A Guide to Sample Size Calculations for Random Effect Models via Simulation and the MLPowSim Software Package

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1 Introduction

1.1 Scope of document

This manual has been written to support the development of the software package MLPowSim which has been written by the authors as part of the work in ESRC grant R000231190 entitled 'Sample Size, Identifiability and MCMC Efficiency in Complex Random Effect Models.'

The software package MLPowSim creates R command scripts and MLwiN macro files which, when executed in those respective packages, employ their simulation facilities and random effect estimation engines to perform sample size calculations for user-defined random effect models. MLPowSim has a number of features novel to this software: for example, it can create scripts to perform sample size calculations for models which have more than two levels of nesting, for models with crossed random effects, for unbalanced data, and for non-normal responses.

This manual has been written to take the reader from the simple question of 'what is a sample size calculation and why do I need to perform one?' right up to 'how do I perform a sample size calculation for a logistic regression with crossed random effects?' We will aim to cover some of the theory behind commonly-used sample size calculations, provide instructions on how to use the MLPowSim package and the code it creates in both the R and MLwiN packages, and also examples of its use in practice.

In this introductory chapter we will go through this whole process using a simple example of a single-level normal response model designed to guide the user through both the basic theory, and how to apply MLPowSim's output in the two software packages R and MLwiN. We will then consider three different response types in the next three chapters: continuous, binary and count. Each of these chapters will have a similar structure. We will begin by looking at the theory behind sample size calculations for models without random effects, and then look at how we can use MLPowSim to give similar results. We will next move on to consider sample size calculations for simple random effect models, and then increase the complexity as we proceed, in particular for the continuous response models.

Please note that as this is the first version of MLPowSim to be produced, it does not have a particularly user-friendly interface, and also supports a limited set of models. It is hoped that in the future, with further funding, both these limitations can be addressed. However, in Chapter 5 we suggest ways in which the more expert user can extend models and give some more details on how the code produced for MLwiN and R actually works.

Good luck with your sample size calculating!

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March 2009

1.2 Sample size / Power Calculations

1.2.1 What is a sample size calculation?

As the name suggests, in simplest terms a sample size calculation is a calculation whose result is an estimate of the size of sample that is required to test a hypothesis. Here we need to quantify more clearly what we mean by 'required' and for this we need to describe some basic statistical hypothesis-testing terminology.

1.2.2 What is a hypothesis test?

When an applied researcher (possibly a social scientist) decides to do research in a particular area, they usually have some research question/interest in mind. For example, a researcher in education may be primarily interested in what factors influence students' attainment at the end of schooling. This general research question may be broken down into several more specific hypotheses: for example, 'boys perform worse than average when we consider total attainment at age 16,' or a similar hypothesis that 'girls perform better than boys.'

1.2.3 How would such hypotheses be tested?

For the first hypothesis we would need to collect a measure of total attainment at age 16 for a random sample of boys, and we would also need a notional overall average score for pupils. Then we would compare the boys' sample mean with this overall average to give a difference between the two and use the sample size and variability in the boys' scores to assess whether the difference is more than might be expected by chance. Clearly, an observed difference based on a sample average derived from just two boys might simply be due to the chosen boys (i.e. we may have got a very different average had we sampled two different boys) whereas the same observed difference based on a sample average of 2,000 boys would be much clearer evidence of a real difference. Similarly, if we observe a sample mean that is 10 points below the overall average, and the boys' scores are not very variable (for example, only one boy scores above the overall average), then we would have more evidence of a significant difference than if the boys' scores exhibit large variability and a third of their scores are in fact above the overall average.

For the second hypothesis ('girls perform better than boys') we could first collect a measure of total attainment at age 16 for a random sample of both boys and girls, and compare the sample means of the genders. Then, by using their sample sizes and variabilities, we could assess whether any difference in mean is more than might be expected by chance.

For the purposes of brevity we will focus on the first hypothesis in more detail and then simply explain additional features for the second hypothesis. Therefore our initial hypothesis of interest is 'boys perform worse than average'; this is known as the alternative hypothesis (H_1), which we will compare with the null hypothesis (H_0, so-

called because it nullifies the research question we are hoping to prove) which in this case would be 'boys perform no different from the average'. Let us assume that we have transformed the data so that the overall average is in fact 0.

We then wish to test the hypotheses

H_0: $\mu_B=0$ versus H_1: $\mu_B<0$

where μ_B is the underlying mean score for the whole population of boys (the population mean).

We now need a rule/criterion for deciding between these two hypotheses. In this case, a natural rule would be to consider the value of the sample mean $\bar{x}$ and then reject the null hypothesis if $\bar{x} \le c$ where c is some chosen constant. If $\bar{x} > c$ then we cannot reject H_0 as we do not have enough evidence to say that boys definitely perform worse than average. We now need to find a way to choose the threshold c at which our decision will change. The choice of c is a balance between making two types of error. The larger we make c the more often we will reject the null hypothesis both if it is false but also if it is true. Conversely the smaller we make c the more often we fail to reject the null hypothesis both if it is true but also if it false.

The error of rejecting a null hypothesis when it is true is known as a Type I error, and the probability of making a Type I error is generally known as the *significance level,* or *size,* of the test and denoted α. The error of failing to reject a null hypothesis when it is false is known as a Type II error, and the probability of making a Type II error is denoted β. The quantity 1- β, which represents the probability of rejecting the null hypothesis when it is false, is known as the *power* of a test.

Clearly, we only have one quantity, c, which we can adjust for a particular sample, and so we cannot control the values of both α and β. Generally we choose a value of c that enables us to get a particular value for α, and this is done as follows. If we can assume a particular distributional form for the sample mean (or a function of it) under H_0 then we can use properties of the distribution to find the probability of rejecting H_0 for various values of c. In our example, we will assume the attainment score for each individual boy (x_i) comes from an underlying Normal distribution with mean μ_B and unknown variance σ^2_B. If we knew the variance then we could assume that the sample mean also came from a Normal distribution with mean μ_B and variance σ^2_B/n where n is our sample size. From this we could also see that

$\frac{\bar{x}-\mu_B}{\sigma_B/\sqrt{n}}$ follows a standard normal distribution from which we can conclude that if

we wish $P(\bar{x} \le c) = \alpha$ then $P(\bar{x} \le c) = P\left[\frac{\bar{x}-\mu_B}{\sigma_B/\sqrt{n}} \le \frac{c-\mu_B}{\sigma_B/\sqrt{n}}\right] = \alpha$

implies $\frac{c-\mu_B}{\sigma_B/\sqrt{n}} = Z_\alpha$ where Z_α is the α-th quantile of the Normal distribution.

Rearranging gives $c = \mu_B + Z_\alpha \sigma_B/\sqrt{n}$.

In the usual case when σ^2_B is unknown we substitute the sample variance s^2_B but as this is an estimate for σ^2_B we now also need to take its distribution into account. This results in using a t_{n-1} distribution in place of a Normal distribution and we have $c = \mu_B + t_{n-1,\alpha} s_B / \sqrt{n}$ as our formula for the threshold. Note that as the sample size *n* increases, the *t* distribution approaches the Normal distribution, and so often we will simply use the Normal distribution quantiles as an approximation to the t distribution quantiles.

1.2.4 What is Power?

As previously defined, power is the probability of rejecting the null hypothesis when it is false. In the case of our example, we have a null hypothesis H_0: $\mu_B=0$; this is known as a simple hypothesis since there is only one possible value for μ_B if the hypothesis is true. The alternative hypothesis H_1: $\mu_B<0$ has an infinite number of possible values and is known as a composite hypothesis. The power of the test will therefore depend on the true value of μ_B. Clearly the further μ_B is from 0, the greater the likelihood that a chosen sample will result in rejecting H_0, and so the power is consequently a function of μ_B.

We can evaluate the power of the test for a particular value of μ_B: for example, if we believe that the true value of $\mu_B=-1$ then we could estimate the power of the test given this value. This would give us how often we would reject the null hypothesis if the specific alternative $\mu_B=-1$ was actually true. We have Power = P ($\bar{x} \le c \mid \mu_B=-1$) where *c* is calculated under the null hypothesis, i.e.:

$$\text{Power} = t^{-1}_{n-1}\left(\frac{c+1}{s_B/\sqrt{n}}\right) = t^{-1}_{n-1}\left(\frac{(t_{n-1,\alpha/2} s_B/\sqrt{n})+1}{s_B/\sqrt{n}}\right)$$

So, for example, if n = 100 and $s_B=1$ and $\alpha=0.05$(2-sided)[1] we have $t_{99,\,0.05/2} = -1.98$ approximately and

Power = $t^{-1}_{99}((-0.198 + 1) / 0.1) = t^{-1}_{99}(8.02)$ = huge! (approximately 1).

So here 100 boys is more than ample to give a large power.
However, if we instead believed the true value of μ_B was only -0.10 then we would have

Power = $t^{-1}_{99}((-0.198 + 0.10) / 0.1) = t^{-1}_{99}(-0.98) = 0.165$.

[1] NB Whilst many of the alternative hypotheses we use as examples in this manual will be directional (e.g. H_1: $\mu_B<0$ rather than H_1: $\mu_B\neq0$), we generally use 2-sided tests of significance, rather than 1-sided. This is simply because, in practice, many investigators are likely to adopt 2-sided tests, even if *a priori* they formulate directional alternative hypotheses. Of course, there may be circumstances in which investigators decide to employ 1-sided tests instead: for example, if it simply isn't scientifically feasible for the alternative hypothesis to be in a direction (e.g. H_1: $\mu_B>0$) other than that proposed *a priori* (in this case H_1: $\mu_B<0$), or, if it were, if that outcome were of no interest to the research community.

Here the power is rather low and we would need to have a larger sample size to give sufficient power. If we want to find a sample size that gives a power of 0.8, we would need to solve for *n*; this is harder in the case of the *t* distribution compared to the Normal, since the distribution function of *t* changes with *n*. However, as *n* gets large the *t* distribution gets closer and closer to a Normal distribution; if we then assume a Normal distribution in this case, we have the slightly simpler formulation:

$$\text{Power} = \Phi\left(\frac{c+0.1}{s_B/\sqrt{n}}\right) = \Phi\left(\frac{(Z_{\alpha/2}s_B/\sqrt{n})+0.1}{s_B/\sqrt{n}}\right)$$

where $\Phi=Z^{-1}$ is the inverse of the standard normal CDF. In the case where $s_B=1$ and $Z_{\alpha/2} = -1.96$ we have:

$$\text{Power} = \Phi\left[\frac{(-1.96/\sqrt{n})+0.1}{1/\sqrt{n}}\right] \text{ which means for a Power of at least 0.8 we have}$$

$$\Phi\left[\frac{(-1.96/\sqrt{n})+0.1}{1/\sqrt{n}}\right] \geq 0.8 \rightarrow \frac{(-1.96/\sqrt{n})+0.1}{1/\sqrt{n}} \geq 0.842$$

Solving for *n* we get $n \geq (10\times(0.842+1.96))^2 = 785.1$ thus we would need a sample size of at least 786. Here 0.842 is the value in the tail of the Normal distribution associated with a Power of 0.8 (above which 20% of the distribution lies).

1.2.5 Why is Power important?

When we set out to answer a research question we are hoping both that the null hypothesis is false and that we will be able to reject it based on our data. If, given our believed true estimate, we have a hypothesis test with low power, then this means that even if our alternative hypothesis is true, we will often not be able to reject the null hypothesis. In other words, we can spend money collecting data in an effort to disprove a null hypothesis, and fail to do so.

On closer inspection the power formula is a function of the size of the data sample that we have collected. This means that we can increase our power by collecting a larger sample size. Hence a power calculation is often turned on its head and described as a sample size calculation. Here we set a desired power which we fix, and then we solve for *n* the sample size instead.

1.2.6 What Power should we aim for?

In the literature the desired power is often set at 0.8 (or 0.9): i.e. in 80% (or 90%) of cases we will (subject to the accuracy of our true estimates) reject the null hypothesis. Of course, in big studies there will be many hypotheses and many parameters that we might like to test, and there is a unique power calculation for each hypothesis. Sample size calculations should be considered as rough guides only, as there is always uncertainty in the true estimates, and there are often practical limitations to consider as well, such as maximum feasible sample sizes and the costs involved.

1.2.7 What are effect sizes?

In sample size calculations the term *effect size* is often used to refer to the magnitude of the difference in value expected for the parameter being tested, between the alternative and null hypotheses. For example, in the above calculations we initially believed that the true value of μ_B=-1 which, as the null hypothesis would correspond to μ_B=0, would give an effect size of 1 (note: it is common practice to assume an effect size is positive). We will use the term *effect size* both in the next section, and when we later use the formula to give theoretical results for comparison. However, in the simulation-based approach, we often use the signed equivalent of the effect size and so we drop this term and use the terms *parameter estimate* or *fixed effect estimate*.

1.2.8 How are power/sample size calculations done more generally?

Basically, for many power/sample size calculations there are four related quantities: size of the test, power of the test, effect size, and standard error of the effect size (which is a function of the sample size). The following formula links these four quantities when a normal distributional assumption for the variable associated with the effect size holds, and can be used approximately in other situations:

$$\frac{\gamma}{SE(\gamma)} \approx z_{1-\alpha/2} + z_{1-\beta}$$

Here α is the size of the test, 1-β is the power of the test, γ is the effect size, and we assume that the Null hypothesis is that the underlying variable has value 0 (another way to think of this is that the effect size represents the increase in the parameter value).

Note that the difficulty here is in determining the standard error formula (SE(γ)). For specific sample sizes/designs; this can be done using theory employed by the package PINT (e.g. see Section 2.3.2). In MLPowSim we adopt a different approach which is more general, in that it can be implemented for virtually any parameter, in any model; however, it can be computationally very expensive!

