## A. 4 Ordered Multinomial

$o_{c}^{(s)}$ is the cumulative probability for category $s$ in an ordered set of categories

$$
\begin{aligned}
o_{c}^{(s)} & =\sum_{a=1}^{s} p_{c}^{(a)} \quad s=1: A-1 \\
f\left(o_{c}^{(s)}\right) & =\operatorname{logit}\left(o_{c}^{(s)}\right) \\
p_{c}^{(s)} & =f^{\prime}(\beta, s, c)= \begin{cases}1 & a=A \\
\operatorname{antilogit}\left(x_{c} \beta\right) & \text { otherwise }\end{cases}
\end{aligned}
$$

Since we are working with predictions now on the logit scale, we can proceed with customised predictions as described for the binary, logistic case (as in section A.2)

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## Index

3D Graphics
commands
SCATt, 56, 60
SHOW, 56
SURF, 56
3D scatter plot, 60
SCAtt, 56, 60
ADDT, 14, 15
Around value, 3
Autocorrelated errors, 69
autocorrelation function, 72
SETD, 72
SUBS, 70
Autocorrelation, 69
autocorrelation function, 72
SETD, 72
SUBS, 70
Autocorrelation function, 72
Blue estimates, 86
Categorical variables, 78
Categories
Copy, 80
Copy button, 80
Copy: command, 81
paste, 80
Paste button, 80
Paste: command, 81
Regenerate, 79
Regenerate button, 79
Regenerate:command, 81
View button, 78
Categories button, 78
CCAT, 81
CENT, 15
Centred around means, 3
Centring, 1, 15
around value, 3
by groups defined by, 3
centred around means, 3
grand mean, 3
uncentred, 3
Change range, 18
for categorical explanatory variables, 25
nested means tab, 24
percentiles tab, 23
range tab, 19
values tab, 23
Cluster specific predictions, 36
Column
Name button, 76
Column descriptions, 76
DESC, 80
Description button, 76
COMB, 81
Combining categorical columns, 81
Command line, 89
Commands, 29, 40, 74, 80, 88
ADDT, 14
and string variables, 88
CCAT, 81
CENT, 15
COMB, 81
COPY, 80
CTOL, 7
DESC, 80
DOFF, 88
ESTM, 87
EXPA, 87
for building customised predictions for Normal response models, 29
for coverages for predictions, 30, 31, 40
for plotting customised predictions, 31
for predicted differences, 30, 40
for predictions for binomial response models, 40
for predictions for continuous response models, 29
for predictions for discrete response models, 40
for predictions for multinomial response models, 40
for predictions for multivariate response models, 30, 40
for predictions for Normal response models, 29
for specifying terms in models, 14
ADDT, 14
CENT, 15
SWAP, 14
for storing and comparing model results, 65
INDE, 87
LFUN, 87
LINE, 87
MCOM, 65
MERA, 65
MPRI, 65
MSTO, 65
MVIE, 71
MWIP, 65
NEXT, 85
NMST, 88
NMVA, 87
NOTA, 87
PASTe, 80
PAUSe, 86
PCAT, 81
PGDE, 29
PGRI, 29
PLTP, 31
predictions for multivariate response models, 31
PREG, 30, 40
for discrete response models, 40
for normal response models, 30
RCAT, 81
RDISt, 87
RMTW, 74
RSAS, 74
RSPS, 74
RSTA, 74
SCATt, 56, 60
SETD, 72
SHOW, 56
SJOI, 88
SMTW, 74
SSAS, 74
SSPS, 74
SSTA, 74
STARt, 85
SUBS, 70
SURF, 56
SWAP, 14

UCOM, 82
UNIQ, 82
UNVE, 83
ZRET, 75
ZSAV, 75
Commands for storing and comparing model results, 65
MCOM, 65
MERA, 65
MPRI, 65
MSTO, 65
MWIP, 65
Compressed worksheets, 75
Confidence intervals for customised predictions, 22
Controlling the equations window from a macro, 87
COPY, 80
Copy
categories, 80
categories: command, 81
command, 80
Data, 77
Data: command, 80
Copy button
Categories, 80
Data, 77
Copying stored model results, 63
Coverages for predictions, 30, 31, 40
CTOL, 7, 14
Customised prediction plot window, $20,27,28,38,43$
and customised graph window, 28
for binomial response models, 38
for multinomial response models, 43
Customised predictions, 16
algorithms, 90
binomial response models, 92
continuous response models, 90
coverage intervals for binomial
response models, 92
coverage intervals for multinomial response models, 94
coverage intervals for Normal response models, 91
differences for binomial response models, 92, 93
differences for multinomial response models, 94, 95
differences for Normal response models, 91
mean (population average) predictions for binomial response models, 93
mean (population average) predictions for multinomial response models, 95
median (cluster specific) predictions for binomial response models, 92
median (cluster specific) predictions for multinomial response models, 94
Normal response models, 90
ordered multinomial response models, 95
unordered multinomial response models, 93
binomial response models, 32
algorithms, 92
cluster specific and population average, 36
commands, 40
differences on logit scale, 39
differences on probability scale, 38
log odds ratio, 39
on logit or probability scale, 34 , 41
on probability scale, 38
predicting mean and median, 32 , 36
predicting mean or median, 34 , 40
prediction distribution, 34
commands, 29, 40
for binomial response models, 40
for continuous response models, 29
for coverages, 30, 31, 40
for discrete response models, 40
for multinomial response models, 40
for multivariate response mod-
els, 30, 31, 40
for Normal response models, 29
for plotting predictions, 31
for predicted differences, 30, 40
PGDE, 29
PGRI, 29
PLTP, 31
PREG, 30, 40
confidence intervals, 22
continuous response models, 16
algorithms, 90
coverage intervals
algorithms, 91, 92, 94
coverages, 30, 31, 40
commands, 30, 31, 40
Customised prediction plot window, 20
Customised predictions window, 16
differences, 21
algorithms, 91-95
commands, 30, 40
discrete response models
commands, 40
mean (population average) predictions
algorithms, 93, 95
mean or median
derived from simulation, 35
median (cluster specific) predictions
algorithms, 92, 94
multinomial response models, 41
algorithms (ordered multinomial), 95
algorithms (unordered multinomial), 93
commands, 40
differences for ordered multinomial models, 51
differences on logit scale, 48
differences on probability scale, 46
log odds ratio, 48
on probability scale, 43, 51
ordered, 49
predicting median, 43, 51
unordered, 41
multivariate response models, 53 commands, 30, 31, 40
Normal response models, 16 algorithms, 90
out of date, 26
plot grid, 20
Poisson response models, 51
predicting mean and median, 52
selecting the response for a multivariate model, 54
setting values as a range, 19
simulation, 35
Customised predictions window, 16
$95 \%$ confidence interval check box, 22
algorithms, 90
binomial response models, 92
continuous response models, 90
coverage intervals for binomial response models, 92
coverage intervals for multinomial response models, 94
coverage intervals for Normal response models, 91
differences for binomial response models, 92, 93
differences for multinomial response models, 94, 95
differences for Normal response models, 91
mean (population average) predictions for binomial response models, 93
mean (population average) predictions for multinomial response models, 95
median (cluster specific) predictions for binomial response models, 92
median (cluster specific) predictions for multinomial response models, 94
Normal response models, 90
ordered multinomial response models, 95
unordered multinomial response models, 93
binomial response models, 32
algorithms, 92
cluster specific and population average, 36
differences on logit scale, 39
differences on probability scale, 38
log odds ratio, 39
on logit or probability scale, 34 , 41
on probability scale, 38
predicting mean and median, 32 , 36
predicting mean or median, 34, 40
prediction distribution, 34
change range, 18
clear button, 26
confidence intervals, 22
continuous response models, 16
algorithms, 90
coverage intervals
algorithms, 91, 92, 94
Customised prediction plot window, 38, 43
customised predictions plot window, 27, 28
differences, 21
algorithms, 91-95
Differences checkbox, 21, 29
draws from $\operatorname{cov}($ Beta $), \#, 36$
fill grid, 19
mean (population average) predictions
algorithms, 93, 95
mean or median
derived from simulation, 35
mean.high.pred, 20
mean.low.pred, 20
mean.pred, 20
median (cluster specific) predictions
algorithms, 92, 94
multinomial response models, 41
algorithms (ordered multinomial), 95
algorithms (unordered multinomial), 93
differences for ordered multino-
mial models, 51
differences on logit scale, 48
differences on probability scale, 46
log odds ratio, 48
on probability scale, 43,51
ordered, 49
predicting median, 43, 51
unordered, 41
multivariate response models, 53
nested draws from $\operatorname{cov}(\mathrm{u}), \#, 36$
Normal response models, 16
algorithms, 90
out of date, 26
Poisson response models, 51
predicting mean and median, 52
predict, 19
predicted cases, \#, 36
prediction grid, 20
predictions tab, 19
selecting the response for a mul-
tivariate model, 54
setting values as a range, 19
simulation, 35
simulations, \#, 36
values to include window, 18,19
Data
Copy button, 77
Delete button, 77
Paste button, 77
View button, 77
Delete button, 77
Denominator
command for specifying, 88
DESC, 80
Description button, 76
Design matrix, 72
Differences (predictions), 21
DOFF, 88
Equations window
controlling from a macro, 87
Store button, 62
Estimate tables, 62
commands, 65
copying results table, 63
delete models, 64, 65
view selected models, 65