1.3 Introduction to MLPowSim

For standard cases and single-level models we can analytically do an exact (or approximate) calculation for the power, and we will discuss some of the formulae for such cases in later sections. As a motivation for a different simulation-based approach, let us consider what a power calculation actually means. In some sense, the *power* can be thought of as how often we will reject a null hypothesis given data that comes from a specific alternative. In reality we will collect one set of data and we will either be able to reject the null hypothesis, or not. However *power*, as a concept coming from frequentist statistics, has a frequentist feel to it in that if we were to repeat our data-collecting many times we could get a long term average of how often we can reject the null hypothesis: this would correspond to our *power*.

In reality, we do not go out on the street collecting data many times, but instead use the computer to do the hard work for us, via simulation. If we were able to generate data that comes from the specific alternative hypothesis (many times), then we could count the percentage of rejected null hypotheses, and this should estimate the required power. The more sets of data (simulations) we use, the more accurate the estimate will be. This approach is particularly attractive as it replicates the procedure that we will perform on the actual data we collect, and so it will take account of the estimation method we use and the test we perform.

This book will go through many examples of using MLPowSim (along with MLwiN and R) for different scenarios, but here we will replicate the simple analysis that we described earlier, in which we compared boys' attainment to average attainment; this boils down to a Z or t test.

1.3.1 A note on retrospective and prospective power calculations

At this point we need to briefly discuss retrospective power calculations. The term refers to power calculations based on the currently collected data to show how much power it specifically has. These calculations are very much frowned upon, and really give little more information than can be obtained from P-values. In the remainder of the manual we will generally use existing datasets to derive estimates of effect sizes, predictor means, variabilities, and so on. Here, the idea is NOT to perform retrospective power calculations, but to use these datasets to obtain (population) estimates for what we might expect in a later sample size collection exercise. Using large existing datasets has the advantage that the parameter estimates are realistic, and this exercise likely mirrors what one might do in reality (although one might round the estimates somewhat, compared to the following example, in which we have used precise estimates from the models fitted to the existing datasets).

1.3.2 Running MLPowSim for a simple example

MLPowSim itself is an executable text-based package written in C which should be used in conjunction with either the MLwiN package or the R package. It can be thought of as a 'program-generating' program, as it creates macros or functions to be run using those respective packages.

In the case of our example, the research question is whether boys do worse than average in terms of attainment at age 16. For those of you familiar with the MLwiN package and its User's Guide (Rasbash et al, 2004), the tutorial example dataset is our motivation here. In the case of that dataset, exam data were collected on 4,059 pupils at age 16, and the total exam score at age 16 was transformed into a normalised response (having mean 0 and variance 1). If we consider only the boys' subset of the data, and this normalised response, we have a mean of -0.140 and a variance of 1.051. Clearly, given the 1,623 boys in this subset, we have a significant negative effect for this specific dataset. Let us now assume that this set of pupils represents our population of boys, and we wish to see how much power different sample sizes produce.

We could consider sub-sampling from the data (see Mok (1995) and Afshartous (1995) for this approach with multilevel examples) if this genuinely is our population, but here let us assume that all we believe is that the mean of the underlying population of boys is -0.140 and the variance is 1.051.

Now we will fire up the MLPowSim executable and answer the questions it asks. In the case of our example, appropriate questions and responses in MLPowSim are given below:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **1**
Please input the random number seed: **1**
Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **0**

Sample size set up

Please input the smallest sample size : **20**
Please input the largest sample size : **600**
Please input the step size: **20**

Parameter estimates

Please input estimate of beta_0: **-0.140**

Please input estimate of sigma^2_e: **1.051**

Files to perform power analysis for the 1 level model with the following sample criterion have been created
Sample size starts at 20 and finishes at 600 with the step size 20
1000 simulations for each sample size combination will be performed

Press any key to continue…

If we analyse these inputs in order, we begin by stating that we are going to use MLwiN for a 1-level (single-level) model. We then input a random number seed[2], and state that we are going to use a significance level (size of test) of 0.025. Note that MLPowSim asks for the significance level for a 1-sided test; hence, when we are considering a 2-sided test, we divide our significance level by 2 (i.e. 0.05 / 2 = 0.025). For a 1-sided test, we would therefore input a significance level of 0.05. We then state that we will use 1000 simulated datasets for each sample size, from which we will calculate our power estimates.

We are next asked what response type and estimation methods we will use. For our example we have a normal response, and we will use the IGLS estimation method. Note that as this method gives maximum likelihood (ML) estimates, it is preferred to RIGLS for testing the significance of estimates, since hypothesis-testing is based on ML theory.

We then need to set up the model structure; in our case this is simply an intercept (common mean) with no predictor variables. Next, we are asked to give limits to the sample sizes to be simulated, and a step size. So, for our example we will start with samples of size 20 and move up in increments of 20 through 40,60,… etc., up to 600.

We then give an effect size estimate for the intercept (beta_0) and an estimate for the underlying variance (sigma^2_e). When we have filled in all these questions, the program will exit having generated several macro files to be used by MLwiN.

1.4 Introduction to MLwiN and MLPowSim

The MLPowSim program will create several macro files which we will now use in the MLwiN software package. The files generated for a 1-level model are *simu.txt*, *setup.txt*, *analyse.txt* and *graphs.txt*. In this introductory section we will simply give instructions on how to run the macros and view the power estimates. In later sections we will give further details on what the macro commands are actually doing.

The first step to running the macros is to start up MLwiN. As the macro files call each other (i.e. refer to each other whilst they are running), after starting up MLwiN we need to let it know in which directory these files are stored. We can do this by changing the current directory, as follows:

Select **Directories** from the **Options** menu.
In the **current directory** box change this to the directory containing the macros.
Click on the **Done** button.

We next need to find the macro file called *simu.txt*, as follows:

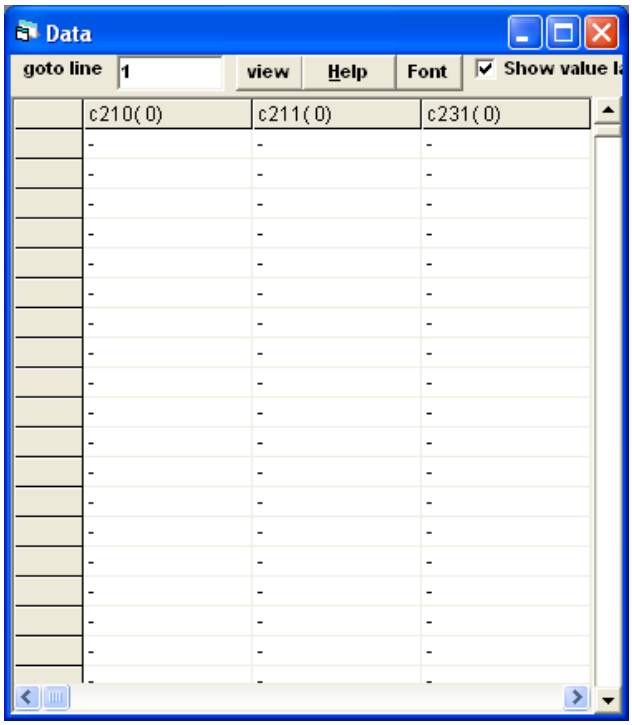
[2] Note that different random number seeds will result in the generation of different random numbers, and so sensitivity to a particular seed can be tested (e.g. one can test how robust particular estimates are to different sets of 'random' numbers). However, using the same seed should always give the same results (since it always generates the same 'random' numbers), and so if the user adopts the same seed as used in this manual, then they should derive exactly the same estimates (see e.g. Browne, 2003, p.59).

Select **Open Macro** from the **File** menu.
Find and select the file *simu.txt* in the **filename** box.
Click on the **Open** button.

A window containing the file *simu.txt* now appears. Note that some of the lines of code in the macro begin with the command NAME, which renames columns in MLwiN. Before starting the macro it is useful to open the data window and select columns of interest to view so that we can monitor the macro's progress. Here we will select columns c210, c211 & c231; from the code we can see that the macro will name these 'Samplesize', 'zpow0' and 'spow0', respectively. These three columns will hence contain the sample size, and the power estimate ('pow') for the intercept ('0') derived from the zero/one ('z') and standard error ('s') methods, respectively (see Sections 1.4.1 & 1.4.2 for a discussion of these methods). We do this as follows:

Select **View or Edit Data** from the **Data Manipulation** menu.
Click on the **view** button to select which columns to show.
Select columns C210, C211 and C231.
Note you will need to hold down the Ctrl button when selecting the later columns to add them to the selection.
Click on the **OK** button

If you have performed this correctly, the window will look as follows:



If you now run the macro by pressing the **Execute** button on the **Macro** window, the data window will fill in the sample size calculations as they are computed. Upon completion of the macro, the window will look as follows:

Data

goto line 1 view Help Font Show value la

	Samplesize(30)	zpow0(30)	spow0(30)
1	20.000	0.103	0.091
2	40.000	0.151	0.140
3	60.000	0.192	0.188
4	80.000	0.255	0.234
5	100.000	0.287	0.279
6	120.000	0.318	0.324
7	140.000	0.361	0.367
8	160.000	0.398	0.409
9	180.000	0.437	0.451
10	200.000	0.481	0.491
11	220.000	0.534	0.528
12	240.000	0.598	0.564
13	260.000	0.610	0.599
14	280.000	0.629	0.630
15	300.000	0.668	0.660
16	320.000	0.672	0.689
17	340.000	0.723	0.715
18	360.000	0.723	0.737
19	380.000	0.732	0.759
20	400.000	0.782	0.781
21	420.000	0.807	0.801
22	440.000	0.800	0.817
23	460.000	0.857	0.835
24	480.000	0.844	0.851
25	500.000	0.849	0.864
26	520.000	0.877	0.877
27	540.000	0.879	0.888
28	560.000	0.898	0.899
29	580.000	0.910	0.909
30	600.000	0.924	0.917

So here we see estimates of power of around 0.1 for just 20 boys, and above 0.9 for 600 boys. Next, we give more details on the two methods used to estimate power with the IGLS method.

1.4.1 Zero/One method

The first method used is perhaps the most straightforward, but can take a long time to get accurate estimates. For each simulation we get an estimate of each parameter of interest (in our case just an intercept) and the corresponding standard error. We can then calculate a (Gaussian) confidence interval for the parameter. If this confidence interval does not contain 0 we can reject the null hypothesis and give this simulation a score of 1. However, if the confidence interval *does* contain 0, we cannot reject the null hypothesis and so the simulation scores 0. To work out power across the

corresponding set of simulations we simply take the average score (i.e. # of 1s / total number of simulations).

1.4.2 Standard error method

A disadvantage of the first method is that to get an accurate estimate of power we need a lot of simulations. An alternative method (suggested by Joop Hox, 2007) is to simply look at the standard error for each simulation. If we take the average of these estimated standard errors over the set of simulations, together with the 'true' effect size γ, and the significance level α, we can use the earlier given formula:

$$\frac{\gamma}{SE(\gamma)} \approx z_{1-\alpha/2} + z_{1-\beta}$$

and solve for the power (1-β). This method works really well for the normal response models that we first consider in this guide, but will not work so well for the other response types that we investigate later.

If we look closely at the two columns on the right, we see that the differences between consecutive values produced using the zero/one method (i.e. those in the column headed 'zpow0') are quite variable and can be negative, whilst the values estimated using the standard error method ('spow0') demonstrate a much smoother pattern. If we are interested in establishing a power of 0.8 then both methods suggest a sample size of 420 will be fine. We can also plot these power curves in MLwiN, and indeed MLPowSim outputs another macro, *graphs.txt*, specifically for this purpose.

1.4.3 Graphing the Power curves

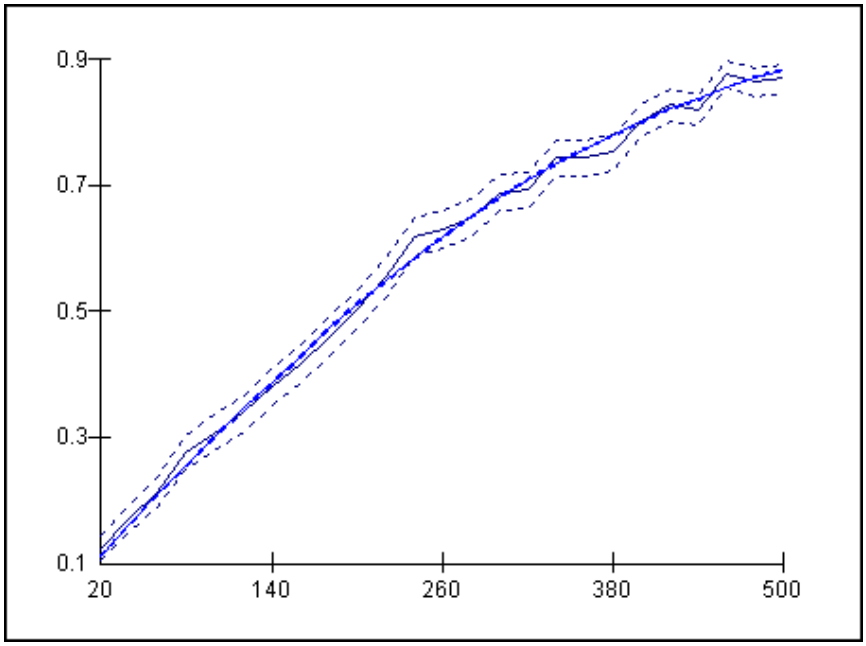
To plot the power curves, we need to find the graphing macro file called *graphs.txt*, as follows:

Select **Open Macro** from the **File** menu.
Select the file *graphs.txt* in the **filename** box.
Click on the **Open** button.
On the **graph macro** window click on the **Execute** button.

This has set up graphs in the background that can be viewed as follows:

Select **Customised graph(s)** from the **Graphs** menu.
Click on the **Apply** button on the **Customised graph(s)** window.

The following graph will appear:



This graph contains two solid lines along with confidence intervals (dashed lines). Here, the smoother brighter blue line is the standard error method, and has confidence interval lines around it that are actually indistinguishable from the line itself. The darker blue line plots the results from the zero/one method, and we can see that, in comparison, it is not very smooth and has wide confidence intervals; however, it does seem to track the brighter line, and with more simulations per setting we would expect closer agreement.

We can use this graph to read off the power for intermediate values of *n* that we did not simulate. Note that the curves here are produced by joining up the selected points, rather than any smooth curve fitting, and so any intermediate value is simply a linear interpolation of the two nearest points.

If we return to the theory, we can plug in the values -0.140 and 1.051 (1.0252^2) into the earlier power calculation to estimate exactly the *n* that corresponds to a power of 0.8 (assuming a normal approximation):

$$\Phi\left[\frac{(-1.96*1.0252/\sqrt{n})+0.14}{1.0252/\sqrt{n}}\right] \geq 0.8 \rightarrow \frac{(-1.96/\sqrt{n})+0.14}{1.0252/\sqrt{n}} \geq 0.842$$

Solving for *n* we get $n \geq (7.142 \times 1.0252 \times (0.842 + 1.96))^2 = 420.9$ thus we would need a sample size of at least 421; therefore, our estimate of around 420 is correct.

We will next look at how similar calculations can be performed with MLPowSim using the R package, instead of MLwiN, before looking at other model types.

1.5 Introduction to R and MLPowSim

As explained earlier, MLPowSim can create output files for use in one of two statistical packages. Having earlier introduced the basics of generating and executing output files for power analyses in MLwiN, here we do the same for the R package.

Once the user has first requested that R code, rather than MLwiN macros, be generated in MLPowSim (by pressing 0 when indicated), most of the subsequent questions and user inputs are the same as for MLwiN, and so we shan't cover all these in detail again. However, there *are* some differences when specifying the model setup, which reflect differences in the methods and terminologies of the estimation algorithms used by the two packages. Therefore, we shall consider these in a little more detail.

The R package is generally slower than MLwiN when simulating and fitting multilevel models. In R, we focus on the *lme* and *nlme* functions, and for single-level models the *glm* function. Employing the same example we studied earlier, the model setup questions, along with the user entries when selecting R, look like this:

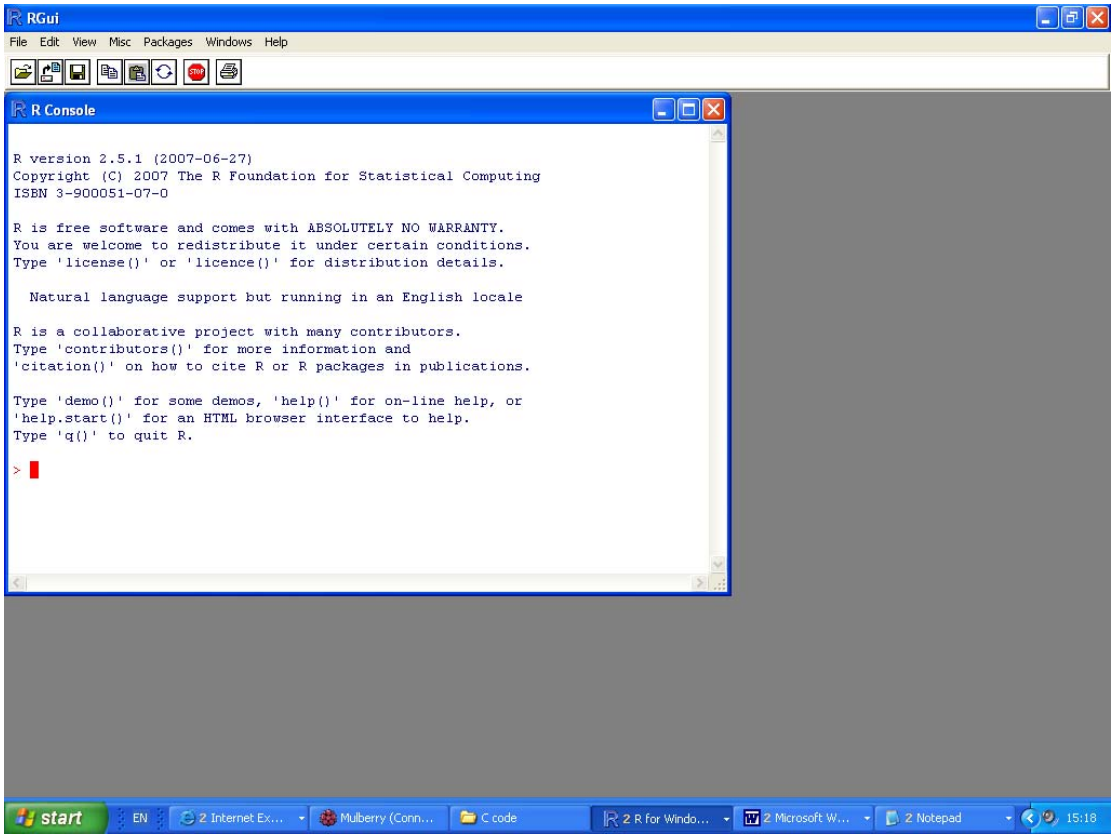
```
                              Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : 0
Do you want to include the fixed intercept in your model (1=YES  0=NO )? 1

                              Predictor(s) input
Do you want to include any explanatory variables in your model (1=YES 0=NO)? 0
```

R does not provide a choice of estimation methods for single-level models, although it does for multilevel models; therefore in the model setup dialogue presented above, there are no questions about estimation methods (unlike the situation we encountered earlier, for MLwiN). This is because the function *glm* is used to fit single-level models in the R package. In this function there is only one method implemented, iteratively reweighted least squares (IWLS).

1.5.1 Executing the R code

Before we introduce the procedure for executing the R code generated by MLPowSim, please note that this manual is written with reference to R version 2.5.1, on a Windows machine. It is possible that there may be some minor differences when executing the R code on other platforms such as Linux, or indeed with other versions of the software.

Upon starting R we will be presented by a screen that looks like this:



In contrast to the output for MLwiN, MLPowSim generates a single file (*powersimu.r*) for the R package. This file has the extension *r* which is the default for R command files. If this file is saved in the same directory as the R package itself, then by entering the following command, R will read the commands contained in the file:

```
source("powersimu.r")
```

If it is not saved in that directory, then one can either give the full path to the output file as an argument (i.e. enter the full path between the brackets in the above command), or change the working directory in R to the one in which the file is saved, as follows:

Select **Change dir …** from the **File** menu.
In the window which appears, do one of the following:
either write the complete pathname to the output file,
or select **Browse** and identify the directory containing the output file.
Click on the **OK** button.

Another simple option is to drag and drop the entire file (i.e. *powersimu.r*) into the R console window.

During the simulation, the R console provides updates, every 10^{th} iteration, of the number of iterations remaining for the current sample size combination being simulated. The start of the simulation for each different sample size combination is also indicated. In the case of our example, part of this output is copied below:

```
> source("powersimu.r")
    The programme was executed at Tue Aug 05 10:13:35 2008
------------------------------------------------------------------
 Start of simulation for sample sizes of  20  units
 Iteration remain= 990
 Iteration remain= 980
 Iteration remain= 970
 Iteration remain= 960
 Iteration remain= 950
 Iteration remain= 940
 Iteration remain= 930
 Iteration remain= 920
 Iteration remain= 910
 Iteration remain= 900
 Iteration remain= 890
 Iteration remain= 880
 Iteration remain= 870
 Iteration remain= 860
 Iteration remain= 850
 Iteration remain= 840
 Iteration remain= 830
 Iteration remain= 820
 Iteration remain= 810
 Iteration remain= 800
 Iteration remain= 790
 Iteration remain= 780
…….
…….
…….
```

The first line of the above screen indicates the date and time *powersimu.r* was executed in R. There is also another date at the top of the file itself (not shown here) indicating the time MLPowSim produced the R code. When the cursor appears in front of the command line again (i.e. in front of sign >), the power calculations are complete, and the power estimates and their confidence intervals (if the user has answered YES, in MLPowSim, to the question of whether or not they wish to have confidence intervals), for the various sample size combinations chosen by the user, will automatically be saved as *powerout.txt*. Since it is a text file, the results can, of course, be viewed using a variety of means; here, though, we view them by typing the name of the data frame saved by the commands we have just executed in the R console:

```
output
```

In the case of our example, the results look like this:

n	zLb0	zpb0	zUb0	sLb0	spb0	sUb0
20	0.073	0.091	0.109	0.089	0.09	0.091
40	0.129	0.151	0.173	0.136	0.137	0.138
60	0.148	0.171	0.194	0.183	0.184	0.186
80	0.214	0.241	0.268	0.229	0.23	0.232
100	0.258	0.286	0.314	0.277	0.279	0.281
120	0.298	0.327	0.356	0.321	0.323	0.325
140	0.351	0.381	0.411	0.365	0.367	0.369
160	0.381	0.411	0.441	0.407	0.409	0.412

180	0.41	0.441	0.472	0.447	0.45	0.452
200	0.457	0.488	0.519	0.486	0.489	0.491
220	0.479	0.51	0.541	0.522	0.524	0.527
240	0.552	0.583	0.614	0.559	0.562	0.564
260	0.56	0.59	0.62	0.594	0.596	0.599
280	0.601	0.631	0.661	0.627	0.629	0.631
300	0.627	0.656	0.685	0.655	0.657	0.659
320	0.664	0.693	0.722	0.684	0.686	0.688
340	0.679	0.707	0.735	0.71	0.712	0.714
360	0.727	0.754	0.781	0.734	0.736	0.738
380	0.731	0.758	0.785	0.757	0.759	0.761
400	0.755	0.781	0.807	0.777	0.778	0.78
420	0.761	0.786	0.811	0.797	0.799	0.8
440	0.793	0.817	0.841	0.816	0.818	0.819
460	0.804	0.827	0.85	0.833	0.834	0.836
480	0.823	0.845	0.867	0.848	0.849	0.85
500	0.823	0.845	0.867	0.863	0.865	0.866
520	0.864	0.884	0.904	0.875	0.876	0.877
540	0.859	0.879	0.899	0.886	0.887	0.889
560	0.87	0.889	0.908	0.898	0.899	0.9
580	0.906	0.923	0.94	0.907	0.908	0.909
600	0.911	0.927	0.943	0.917	0.918	0.918

The first column in this output file contains the sample size. In multilevel models, depending on the model type chosen by the user, we might have one, two or three columns representing the various sample size combinations at each level. The rest of the columns are either the estimated power or the lower/upper bounds, calculated using the methods described earlier (i.e. in Sections 1.4.1 and 1.4.2).

The column headings on the first row denote the specific method, statistic and parameter. This nomenclature uses the prefixes z and s for the zero/one and standard error methods of calculating power, respectively. Furthermore, the characters L and U indicate the lower (L) and upper (U) bounds of the confidence intervals, whilst the character p stands for the power estimate. Finally, in keeping with common notation for estimated parameters (i.e. β_0, β_1 etc.), the characters b0, b1, etc., finish the column headings.

The results indicate a sample size of between 420 and 440 should be sufficient to achieve a power of 0.8; this is very similar to our earlier finding using MLwiN, and indeed our theory-based calculations (Section 1.4).

1.5.2 Graphing Power curves in R

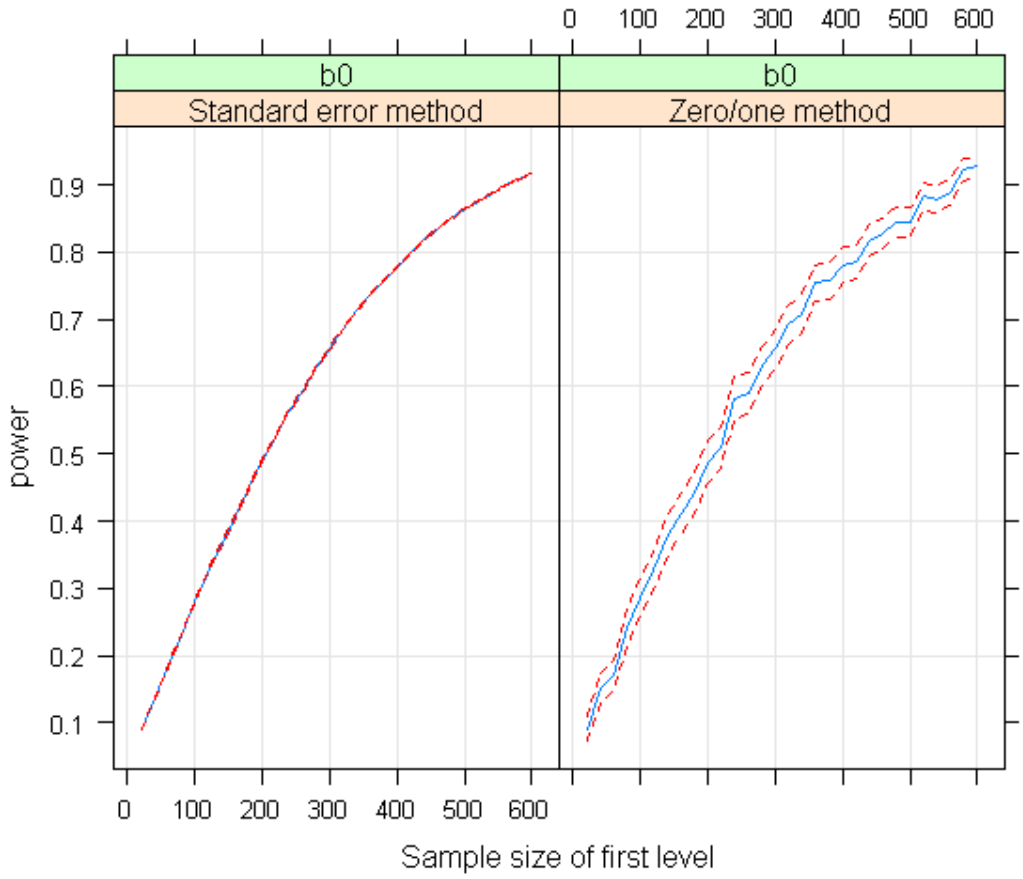
R has many facilities for producing plots of data, and users can load a variety of libraries and expand these possibilities further.