Estimates in blue, 86
ESTM, 87
Executing models from macros, 85
blue estimates, 86
controlling the equations window from a macro, 87
estimates in blue, 86
EXPA, 87
Fill grid, 19
Finding unique codes, 82
Grand mean, 3
Graph trellis, 32, 45
Groups defined by, 3
INDE, 87
Interaction term, 14
Interactions, 1, 14
and polynomials, 3, 14
Invoking MLwiN from a command line, 89

LFUN, 87
LINE, 87
Link function
command for specifying, 87
Longitudinal data, 9, 69
autocorrelation function, 72
SETD, 72
SUBS, 70
Macro programming, 85
blue estimates, 86
controlling the equations window from a macro, 87
DOFF, 88
estimates in blue, 86
ESTM, 87
executing models from macros, 85
EXPA, 87
INDE, 87
LFUN, 87
LINE, 87
NMST, 88
NMVA, 87
NOTA, 87
RDISt, 87
running models from macros, 85
SJOI, 88

MCOM, 65
mean.high.pred, 20
mean.low.pred, 20
mean.pred, 20
MERA, 65
Minitab worksheets, 74
Model comparison tables, 62
commands, 65
copy button, 63
copying results table, 63
delete models, 64,65
view selected models, 65
Modify term, 9
MPRI, 65
MQL
command for specifying, 87
MSTO, 65
MVIE, 71
MWIP, 65
Name button
Names window, 76
Names window
categorical variables, 78
Categories button, 78
Categories: Copy button, 80
Categories: Paste button, 80
Categories: Regenerate button, 79
Categories: View button, 78
column descriptions, 76
Copy button, 80
Data: Copy button, 77
Data: Delete button, 77
Data: Paste button, 77
Data: View button, 77
Description button, 76
Name button, 76
Paste button, 80
Regenerate button, 79
Toggle categorical button, 78
viewing data, 77
Nested means, 5, 24
Nested means tab, 24
NEXT, 85
NMST, 88
NMVA, 87
Nonlinear estimation command for specifying, 87