When fitting a multilevel (mixed effect) model in R we have a grouped data structure, and a number of specific commands have been written to visualise such data (see, for example, Venables and Ripley, 2002, Pinheiro and Bates, 2000). For instance, the *trellis* graphing facility in the *lattice* package is useful for plotting grouped data, and many other complex multivariate data as well. Among the many plotting commands and functions in the trellis device, the command *xyplot ( )*, combined with others such

as *lines ( )*, via the function *panel*, are useful tools. For example, one can employ code such as the following:

```
library(lattice)
output<-read.table("powerout.txt",header =T,sep = " ", dec = ".")
method<-rep(c("Zero/one method","Standard error method"),each=length(n1range),times=betasize)
sample<-rep(n1range,times=2*betasize)
parameter<-rep(c("b0"),each=2*length(n1range))
power<-c(output$zpb0,output$spb0)
Lpower<-c(output$zLb0,output$sLb0)
Upower<-c(output$zUb0,output$sUb0)
dataset<-data.frame(method,sample,parameter,Lpower,power,Upower)
xyplot(power~sample | method*parameter ,data=dataset,xlab="Sample size of first level",
        scales=list(x=list(at=seq(0,600,100)),y=list(at=seq(0,1,.1))),
        as.table=T,subscripts=T,
        panel=function(x,y,subscripts)
{
         panel.grid(h=-1,v=-1)
        panel.xyplot(x,y,type="l")
       panel.lines(dataset$sample[subscripts],dataset$Lpower[subscripts],lty=2,col=2)
      panel.lines(dataset$sample[subscripts],dataset$Upower[subscripts],lty=2,col=2)
      })
```

This will produce the following graphs:



The curves are shown in two different panels to make comparison easier. In both panels, the solid lines (in blue) indicate the estimated powers while the broken lines

(in red) are the confidence bounds. It can be seen that the bound interval of the estimated power in the zero/one method is wider than that in standard error method.

If one wanted to read off the predicted power for a predefined sample size (or *vice versa*), one could make the grids in the panels thinner, via the available parameters in the panel function. However, it's likely that visual interpolation with the coarse grid above will give approximately the same result.

For further guidance on plotting power estimates in R, please see Section 5.3.3.

2 Continuous Response Models

In this section we describe sample size calculations for continuous (normally-distributed) response models in general. For these models there exists further exact formulae that can be used for other single-level models, and also an existing piece of software (PinT) that gives sample size formulae for balanced 2-level nested models. In Section 2.1 we will review some of the single-level model formulae while comparing results in Section 2.2 with the simulation approach. In Section 2.3 we look at 2-level nested variance components models and describe the design effect formula, the PinT software package, and the simulation-based approach we adopt in MLPowSim. Finally, in Sections 2.4 to 2.6 we discuss extending our calculations to other 2-level nested models, 3-level models and cross-classified models.

2.1 Standard Sample size formulae for continuous responses

In the introductory chapter we described how one approximate formula can link power, significance level, effect size and sample size (through the standard error of the effect size). This formula is as follows:

$$\frac{\gamma}{SE(\gamma)} \approx z_{1-\alpha/2} + z_{1-\beta}$$

The approximation here is in terms of assuming an underlying normal distribution for γ when in reality this is only asymptotically correct: i.e. we should really use a *t* distribution; however, this will not matter much as long as the sample size is reasonable. When we are sure about the size and power we require, we can simplify this further by plugging these values in and having a simple relationship linking the effect size and its standard error, as described in Chapter 20 of Gelman and Hill (2007). They consider as we do in general two-sided tests with a significance level of 0.05 and a power of 0.8 which results in $\gamma = (1.96+0.84)SE(\gamma) = 2.8SE(\gamma)$.[3]

[3] Note that if we were considering a one-sided test with the same significance level and power, this would result in $\gamma = (1.645+0.842)SE(\gamma) = 2.487SE(\gamma)$.

2.1.1 Single mean – one sample t-test

In the introduction we showed that to test whether a sample mean is greater than 0 we needed to perform a one sample t-test which could be approximated by a Z test for suitably large sample sizes.

To repeat the theory, we plugged in the values -0.140 and 1.051 (1.0252^2) into the power calculation to estimate exactly the *n* that corresponds to a power of 0.8 (assuming a normal approximation):

$$\Phi\left[\frac{(-1.96*1.0252/\sqrt{n})+0.14}{1.0252/\sqrt{n}}\right] \geq 0.8 \rightarrow \frac{(-2.01/\sqrt{n})+0.14}{1.0252/\sqrt{n}} \geq 0.842$$

Solving for *n* we get $n \geq (7.142 \times 1.0252 \times (0.842 + 1.96))^2 = 420.9$ thus we would need a sample size of at least 421.

With our simplified formula we have:

$$\gamma = 2.802SE(\gamma)$$
$$\rightarrow 0.140 = 2.802 \times \frac{1.0252}{\sqrt{n}} \rightarrow \sqrt{n} = \frac{2.87}{0.14} = 20.5$$
$$\rightarrow n = 421$$

which is exactly the same calculation.

2.1.2 Comparison of two means – two-sample t-test

If we have a binary predictor variable then we have a predictor that essentially splits our dataset in two. We might then be interested in whether these two groups have significantly different means, or equivalently in a linear modelling framework (see Section 2.1.5), whether the predictor has a significant effect on the response.

The common approach for testing the hypothesis that two independent samples have differing means is the two-sample t-test which can be approximated for large sample sizes by the Z test using the standard formula.

Letting y_{1i} be the *i*th observation in the first sample, and y_{2j} be the *j*th observation in the second sample, then the test statistic that will play the role of γ is the difference in sample means $\bar{y}_1 - \bar{y}_2$, which has associated (pooled) standard error

$$\sqrt{\sigma_1^2/n_1 + \sigma_2^2/n_2}\ .$$

Here we can see that to perform a power calculation we need to estimate the difference between the means, the variances of the two groups and the sizes of the samples in the two groups. We can then work out the power for any combination of sample sizes.

So we can calculate the power associated with various combinations of group 1 sample sizes, and group 2 sample sizes. If the variability within each group is different, it may be advantageous to sample more from the group which has the highest variance to reduce the standard error of the difference. In an experimental setting it is easy to sample the two groups independently, and if the effect of the two groups is of great interest and/or one of the two groups is rare, it might be useful to do so explicitly (a form of stratified sampling).

In observational studies, on the other hand, we will generally sample at random from the population, and the group identifier/binary predictor will simply be recorded. Here the two group sample sizes will be replaced by an overall sample size, together with a probability of group membership. The uncertainty in actual group sample sizes will have an impact on power, but a simulation approach can cope with this. As later discussed in Section 2.1.5, we can calculate desired sample sizes conditional on the probability of group membership.

2.1.3 Simple linear regression

The simple linear regression model can be written as follows:

$$y_i = \beta_0 + \beta_1 x_i + e_i, e_i \sim N(0, \sigma^2)$$

Here we are aiming to look at the relationship between a (typically continuous) predictor variable *x*, and the response variable *y*, where *i* indexes the individuals. Our null hypothesis will generally be that the predictor has no effect, i.e. $\beta_1=0$, although we might also wish to test for a strictly non-zero intercept as well, i.e. $\beta_0=0$.

From regression theory we can calculate the standard errors for the two quantities β_0 and β_1 which are $\sigma\sqrt{\frac{1}{n}+\frac{\bar{x}^2}{S_{xx}}}$ and $\sigma/\sqrt{S_{xx}}$ where $S_{xx} = \sum_i x_i^2 - \frac{(\sum_i x_i)^2}{n}$ respectively. It is important to note the meaning of σ has changed from the simple mean model. In this case it is the residual variation after accounting for the predictor *x*. This is important to note when choosing an estimate for σ to perform the power calculation. From the standard error formulae we can see that we also need to give an estimate for S_{xx} to perform a sample size calculation. This quantity is not an intuitive one to estimate, so it makes more sense to make use of the fact that
$S_{xx} = \sum_i (x_i - \bar{x})^2 = (n-1)\,\mathrm{var}(x_i)$
and instead estimate the variance of the predictor variable.

2.1.4 General linear model

In the general linear modelling framework, we have the following:

$$y_i = X_i^T \beta + e_i, e_i \sim N(0, \sigma^2)$$

Here X_i is a vector of predictor variables for individual *i* that are associated with response y_i. The corresponding coefficient vector β represents the effects of the various predictor variables. Usually our null hypotheses will be based on specific elements of the vector β, and whether they are zero. For this we will require the standard errors for β. The variance matrix associated with the β predictors has formula $\sigma^2 (X^T X)^{-1}$ from which we can pick out the standard errors for specific β_i. The standard error formula will then be a function of the sample size, the variance of the particular predictor, and the covariances between the predictors. Therefore, as we will see in Section 2.2, if we specify that our predictors are multivariate normally-distributed, then we will need to specify both their means and also their covariance matrix.

2.1.5 Casting all models in the same framework

For normal response models which do not involve higher-level random structure, the linear modelling framework covers most cases. There is one minor exception which we have already looked at briefly: namely the two population different means (two sample t / Z test) hypothesis. Here we can write out the linear regression model

$$y_i = \beta_0 + \beta_1 x_i + e_i, e_i \sim N(0, \sigma^2)$$

where x_i is a binary indicator that an observation belongs to group 2. Clearly this model is a member of the linear model family and testing the hypothesis that $\beta_1=0$ is equivalent to the hypothesis that the two group means differ. However, this model makes the implicit assumption that the two group variances are equal, and equal to σ^2. To allow a model with differing group variances we would need the more general model:

$$y_i = \beta_0 + \beta_1 x_i + e_i, e_i \sim N(0, \sigma_i^2)$$

which allows different variances for each observation. We would then need to implicitly set the variances for each observation in group 1 to be equal and similarly set the variances for each observation in group 2 to be equal. Such a model is fitted easily in packages such as MLwiN, with which a simulation study can be conducted to work out power. For this first version of MLPowSim, however, we have assumed that single-level models fit in the standard linear modelling framework with constant residual variation.

We will now introduce a selected range of the possible single-level models that MLPowSim can fit, using the tutorial example introduced in the last chapter.

2.2 Equivalent results from MLPowSim

In this section we will begin each example by describing the research question, and then show how to set up the model in MLPowSim. We will then look at the answers produced in MLwiN, and compare them with theoretical results. Note that similar results would be attained via R, but these are not included for brevity.

2.2.1 Testing for differences between two groups

The tutorial dataset contains a gender predictor for each pupil. In the introduction we looked at the hypothesis that boys did worse than an average value. Perhaps a more sensible hypothesis would be that girls do better than boys. We will here consider the hypothesis within a regression framework, and consider the model:

$$y_i = \beta_0 + \beta_1 x_i + e_i, e_i \sim N(0, \sigma^2)$$

where x_i takes value 1 for a girl, and 0 for a boy. Our null hypothesis is that $\beta_1=0$, with an alternative hypothesis $\beta_1>0$. To fit this model we need estimates for β_0, β_1 and σ^2, along with some information about the predictor.

We will take estimates from the full tutorial dataset, and so we have β_0=-0.140, β_1=0.234 and σ^2=0.985.
In the population we have 60% girls and 40% boys and so we will consider two possible ways of including information about the predictor:

(i) assume x_i is Bernouilli-distributed, with underlying probability 0.6;
(ii) assume a normal approximation, and so x_i ~N(0.6,0.24).

We will describe each of these, in turn, below. We will fire up the MLPowSim executable and answer the questions it asks. Using our tutorial example, here we present questions and responses corresponding to (i):

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **1**
Please input the random number seed: **1**
Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**
How many explanatory variables do you want to include in your model? **1**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **1**

Please input probability of a 1 for x1 : **0.6**

Sample size set up

Please input the smallest sample size : **50**
Please input the largest sample size : **1500**
Please input the step size: **50**

Parameter estimates

Please input estimate of beta_0: **-0.140**
Please input estimate of beta_1: **0.234**

Please input estimate of sigma^2_e: **0.985**

Files to perform power analysis for the 1 level model with the following sample criterion have been created
Sample size starts at 50 and finishes at 1500 with the step size 50
1000 simulations for each sample size combination will be performed

Press any key to continue…

We will now run the code in MLwiN as we did in the introductory example (see Section 1.4 for information on starting up MLwiN and changing directories). Again, before starting the macro, it is useful to open the **View/Edit Data** window to view its progress (Section 1.4 details how to do this). In this case, it is useful to select columns c210, c211, c212, c231 and c232 to view, since, as the coding in the macro indicates, it will place the sample sizes in the first of these columns, and the estimated powers for the two predictors, using two different methods detailed earlier (Sections 1.4.1 & 1.4.2), in the last four of these columns.