NOTA, 87
Numeric grids, 82
Offset
command for specifying, 88
Opening worksheets, 74, 75
commands, 74, 75
Minitab worksheets, 74
commands, 74
RMTW, 74
RSPS, 74
RSTA, 74
SAS worksheets
commands, 74
SPSS worksheets, 74
commands, 74
Stata worksheets, 74
commands, 74
zipped worksheets, 75
ZRET, 75
Orthogonal polynomial, 4, 9, 14
Out of sample predictions, 16
algorithms, 90
binomial response models, 92
continuous response models, 90
coverage intervals for binomial response models, 92
coverage intervals for multinomial response models, 94
coverage intervals for Normal response models, 91
differences for binomial response models, 92, 93
differences for multinomial response models, 94, 95
differences for Normal response models, 91
mean (population average) predictions for binomial response models, 93
mean (population average) predictions for multinomial response models, 95
median (cluster specific) predictions for binomial response models, 92
median (cluster specific) predictions for multinomial response
models, 94
Normal response models, 90
ordered multinomial response models, 95
unordered multinomial response models, 93
binomial response models, 32
algorithms, 92
cluster specific and population average, 36
commands, 40
differences on logit scale, 39
differences on probability scale, 38
log odds ratio, 39
on logit or probability scale, 34, 41
on probability scale, 38
predicting mean and median, 32 , 36
predicting mean or median, 34 , 40
prediction distribution, 34
commands, 29, 40
for binomial response models, 40
for continuous response models, 29
for coverages, 30, 31, 40
for discrete response models, 40
for multinomial response models, 40
for multivariate response models, 30, 31, 40
for Normal response models, 29
for plotting predictions, 31
for predicted differences, 30, 40
PGDE, 29
PGRI, 29
PLTP, 31
PREG, 30, 40
confidence intervals, 22
continuous response models, 16
algorithms, 90
coverage intervals
algorithms, 91, 92, 94
coverages, 30, 31, 40
commands, 30, 31, 40

Customised predictions window, 16
differences, 21
algorithms, 91-95
commands, 30, 40
discrete response models
commands, 40
mean (population average) predictions
algorithms, 93, 95
mean or median
derived from simulation, 35
median (cluster specific) predictions
algorithms, 92, 94
multinomial response models, 41
algorithms (ordered multinomial), 95
algorithms (unordered multinomial), 93
commands, 40
differences for ordered multinomial models, 51
differences on logit scale, 48
differences on probability scale, 46
log odds ratio, 48
on probability scale, 43,51
ordered, 49
predicting median, 43, 51
unordered, 41
multivariate response models, 53
commands, 30, 31, 40
Normal response models, 16
algorithms, 90
out of date, 26
Poisson response models, 51
predicting mean and median, 52
selecting the response for a multivariate model, 54
setting values as a range, 19
simulation, 35
PASTe, 80
Paste
categories, 80
categories: command, 81
command, 80

Data, 77
Data: command, 80
Paste button
Categories, 80
Data, 77
PAUSe, 86
PCAT, 81
Percentiles tab, 23
PGDE, 29
PGRI, 29
Plot grid, 20
PLTP, 31
Polynomial, 1, 3, 14
Polynomials
and interactions, 3,14
Population average predictions, 36
PQL
command for specifying, 87
Predict, 19
Prediction
out of date, 26
Prediction distribution, 34
Prediction grid, 20
Predictions, 16
algorithms, 90
binomial response models, 92
continuous response models, 90
coverage intervals for binomial response models, 92
coverage intervals for multinomial response models, 94
coverage intervals for Normal response models, 91
differences for binomial response models, 92, 93
differences for multinomial response models, 94, 95
differences for Normal response models, 91
mean (population average) predictions for binomial response models, 93
mean (population average) predictions for multinomial response models, 95
median (cluster specific) predictions for binomial response models, 92
median (cluster specific) predictions for multinomial response models, 94
Normal response models, 90
ordered multinomial response models, 95
unordered multinomial response models, 93
binomial response models, 32
algorithms, 92
cluster specific and population average, 36
commands, 40
differences on logit scale, 39
differences on probability scale, 38
log odds ratio, 39
on logit or probability scale, 34 , 41
on probability scale, 38
predicting mean and median, 32, 36
predicting mean or median, 34, 40
prediction distribution, 34
commands, 29, 40
for binomial response models, 40
for continuous response models, 29
for coverages, 30, 31, 40
for discrete response models, 40
for multinomial response models, 40
for multivariate response models, 30, 31, 40
for Normal response models, 29
for plotting predictions, 31
for predicted differences, 30, 40
PGDE, 29
PGRI, 29
PLTP, 31
PREG, 30, 40
confidence intervals, 22
continuous response models, 16
algorithms, 90
coverage intervals
algorithms, 91, 92, 94
coverages, 30, 31, 40
commands, 30, 31, 40
Customised predictions window, 16
differences, 21
algorithms, 91-95
commands, 30, 40
discrete response models
commands, 40
mean (population average) predictions
algorithms, 93, 95
mean or median
derived from simulation, 35
median (cluster specific) predictions
algorithms, 92, 94
multinomial response models, 41
algorithms (ordered multinomial), 95
algorithms (unordered multinomial), 93
commands, 40
differences for ordered multinomial models, 51
differences on logit scale, 48
differences on probability scale, 46
log odds ratio, 48
on probability scale, 43, 51
ordered, 49
predicting median, 43, 51
unordered, 41
multivariate response models, 53
commands, 30, 31, 40
Normal response models, 16
algorithms, 90
Poisson response models, 51
predicting mean and median, 52
selecting the response for a multivariate model, 54
setting values as a range, 19
simulation, 35
Predictions tab, 19
PREG, 30
for discrete response models, 40
for normal response models, 30