If we now run the macro by pressing the **Execute** button on the **Macro** window the data window will fill in the sample size calculations as they are computed. Upon completion of the macro, the window will look as follows:

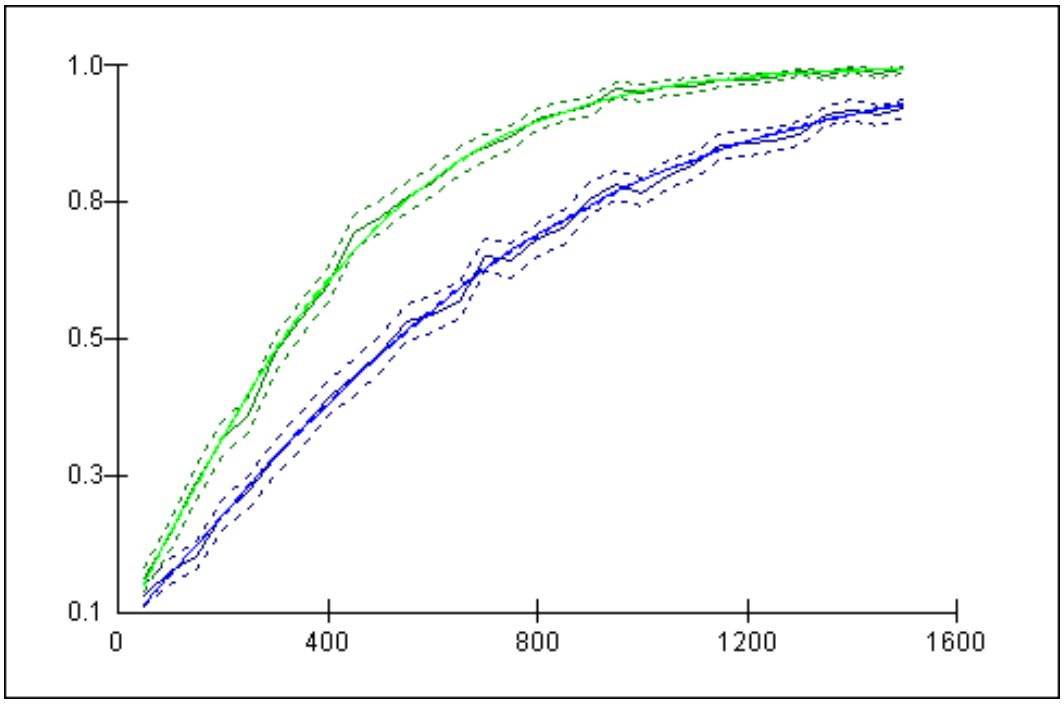
Data

goto line 1 | view | Help | Font | Show value labels

	Samplesize(30)	zpow0(30)	zpow1(30)	spow0(30)	spow1(30)
1	50.000	0.109	0.136	0.094	0.128
2	100.000	0.148	0.209	0.144	0.213
3	150.000	0.176	0.298	0.193	0.294
4	200.000	0.244	0.372	0.243	0.373
5	250.000	0.283	0.412	0.292	0.447
6	300.000	0.337	0.514	0.341	0.518
7	350.000	0.385	0.573	0.386	0.581
8	400.000	0.441	0.632	0.432	0.638
9	450.000	0.477	0.720	0.474	0.689
10	500.000	0.516	0.745	0.515	0.734
11	550.000	0.567	0.776	0.554	0.774
12	600.000	0.581	0.804	0.587	0.807
13	650.000	0.603	0.838	0.625	0.839
14	700.000	0.680	0.861	0.657	0.865
15	750.000	0.672	0.878	0.688	0.887
16	800.000	0.706	0.907	0.713	0.905
17	850.000	0.726	0.921	0.739	0.920
18	900.000	0.775	0.929	0.762	0.933
19	950.000	0.798	0.959	0.788	0.946
20	1000.000	0.786	0.952	0.807	0.955
21	1050.000	0.814	0.962	0.825	0.963
22	1100.000	0.832	0.965	0.841	0.969
23	1150.000	0.864	0.974	0.858	0.975
24	1200.000	0.868	0.975	0.872	0.980
25	1250.000	0.873	0.978	0.885	0.983
26	1300.000	0.884	0.987	0.895	0.986
27	1350.000	0.914	0.982	0.907	0.989
28	1400.000	0.923	0.991	0.916	0.991
29	1450.000	0.915	0.985	0.925	0.993
30	1500.000	0.927	0.991	0.933	0.994

So here we see estimates of power for the intercept of around 0.1 for 50 pupils, and up to 0.92 for 1500 pupils (see columns 'zpow0' & 'spow0'). More importantly, for the gender effect ('zpow1' & 'spow1') we have power of around 0.13 for 50 pupils, rising to 0.991 for 1500 pupils, with around 600 pupils giving a power of 0.8.

If we graph the curves (see Section 1.4.3 on finding and executing the *graphs.txt* macro, and then viewing the resulting graph), they look as follows:



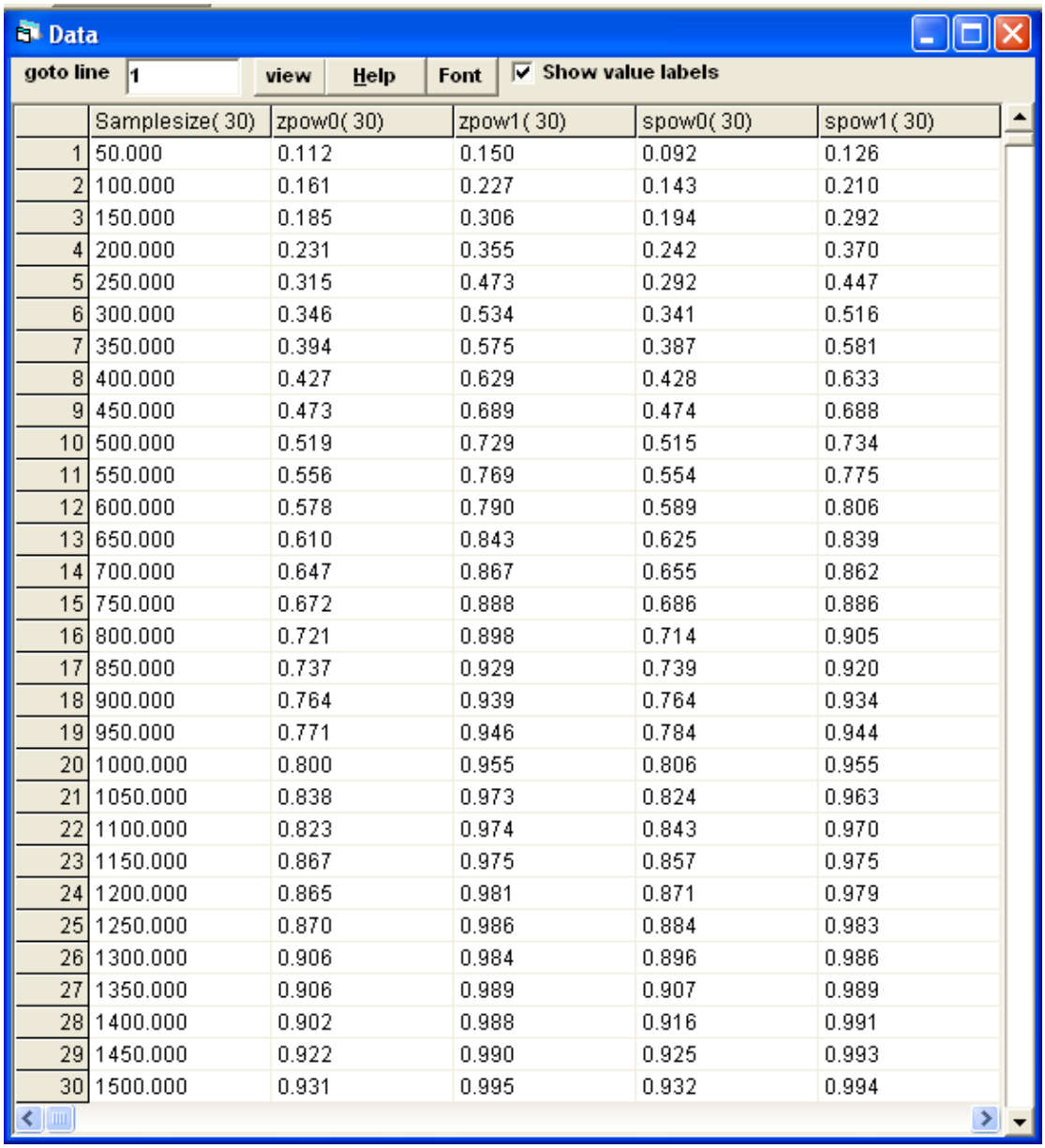
This graph contains two lines, along with confidence intervals, for each parameter, with the intercept in blue and the gender effect in green. The smoother brighter lines correspond to the standard error method and have confidence interval lines around them that are actually indistinguishable from the lines themselves. The darker lines are the zero/one method results and we can see they are not very smooth and have wide confidence intervals; however, as we mentioned in Section 1.4.3, they do seem to track the brighter lines and with more simulations per setting we would expect more agreement.

We next consider option (ii), and look at the effect of assuming an approximate normal distribution for gender: i.e. in the simulated dataset that generated 0 and 1 values for boys and girls, we will have a continuous predictor with mean and variance equal to the mean and variance of the binary predictor considered in option (i), remembering the mean of a Bernouilli(p) distributed variable is p and the variance is $p(1-p)$. In our case we have p = 0.6.

To do this, we have to make some minor changes to the questions in MLPowSim regarding types of predictor. Rather than repeat all the code from the example relating to (i), we only show the relevant changes below:

Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **2**
Assuming normality, please input its parameters here:
The mean of the predictor x1: **0.6**
The variance of the predictor x1: **0.24**

Running this model results in the following table of output:



	Samplesize(30)	zpow0(30)	zpow1(30)	spow0(30)	spow1(30)
1	50.000	0.112	0.150	0.092	0.126
2	100.000	0.161	0.227	0.143	0.210
3	150.000	0.185	0.306	0.194	0.292
4	200.000	0.231	0.355	0.242	0.370
5	250.000	0.315	0.473	0.292	0.447
6	300.000	0.346	0.534	0.341	0.516
7	350.000	0.394	0.575	0.387	0.581
8	400.000	0.427	0.629	0.428	0.633
9	450.000	0.473	0.689	0.474	0.688
10	500.000	0.519	0.729	0.515	0.734
11	550.000	0.556	0.769	0.554	0.775
12	600.000	0.578	0.790	0.589	0.806
13	650.000	0.610	0.843	0.625	0.839
14	700.000	0.647	0.867	0.655	0.862
15	750.000	0.672	0.888	0.686	0.886
16	800.000	0.721	0.898	0.714	0.905
17	850.000	0.737	0.929	0.739	0.920
18	900.000	0.764	0.939	0.764	0.934
19	950.000	0.771	0.946	0.784	0.944
20	1000.000	0.800	0.955	0.806	0.955
21	1050.000	0.838	0.973	0.824	0.963
22	1100.000	0.823	0.974	0.843	0.970
23	1150.000	0.867	0.975	0.857	0.975
24	1200.000	0.865	0.981	0.871	0.979
25	1250.000	0.870	0.986	0.884	0.983
26	1300.000	0.906	0.984	0.896	0.986
27	1350.000	0.906	0.989	0.907	0.989
28	1400.000	0.902	0.988	0.916	0.991
29	1450.000	0.922	0.990	0.925	0.993
30	1500.000	0.931	0.995	0.932	0.994

There is very little difference between the results produced using the normal approximation, and the results produced using the binary predictor, which suggests that we might like to consider using the normal approximation at all times, particularly as it makes it easy to include correlations between predictors (see Section 2.2.3). One word of caution, though: in this case we have an underlying probability of 0.6, and reasonable sample sizes; the normal approximation works best in these situations but may not be so good when the probability is more extreme or the sample size is small.

From a theory point of view, we can consider the 2-sample Z-test with fixed sample size ratio of 60% girls and 40% boys and equal variance (0.985), and an effect size of 0.234.

Then the sample size calculation becomes:

$$\gamma = 2.802 SE(\gamma)$$
$$\rightarrow 0.234 = 2.802 \times \sqrt{\sigma^2 / 0.4n + \sigma^2 / 0.6n}$$
$$\rightarrow 0.234 = 2.802 \times \sqrt{0.985 / 0.24n}$$
$$\rightarrow n = (2.802 / 0.234)^2 \times 0.985 / 0.24 = 588.5$$

So if we had fixed ratios in our 2-sample Z-test, we would need a sample of at least 589 pupils. Even though our simulation is based on observational data, where the ratio 6:4 is just the expected ratio, we still get a similar estimate of the sample size required.

2.2.2 Testing for a significant continuous predictor

The main predictor of interest in the tutorial example in the MLwiN User's Guide is a prior ability measure: namely the London Reading Test (LRT; this predictor is standardised using Z-scores in the User's Guide, and is named 'standlrt') which the students take at age 11 prior to taking their main exams (the response variable) at age 16. This predictor has a very significant effect on the exam response, and consequently we expect that we will need a small sample size to gain a power of 0.8.

We can run MLPowSim in a similar way as we did for the gender predictor in Section 2.2.1 when we assumed a normal approximation. The inputs that will change are outlined below:

Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **2**
Assuming normality, please input its parameters here:
The mean of the predictor x1: **0**
The variance of the predictor x1: **1**

Sample size set up

Please input the smallest sample size : **5**
Please input the largest sample size : **50**
Please input the step size: **5**

Parameter estimates

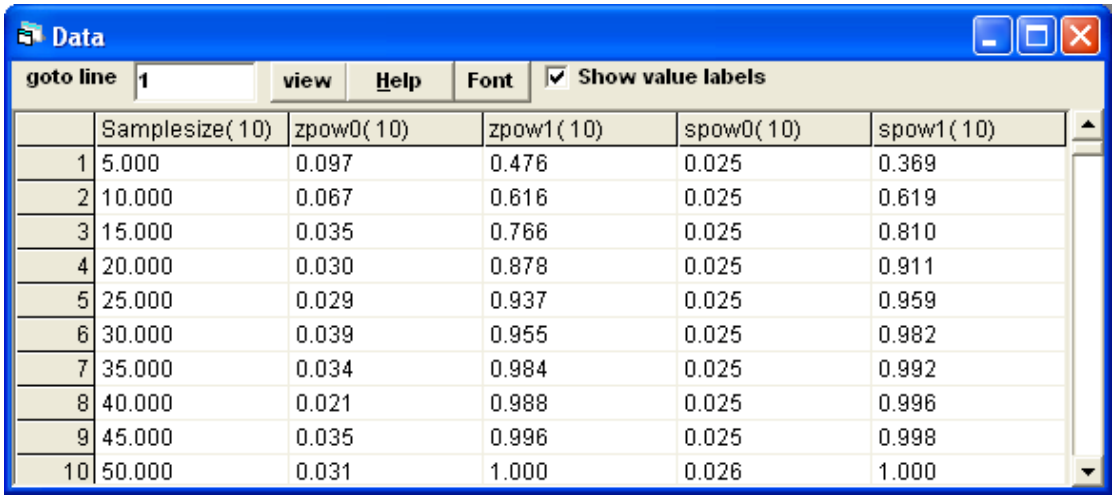
Please input estimate of beta_0: **-0.001**
Please input estimate of beta_1: **0.595**

Please input estimate of sigma^2_e: **0.648**

Files to perform power analysis for the 1 level model with the following sample criterion have been created
Sample size starts at 5 and finishes at 50 with the step size 5
1000 simulations for each sample size combination will be performed

Press any key to continue…

If we run these new macros in MLwiN as previously described (in Section 1.4) we get the following values in the Data window:



Data

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	Samplesize(10)	zpow0(10)	zpow1(10)	spow0(10)	spow1(10)
1	5.000	0.097	0.476	0.025	0.369
2	10.000	0.067	0.616	0.025	0.619
3	15.000	0.035	0.766	0.025	0.810
4	20.000	0.030	0.878	0.025	0.911
5	25.000	0.029	0.937	0.025	0.959
6	30.000	0.039	0.955	0.025	0.982
7	35.000	0.034	0.984	0.025	0.992
8	40.000	0.021	0.988	0.025	0.996
9	45.000	0.035	0.996	0.025	0.998
10	50.000	0.031	1.000	0.026	1.000

So, looking at columns 'zpow1' and 'spow1' we see that with even around 15 to 20 pupils, we have a power greater than 0.8.

To compare this with the theory, we can look at the following:

$$\gamma = 2.802 SE(\gamma)$$
$$\rightarrow 0.595 = 2.802 \times \sqrt{\sigma^2 / S_{xx}}$$
$$\rightarrow 0.595 = 2.802 \times \sqrt{0.648/(n-1)}$$
$$\rightarrow n - 1 = (2.802/0.595)^2 \times 0.648 \rightarrow n = 14.37$$

and so this clearly agrees with the simulation results.

2.2.3 Fitting a multiple regression model.

We can next consider a model that includes both gender and LRT predictors. We already have sample size estimates for the relationship between each of these two predictors and the response independently, but now we are looking at the relationships conditional on the other predictor. For this model we will get three estimated powers for each sample size: one for each of the relationships, and one for the intercept.

We will once again use the actual estimates obtained from fitting the model to the full tutorial dataset for our effect estimates, our variability, and so on. Note that the estimates are reduced due to the correlation between the two predictors. We will firstly assume independence between the two predictor variables; the MLPowSim session will then proceed as follows:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model

3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **1**
Please input the random number seed: **1**
Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**
How many explanatory variables do you want to include in your model? **2**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **1**
Please input probability of a 1 for x1 : **0.6**
Please choose a type for the predictor x2 (1=Binary 2=Continuous): **2**
Assuming normality, please input its parameters here:
The mean of the predictor x2: **0**
The variance of the predictor x2: **1**

Sample size set up

Please input the smallest sample size : **50**
Please input the largest sample size : **1500**
Please input the step size: **50**

Parameter estimates

Please input estimate of beta_0: **-0.103**
Please input estimate of beta_1: **0.170**
Please input estimate of beta_2: **0.591**

Please input estimate of sigma^2_e: **0.642**

Files to perform power analysis for the 1 level model with the following sample criterion have been created
Sample size starts at 50 and finishes at 1500 with the step size 50
1000 simulations for each sample size combination will be performed

Press any key to continue…

We will now run the macros in the usual way and we will need to look at seven columns to get the power for all three parameters using both methods. For the 0/1 method, the power for the fixed effects starts in column c211 and proceeds sequentially, whilst for the standard error method the power for the fixed effects starts in column c231 and proceeds sequentially. As a side issue, this means that there is an implicit limit of 20 fixed effects in MLPowSim when using MLwiN, as otherwise the columns will start being reused for more than one purpose!

The **Data** window for this model looks as follows:

Data

goto line 1 | view | Help | Font | Show value labels

	Samplesize(30)	zpow0(30)	zpow1(30)	zpow2(30)	spow0(30)	spow1(30)	spow2(30)
1	50.000	0.093	0.107	0.998	0.085	0.113	0.999
2	100.000	0.143	0.188	1.000	0.126	0.180	1.000
3	150.000	0.173	0.255	1.000	0.168	0.247	1.000
4	200.000	0.208	0.313	1.000	0.210	0.314	1.000
5	250.000	0.277	0.396	1.000	0.251	0.377	1.000
6	300.000	0.302	0.443	1.000	0.292	0.438	1.000
7	350.000	0.342	0.520	1.000	0.332	0.496	1.000
8	400.000	0.377	0.545	1.000	0.369	0.547	1.000
9	450.000	0.391	0.592	1.000	0.407	0.597	1.000
10	500.000	0.427	0.651	1.000	0.445	0.643	1.000
11	550.000	0.491	0.680	1.000	0.482	0.685	1.000
12	600.000	0.483	0.704	1.000	0.514	0.723	1.000
13	650.000	0.548	0.761	1.000	0.545	0.755	1.000
14	700.000	0.568	0.785	1.000	0.578	0.787	1.000
15	750.000	0.592	0.818	1.000	0.605	0.812	1.000
16	800.000	0.616	0.820	1.000	0.633	0.837	1.000
17	850.000	0.662	0.862	1.000	0.660	0.858	1.000
18	900.000	0.671	0.878	1.000	0.686	0.878	1.000
19	950.000	0.724	0.903	1.000	0.709	0.894	1.000
20	1000.000	0.714	0.896	1.000	0.730	0.908	1.000
21	1050.000	0.753	0.925	1.000	0.750	0.920	1.000
22	1100.000	0.753	0.931	1.000	0.771	0.932	1.000
23	1150.000	0.786	0.937	1.000	0.788	0.941	1.000
24	1200.000	0.779	0.933	1.000	0.805	0.950	1.000
25	1250.000	0.798	0.947	1.000	0.820	0.957	1.000
26	1300.000	0.838	0.960	1.000	0.835	0.963	1.000
27	1350.000	0.857	0.969	1.000	0.848	0.969	1.000
28	1400.000	0.856	0.975	1.000	0.861	0.973	1.000
29	1450.000	0.863	0.973	1.000	0.873	0.977	1.000
30	1500.000	0.892	0.980	1.000	0.882	0.981	1.000

Here we see that the LRT predictor has associated power (see columns ‘zpow2’ and ‘spow2’) of essentially 1 at sample sizes of only 100 pupils, whilst the gender predictor requires samples of around 750 to gain a power of 0.8 (‘zpow1’ and ‘spow1’). This is higher than the 600 required when LRT was not considered, but this will be in part due to the reduced effect size of 0.170 versus 0.234, which more than outweighs the reduction in unexplained variability (0.642 versus 0.985).

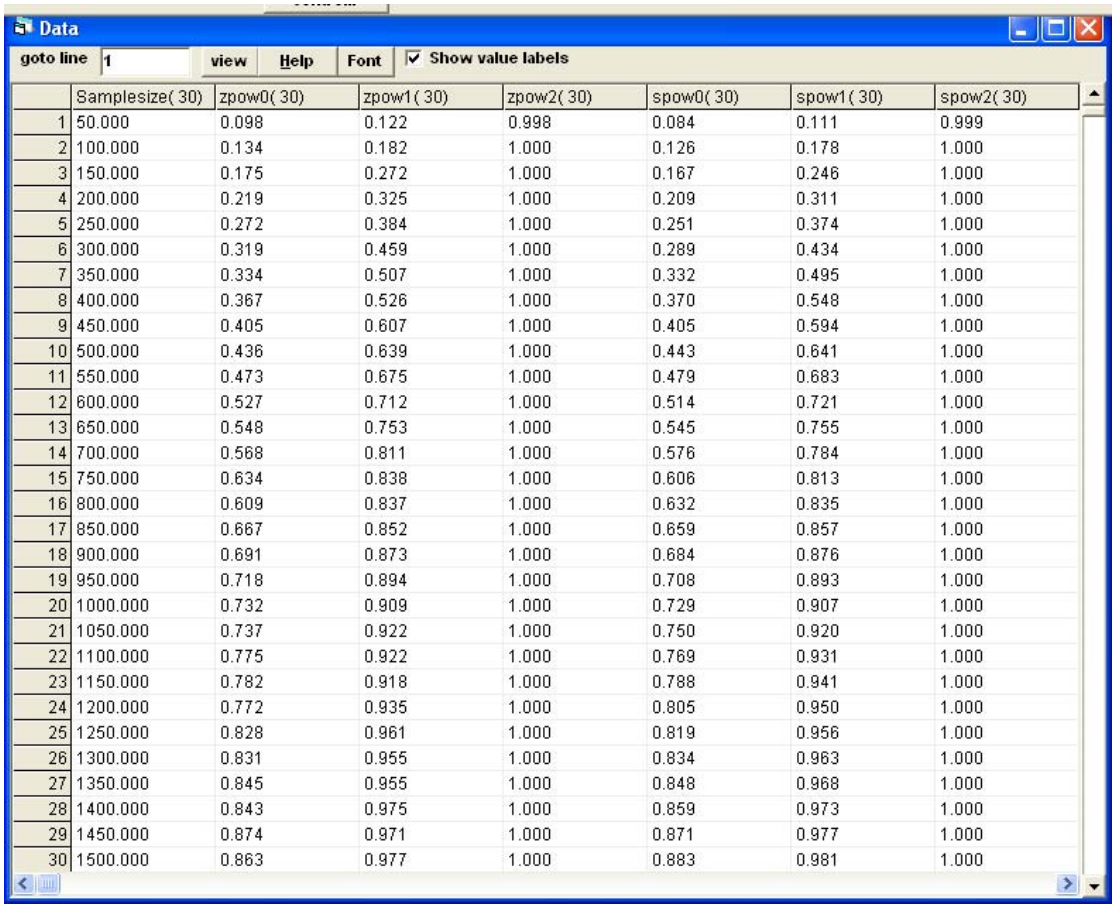
We could also consider including the correlation between our two predictors in our simulation; i.e. at present we are assuming independence between prior attainment and gender, whereas in reality there is a small positive correlation, with girls doing better in the LRT than boys. To do this we need to approximate the 0/1 gender predictor with a continuous predictor for simulation purposes and assume a multivariate normal distribution. This involves minor changes to the above macro as follows:

Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **3**
Assuming multivariate normality, please input its parameters here:
The mean of the predictor x1: **0.6**
The mean of the predictor x2: **0**
The variance matrix of the predictors
The element [1,1]: **0.24**
The element [2,1]: **0.026**
The element [2,2]: **1**

Note that here we have worked out the correlation between the two predictors based on the full tutorial dataset and then converted this to a covariance value of 0.026. In

addition, note that in MLPowSim, one can choose independent combinations of binary and continuous as predictor types, but if MVN is selected, then *all* predictors are treated as such (i.e. as MVN).

So, if we fit this model, we get the following:



Data

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	Samplesize(30)	zpow0(30)	zpow1(30)	zpow2(30)	spow0(30)	spow1(30)	spow2(30)
1	50.000	0.098	0.122	0.998	0.084	0.111	0.999
2	100.000	0.134	0.182	1.000	0.126	0.178	1.000
3	150.000	0.175	0.272	1.000	0.167	0.246	1.000
4	200.000	0.219	0.325	1.000	0.209	0.311	1.000
5	250.000	0.272	0.384	1.000	0.251	0.374	1.000
6	300.000	0.319	0.459	1.000	0.289	0.434	1.000
7	350.000	0.334	0.507	1.000	0.332	0.495	1.000
8	400.000	0.367	0.526	1.000	0.370	0.548	1.000
9	450.000	0.405	0.607	1.000	0.405	0.594	1.000
10	500.000	0.436	0.639	1.000	0.443	0.641	1.000
11	550.000	0.473	0.675	1.000	0.479	0.683	1.000
12	600.000	0.527	0.712	1.000	0.514	0.721	1.000
13	650.000	0.548	0.753	1.000	0.545	0.755	1.000
14	700.000	0.568	0.811	1.000	0.576	0.784	1.000
15	750.000	0.634	0.838	1.000	0.606	0.813	1.000
16	800.000	0.609	0.837	1.000	0.632	0.835	1.000
17	850.000	0.667	0.852	1.000	0.659	0.857	1.000
18	900.000	0.691	0.873	1.000	0.684	0.876	1.000
19	950.000	0.718	0.894	1.000	0.708	0.893	1.000
20	1000.000	0.732	0.909	1.000	0.729	0.907	1.000
21	1050.000	0.737	0.922	1.000	0.750	0.920	1.000
22	1100.000	0.775	0.922	1.000	0.769	0.931	1.000
23	1150.000	0.782	0.918	1.000	0.788	0.941	1.000
24	1200.000	0.772	0.935	1.000	0.805	0.950	1.000
25	1250.000	0.828	0.961	1.000	0.819	0.956	1.000
26	1300.000	0.831	0.955	1.000	0.834	0.963	1.000
27	1350.000	0.845	0.955	1.000	0.848	0.968	1.000
28	1400.000	0.843	0.975	1.000	0.859	0.973	1.000
29	1450.000	0.874	0.971	1.000	0.871	0.977	1.000
30	1500.000	0.863	0.977	1.000	0.883	0.981	1.000

Here we see that, as with the uncorrelated case, we need a sample size of around 750 for a power of 0.8 for the gender predictor (columns 'zpow1' & 'spow1'). Please note that in this case, the correlation between the two predictors is small (0.053). Allowing for correlations between predictors will be more important, however, when those correlations are larger. In fact, if we were to increase the covariance from 0.026 to 0.26 (i.e. a correlation of 0.53 between gender and LRT), then the resulting simulations suggest that we would then need a sample size of around 1000 for a power of 0.8.