Range tab, 19
RCAT, 81
RDISt, 87
Recode, 6
by range, 6
Recoding, 1, 83
Reference category, 1, 14
Regenerate button, 79
Regenerate categories, 79
command, 81
Repeated measures, 9, 69
autocorrelation function, 72
SETD, 72
SUBS, 70
Results table, 62
commands, 65
copy button, 63
copying results table, 63
delete models, 64, 65
view selected models, 65
Retrieving worksheets, 74, 75
commands, 74, 75
Minitab worksheets, 74
commands, 74
RMTW, 74
RSAS, 74
RSPS, 74
RSTA, 74
SAS worksheets commands, 74
SPSS worksheets, 74
commands, 74
Stata worksheets, 74
commands, 74
zipped worksheets, 75
ZRET, 75
RMTW, 74
RSAS, 74
RSPS, 74
RSTA, 74
Running models from macros, 85
blue estimates, 86
controlling the equations window
from a macro, 87
estimates in blue, 86
Saving worksheets, 74, 75
as Minitab worksheets, 74
commands, 74
as SAS worksheets
commands, 74
as SPSS worksheets, 74
commands, 74
as Stata worksheets, 74
commands, 74
commands, 74,75
SMTW, 74
SSAS, 74
SSPS, 74
SSTA, 74
zipped worksheets, 75
ZSAV, 75
SCATt, 56, 60
Scatter plot, 60
SCAtt, 56, 60
SETD, 72
Setting values as a range, 19
SHOW, 56
SJOI, 88
SMTW, 74
Specify term window, 2
around value, 3
by groups defined by, 3
grand mean, 3
polynomial, 3
uncentred, 3
SPSS worksheets, 74
SSAS, 74
SSPS, 74
SSTA, 74
STARt, 85
Stata worksheets, 74
Store button, 62
Storing estimates, 62
commands, 65
copying results table, 63
deleting stored results, 64, 65
viewing selected model estimates, 65
Storing results, 62
commands, 65
copying results table, 63
deleting stored results, 64,65
viewing selected model results, 65
String variables, 88
SUBS, 70

SURF, 56
Surface plotting, 57
SURF, 56
SWAP, 14
Time series, 69
autocorrelation function, 72
SETD, 72
SUBS, 70
Time series macros, 69
Toggle categorical button, 78
Tolerance, 7, 13
UCOM, 82
Uncentred, 3
UNIQ, 82
Unsplit records, 84
Unsplitting records, 83
UNVE, 83
Unvectorising data, 83
Values tab, 23
Values to include window, 18, 19
for categorical explanatory variables, 25
nested means tab, 24
percentiles tab, 23
range tab, 19
values tab, 23
View button
Categories, 78
Data, 77
Viewing data, 77
Window tabs, 76
Worksheet formats, 74, 75
commands, 74
zipped worksheets, 75
Zipped worksheets, 75
ZRET, 75
ZSAV, 75