Perhaps more importantly, the inclusion of the LRT predictor in the model has changed our hypothesis so that we are now investigating the effect of gender on progress made between ages 11 to 16, rather than simply unadjusted attainment at age 16; since this change results in reduced estimates, we now need a larger sample size.

2.2.4 A note on sample sizes for multiple hypotheses, and using sample size calculations as 'rough guides'

This example illustrates several important factors when constructing sample size calculations. Firstly, each hypothesis will have a unique sample size calculation. So, even though we found that a very small sample is required to show the significant relationship between the response and LRT, the same data are to be used to show a significant relationship between the response and gender, and so our chosen sample size will need to satisfy all our hypotheses. Secondly, in this section we have used existing data – in fact the true tutorial dataset – to estimate parameter values, and so we have been able to establish, for example, that there is a reduction in the effect of gender when we include LRT in the model. This illustrates that when conducting our power calculation, it is important to replicate exactly what we expect to happen in our data collection. However, this is easier said than done. This is why sample size calculations can be thought of as a rough guide: in practice, it might be best to treat them with some caution and scale them up to cover factors such as over-optimism in effect sizes, missing variables, and so on. In addition, if we were to switch to a one-sided test, then this would decrease our sample sizes, whereas if we were to choose a power of 0.9, then this would increase our sample sizes.

2.2.5 Using RIGLS

Up to this point we have focussed solely on the IGLS method in the MLwiN package. This is because when fitting models in MLwiN, most people use IGLS. This is because it gives maximum likelihood (ML) estimates and therefore allows likelihood ratio tests to be used when comparing models. In terms of single-level normal models, we do have a bit of a dilemma, since, typically, general purpose statistical software packages output unbiased standard errors for coefficients. These coefficients are equivalent to restricted maximum likelihood (REML) estimates, as used in the RIGLS estimation method. This difference amounts to changing the divisor in the formula for estimating the residual variance from n in the ML estimate, to n-p in the REML estimate, where p is the number of fitted parameters. This will only have a big impact when n is sufficiently small, and in these cases the fact that we are assuming a normal distribution, rather than a t distribution, is also a problem.

In Section 2.2.2 we encountered an example where this would make a difference; there we looked at sample sizes for estimating the effect of LRT (the London Reading Test score indicator). We can repeat this analysis using RIGLS estimation simply by changing our selection, when prompted in MLPowSim, of the estimation method from a 1 to a 0. If we do this, and run the resulting macros in MLwiN, we get the following:

	Samplesize(10)	zpow0(10)	zpow1(10)	spow0(10)	spow1(10)
1	5.000	0.054	0.361	0.025	0.241
2	10.000	0.046	0.548	0.025	0.526
3	15.000	0.027	0.723	0.025	0.753
4	20.000	0.024	0.862	0.025	0.881
5	25.000	0.026	0.931	0.025	0.944
6	30.000	0.031	0.951	0.025	0.974
7	35.000	0.030	0.981	0.025	0.989
8	40.000	0.019	0.988	0.025	0.995
9	45.000	0.030	0.996	0.025	0.998
10	50.000	0.025	0.998	0.026	0.999

For comparison, in the column headed 'spow1' for the IGLS method the first three power estimates are 0.369, 0.619 and 0.810, respectively, and so we see that for very small n, the power can be very different. However, we still come to a similar conclusion that for a power of 0.8, we would need a sample of between 15 and 20 pupils.

2.2.6 Using MCMC estimation

MCMC estimation is another alternative estimation approach available in MLwiN (see Browne, 2003, for details). Later we will see that when we encounter cross-classified models, we turn to MCMC estimation to work out power calculations in MLwiN. One problem with MCMC estimation, however, is its speed, as it is far slower than the IGLS method. This is because it is an iterative procedure, and so for each simulated dataset, the method needs to be run for a large number of iterations. So for example if we require 1,000 simulations per setting and choose to run MCMC for a burn-in of 1,000 iterations and store the following 5,000 iterations we will in effect run for 6 million iterations per setting! This means that it is not desirable to use the MCMC method for many of the examples illustrated here, unless you intend to use MCMC to fit your model in practice (for example, for non-normal responses, where MCMC estimation has some advantages over the classical methods).

At this stage, we will simply illustrate MCMC estimation in the case of the simple example given in Chapter 1, in which we estimated power for a 1-sample mean problem. The MLPowSim program will create MLwiN macro code that utilises MCMC with the MLwiN default prior distributions: improper normal priors for fixed effects and $\Gamma^{-1}(\varepsilon,\varepsilon)$ for variances (with inverse Wishart priors for variance matrices). For the starting values, MCMC uses the IGLS estimates for the fixed effect parameters and the values simulated for the variances to avoid any zero starting values. In multilevel models (unlike running MCMC in MLwiN normally, i.e. from the menu), the residual starting values are not taken from IGLS, and so the method may need to burn in for longer.

The MCMC method requires the user to input both a burn-in length, and main run length, that will be used for each simulated dataset. In calculating the power we can use both the 0/1 approach, and the SE approach (as described in Sections 1.4.1 &

1.4.2), simply by taking the posterior means and standard deviations for each simulated dataset. Here, though, another approach is also available, namely a non-parametric 0/1 method, where for each parameter the chain of stored values is sorted, and the value of the appropriate quantile is calculated from this sorted chain. The sign of this value can then be evaluated to decide if the credible interval contains zero or not. So, when selecting MCMC estimation in MLPowSim, and running the resulting macros in MLwiN, power estimates from *three* different methods are produced. Here we show the relevant MLPowSim inputs for MCMC estimation, using the example from Chapter 1:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **1**
Please input the random number seed: **1**
Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **2**
Please input burnin length for each simulation: **1000**
Please input main run length for each simulation : **5001**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **0**

Sample size set up

Please input the smallest sample size : **20**
Please input the largest sample size : **500**
Please input the step size: **20**

Parameter estimates

Please input estimate of beta_0: **-0.140**

Please input estimate of sigma^2_e: **1.051**

Files to perform power analysis for the 1 level model with the following sample criterion have been created
Sample size starts at 20 and finishes at 500 with the step size 20
1000 simulations for each sample size combination will be performed

Press any key to continue…

Here we see that we have selected a burn-in of 1000 iterations to allow the chains for each model to settle down, and then a main run of 5001 iterations from which we will obtain our power estimates. Note we use 5001, rather than 5000, for ease of calculation of quantiles. The macros take a while to run in MLwiN (approximately 43 minutes on my machine) and if one selects columns c210, c211, c231 and c421 to view in the **View/Edit Data** window, the results can be seen as follows:

Data

goto line 1 | view | Help | Font | Show value labels

	Samplesize(25)	zpow0(25)	spow0(25)	mpow0(25)
1	20.000	0.081	0.083	0.080
2	40.000	0.133	0.134	0.128
3	60.000	0.182	0.182	0.178
4	80.000	0.249	0.229	0.243
5	100.000	0.277	0.276	0.276
6	120.000	0.310	0.320	0.309
7	140.000	0.349	0.363	0.350
8	160.000	0.392	0.406	0.398
9	180.000	0.429	0.448	0.444
10	200.000	0.478	0.489	0.485
11	220.000	0.527	0.525	0.536
12	240.000	0.590	0.561	0.603
13	260.000	0.603	0.596	0.612
14	280.000	0.619	0.628	0.636
15	300.000	0.665	0.659	0.668
16	320.000	0.669	0.688	0.676
17	340.000	0.715	0.714	0.726
18	360.000	0.721	0.737	0.726
19	380.000	0.731	0.759	0.737
20	400.000	0.781	0.781	0.786
21	420.000	0.805	0.801	0.811
22	440.000	0.798	0.818	0.809
23	460.000	0.853	0.836	0.861
24	480.000	0.844	0.851	0.848
25	500.000	0.849	0.864	0.853

Note that the three methods of estimating power give similar results, and the estimates for power are broadly similar to those using IGLS. In addition, for small sample sizes, the power from MCMC is systematically smaller than that for IGLS; again, this is due to the bias of ML variance estimates.

2.2.7 Using R

Whilst RIGLS and MCMC estimation are not offered in MLPowSim when producing output for R (as opposed to producing output for MLwiN), power calculations for the various models we have discussed above can be performed in R, using the default estimation method of iteratively reweighted least squares (IWLS; see Section 1.5 for

notes on both this, and on running the outputted code in R). For illustrative purposes, here we present the results of a power calculation conducted in R for the model we studied in Section 2.2.1 (testing differences between the two genders, treating the predictor as binary):[4]:

n	zLb0	**zpb0**	zUb0	sLb0	**spb0**	sUb0	zLb1	**zpb1**	zUb1	sLb1	**spb1**	sUb1
50	0.085	**0.107**	0.129	0.09	**0.091**	0.092	0.106	**0.13**	0.154	0.123	**0.124**	0.126
100	0.121	**0.146**	0.171	0.141	**0.142**	0.144	0.172	**0.2**	0.228	0.207	**0.209**	0.211
150	0.168	**0.196**	0.224	0.192	**0.193**	0.195	0.253	**0.285**	0.317	0.291	**0.293**	0.295
200	0.208	**0.238**	0.268	0.239	**0.241**	0.243	0.335	**0.369**	0.403	0.368	**0.371**	0.373
250	0.262	**0.294**	0.326	0.289	**0.291**	0.293	0.413	**0.448**	0.483	0.443	**0.446**	0.448
300	0.308	**0.342**	0.376	0.335	**0.337**	0.34	0.497	**0.532**	0.567	0.512	**0.514**	0.516
350	0.35	**0.384**	0.418	0.382	**0.384**	0.387	0.574	**0.609**	0.644	0.576	**0.578**	0.581
400	0.418	**0.453**	0.488	0.428	**0.43**	0.432	0.615	**0.649**	0.683	0.634	**0.636**	0.638
450	0.448	**0.483**	0.518	0.47	**0.473**	0.475	0.665	**0.698**	0.731	0.685	**0.687**	0.69
500	0.485	**0.52**	0.555	0.51	**0.513**	0.515	0.723	**0.754**	0.785	0.73	**0.732**	0.734
550	0.513	**0.548**	0.583	0.549	**0.551**	0.553	0.747	**0.777**	0.807	0.77	**0.771**	0.773
600	0.542	**0.577**	0.612	0.588	**0.59**	0.593	0.763	**0.792**	0.821	0.806	**0.808**	0.809
650	0.565	**0.6**	0.635	0.622	**0.624**	0.626	0.793	**0.82**	0.847	0.836	**0.838**	0.839
700	0.616	**0.65**	0.684	0.653	**0.655**	0.657	0.87	**0.892**	0.914	0.862	**0.863**	0.864
750	0.648	**0.681**	0.714	0.683	**0.685**	0.687	0.85	**0.874**	0.898	0.884	**0.885**	0.886
800	0.655	**0.688**	0.721	0.711	**0.713**	0.715	0.862	**0.885**	0.908	0.903	**0.904**	0.905
850	0.677	**0.709**	0.741	0.737	**0.739**	0.741	0.905	**0.924**	0.943	0.92	**0.921**	0.921
900	0.732	**0.762**	0.792	0.761	**0.763**	0.765	0.919	**0.936**	0.953	0.933	**0.934**	0.935
950	0.777	**0.805**	0.833	0.782	**0.784**	0.785	0.945	**0.959**	0.973	0.944	**0.945**	0.945
1000	0.807	**0.833**	0.859	0.803	**0.805**	0.806	0.939	**0.954**	0.969	0.954	**0.954**	0.955
1050	0.783	**0.811**	0.839	0.822	**0.824**	0.825	0.935	**0.95**	0.965	0.962	**0.963**	0.963
1100	0.833	**0.858**	0.883	0.84	**0.841**	0.843	0.957	**0.969**	0.981	0.969	**0.969**	0.97
1150	0.853	**0.876**	0.899	0.856	**0.857**	0.858	0.975	**0.984**	0.993	0.975	**0.975**	0.975
1200	0.843	**0.867**	0.891	0.87	**0.871**	0.872	0.974	**0.983**	0.992	0.979	**0.979**	0.98
1250	0.869	**0.891**	0.913	0.883	**0.884**	0.885	0.971	**0.981**	0.991	0.983	**0.983**	0.983
1300	0.885	**0.906**	0.927	0.894	**0.895**	0.896	0.993	**0.997**	1	0.986	**0.986**	0.986
1350	0.889	**0.909**	0.929	0.904	**0.905**	0.906	0.98	**0.988**	0.996	0.988	**0.989**	0.989
1400	0.886	**0.907**	0.928	0.915	**0.916**	0.917	0.984	**0.991**	0.998	0.991	**0.991**	0.991
1450	0.893	**0.913**	0.933	0.923	**0.924**	0.925	0.978	**0.986**	0.994	0.992	**0.992**	0.993
1500	0.905	**0.924**	0.943	0.932	**0.933**	0.934	0.986	**0.992**	0.998	0.994	**0.994**	0.994

Here we see the sample size indicated in the column on the far left, with the power estimates (together with upper and lower bounds) of the intercept and the predictor in the remaining columns, for each method of power calculation. As discussed in Section 1.5.1, 'z' and 's' denote the zero/one and standard error methods, respectively, whilst 'p', 'L' and 'U' denote the power estimate, and the lower and upper bounds, respectively, whilst 'b0' and 'b1' denote the intercept (β_0) and predictor (β_1). The results indicate that sampling around 600 pupils should provide a power of 0.8 for the gender predictor (columns 'zpb1' and 'spb1'). These findings are very similar to the results we found earlier when using MLwiN (Section 2.2.1), although performing the above power calculation in R is computationally more expensive (taking approximately 9 minutes (for R) versus a minute or so (for MLwiN) on my machine).

[4] Note that to aid the reader, we have widened the spaces between columns relating to different predictors/methods, and have formatted the power estimates in bold.

2.3 Variance Components and Random Intercept Models

We now turn our attention to multilevel data, as this is one of the chief motivations in writing MLPowSim. This is because apart from simple cases, such as those described in Sections 2.3.1 and 2.3.2, when we move to multilevel modelling, standard sample size formulae do not exist. In Section 2.3.1 we will discuss a specific formula – the design effect formula – that can be used for scaling up sample sizes in variance components models to account for clustering; we will compare results from that formula with MLPowSim. In Section 2.3.2 we will discuss the PINT modelling software that can be used to fit (balanced) two-level nested models, and will again compare results between PINT and MLPowSim.

Before we begin, however, please note that in this section we are considering random intercepts models – i.e. models that can be written as follows:

$$y_{ij} = X_{ij}^T \beta + u_j + e_{ij}, u_j \sim N(0, \sigma_u^2), e_{ij} \sim N(0, \sigma_e^2)$$

where j indexes clusters (schools, in our example) and i indexes units within clusters (pupils, in our example). We also assume that the u_j and the e_{ij} are independent, and we have J clusters with the jth cluster containing n_j units.

2.3.1 The Design Effect formula

In the case of a model where we test just a mean against some known constant (as described in the introductory chapter), but with clustering in the data (i.e. a variance components model) and balance in the clusters (i.e. $n_j=n^C$ for all j), there is a simple scaling formula that can be used.

The design effect formula requires an estimate of ρ, the intra-class correlation. This is a measure of how much correlation exists within clusters. If we initially work out a required sample size without accounting for clustering, then to subsequently account for clustering we need to multiply by the **Design effect = 1 + (n^C-1)ρ** where n^C is the cluster size.

To see this in practice, we will return to the introductory example in which we estimated sample sizes to show that boys do significantly worse at age 16 than average, with a power of 0.8. The tutorial dataset consists of 65 schools with 4059 pupils in total, leaving an average cluster sample size of 62, but 60% of these pupils are, on average, girls and so we will now consider a (balanced) analysis where we take samples of between 10 and 60 boys from each school and we visit between 10 and 50 schools. When we look at the model fitted to all the boys in the tutorial dataset (accounting for clustering) we get an estimate of -0.177. The estimates of the level 1 and level 2 variances are 0.916 and 0.151, respectively.

If we assume a total variance of 0.916+0.151 = 1.067, we can then repeat our calculations from Section 2.1.1 to give:

$$\gamma = 2.802SE(\gamma)$$

$$\rightarrow 0.177 = 2.802 \times \frac{\sqrt{1.067}}{\sqrt{n}} \rightarrow \sqrt{n} = \frac{2.89}{0.177} = 16.352$$

$$\rightarrow n = 267.4$$

which, due to the increased parameter estimate, is smaller than in Chapter 1. With the design effect formula we can now work out total sample sizes required for clusters of sizes 10 to 60. Note that ρ has the formula:

$$\rho = \frac{\sigma_u^2}{\sigma_u^2 + \sigma_e^2} = \frac{0.151}{1.067} = 0.142 \text{ in our example.}$$

Cluster size	Design formula	Total sample size	Number of clusters
10	2.278	610	61
20	3.698	989	50
30	5.118	1369	46
40	6.538	1749	44
50	7.958	2128	43
60	9.378	2508	42

We will now show how to fit this model using MLPowSim to confirm that it gives similar sample sizes. Below, we show how to set up this model (to generate output for MLwiN):

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **2**
Please input the random number seed: **1**
Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **0**

Sample size set up

Please input the smallest number of units for the second level: **10**
Please input the largest number of units for the second level: **50**
Please input the step size for the second level: **10**
Please input the smallest number of units for the first level per second level: **10**
Please input the largest number of units for the first level per second level: **60**
Please input the step size for the first level per second level: **10**

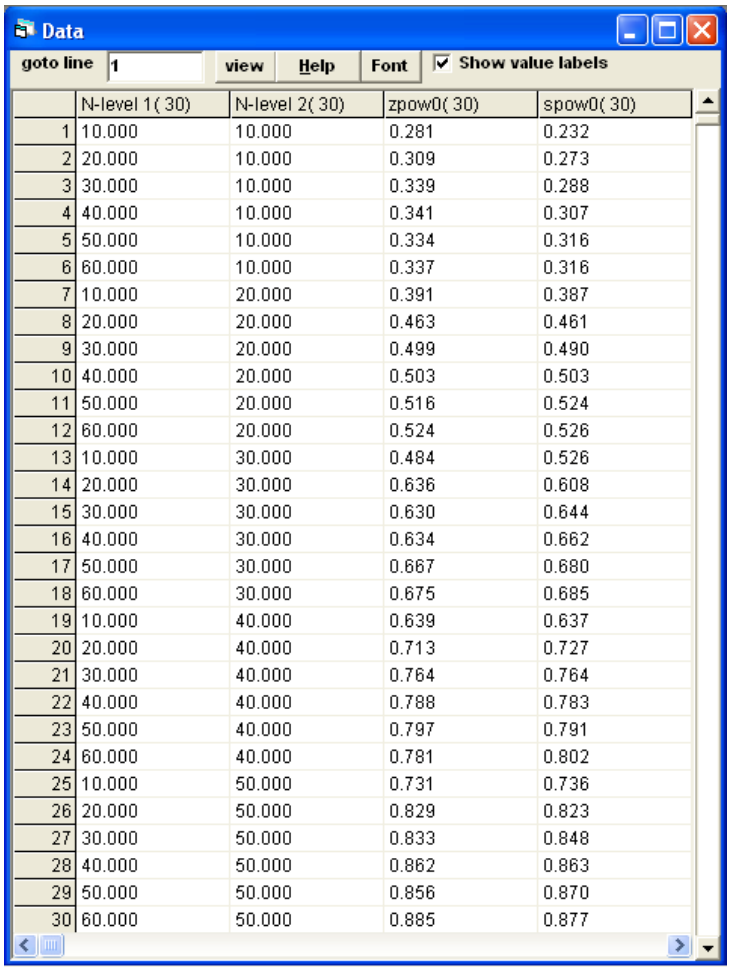
Parameter estimates

Please input estimate of beta_0: **-0.177**
Please input estimate of sigma^2_u: **0.151**
Please input estimate of sigma^2_e: **0.916**

Files to perform power analysis for the 2 level nested model with the following sample criterion have been created
Sample size in the first level starts at 10 and finishes at 60 with the step size 10
Sample size in the second level starts at 10 and finishes at 50 with the step size 10
1000 simulations for each sample size combination will be performed

Press any key to continue…

If we run the macros in MLwiN, we can view the following results via the **View or edit data** menu option:



	N-level 1(30)	N-level 2(30)	zpow0(30)	spow0(30)
1	10.000	10.000	0.281	0.232
2	20.000	10.000	0.309	0.273
3	30.000	10.000	0.339	0.288
4	40.000	10.000	0.341	0.307
5	50.000	10.000	0.334	0.316
6	60.000	10.000	0.337	0.316
7	10.000	20.000	0.391	0.387
8	20.000	20.000	0.463	0.461
9	30.000	20.000	0.499	0.490
10	40.000	20.000	0.503	0.503
11	50.000	20.000	0.516	0.524
12	60.000	20.000	0.524	0.526
13	10.000	30.000	0.484	0.526
14	20.000	30.000	0.636	0.608
15	30.000	30.000	0.630	0.644
16	40.000	30.000	0.634	0.662
17	50.000	30.000	0.667	0.680
18	60.000	30.000	0.675	0.685
19	10.000	40.000	0.639	0.637
20	20.000	40.000	0.713	0.727
21	30.000	40.000	0.764	0.764
22	40.000	40.000	0.788	0.783
23	50.000	40.000	0.797	0.791
24	60.000	40.000	0.781	0.802
25	10.000	50.000	0.731	0.736
26	20.000	50.000	0.829	0.823
27	30.000	50.000	0.833	0.848
28	40.000	50.000	0.862	0.863
29	50.000	50.000	0.856	0.870
30	60.000	50.000	0.885	0.877

Looking at the power estimates we see that with 40 schools (see the column headed ‘N-level 2’), only a cluster size of 60 produces a power around 0.8, but for 50 schools

we have all bar cluster size 10 producing a power above 0.8; this corresponds to the design effect table where the required number of schools for the various cluster sizes is between 40 and 50 for cluster sizes greater than 10.

2.3.2 PINT

The PINT program (Bosker, Snijders and Guldemond, 2003) calculates Power IN Two-level designs and is available at http://stat.gamma.rug.nl/snijders/. PINT takes user input detailing the proposed design, including effect sizes and anticipated variabilities, and for a range of sample sizes, both for the clusters and within clusters, it gives standard error estimates for the fixed effect parameters in the model. The mathematics that it uses to construct its approximation to the standard errors can be found in Snijders and Bosker (1993). It is very fast for the models it fits, as it is simply deriving matrix formulae, but it has some limitations: for example, it only deals with normal response models with equal-sized (balanced) clusters and only one set of clusters.

We will compare the results we get from MLPowSim to PINT in the remaining examples in this section.

2.3.3 Multilevel two sample t-test example

We earlier studied power calculations pertaining to the hypothesis that girls did better than boys, and we saw in Section 2.2.1 how to test this hypothesis with independent samples of girls and boys. We now look at what happens when the girls and boys are clustered together in schools. We will again use the tutorial dataset example to get hold of our parameter estimates. For this model, the tutorial example gives estimates of the intercept and female effects of -0.161 and 0.262, respectively (note in the one-level case, these were -0.140 and 0.234), and the split of the variability is 0.161 at school level with 0.839 left as residual variability.

We will consider two methods of describing the variability in the predictor variable of gender. Firstly, as in Section 2.2.1, we will assume a normal approximation to the Binomial with probability of 0.6 of being a girl, with a mean of 0.6 and a variance of 0.24. Secondly, we will take account of clustering by assuming the variability is split into 0.12 between schools, with 0.12 left as residual variability. In reality, the tutorial dataset has some single sex schools which can explain this clustering, and which we will examine in Section 2.3.4.

Below, we give details of the MLPowSim inputs which have changed from previously:

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**

How many explanatory variables do you want to include in your model? **1**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **2**
Assuming normality, please input its parameters here:
The mean of the predictor x1: **0.6**
The variance of the predictor x1 at level 1: **0.24**
The variance of the predictor x1 at level 2: **0**
Do you want the coefficient associated with explanatory variable x1 to be random (1=YES 0=NO) ? **0**

Sample size set up

Please input the smallest number of units for the second level: **10**
Please input the largest number of units for the second level: **50**
Please input the step size for the second level: **10**
Please input the smallest number of units for the first level per second level: **10**
Please input the largest number of units for the first level per second level: **60**
Please input the step size for the first level per second level: **10**

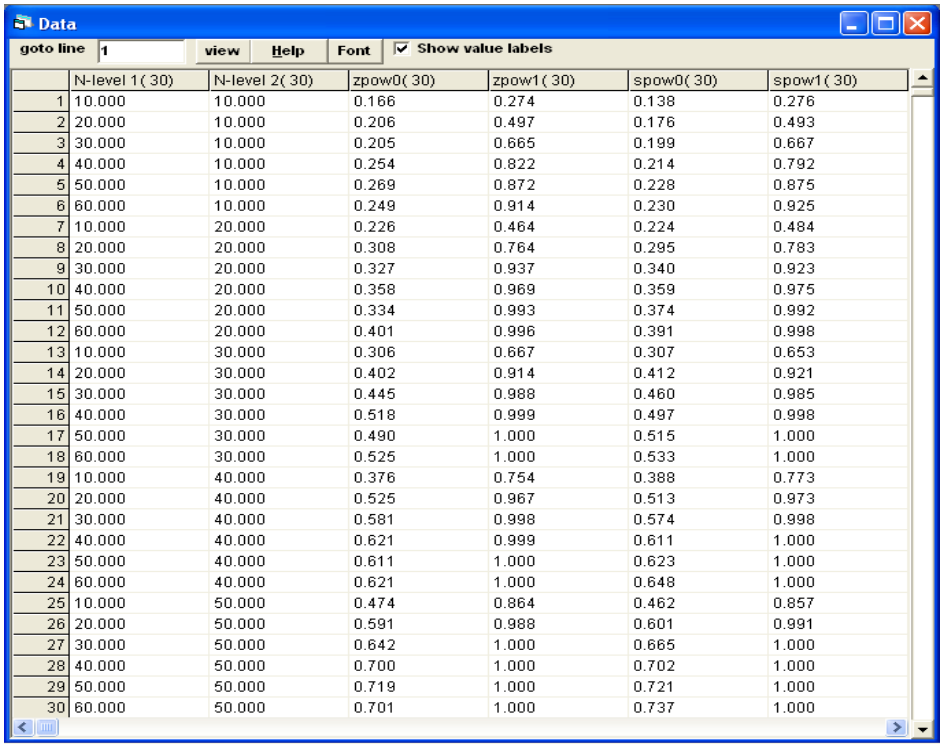
Parameter estimates

Please input estimate of beta_0: **-0.161**
Please input estimate of beta_1: **0.262**
Please input estimate of sigma^2_u: **0.161**
Please input estimate of sigma^2_e: **0.839**

Files to perform power analysis for the 2 level nested model with the following sample criterion have been created
Sample size in the first level starts at 10 and finishes at 60 with the step size 10
Sample size in the second level starts at 10 and finishes at 50 with the step size 10
1000 simulations for each sample size combination will be performed

Press any key to continue…

If we run the macros in MLwiN, and look at the following six columns in the View Data window, we see the following:


Data

goto line 1 | view | Help | Font | Show value labels

	N-level 1(30)	N-level 2(30)	zpow0(30)	zpow1(30)	spow0(30)	spow1(30)
1	10.000	10.000	0.166	0.274	0.138	0.276
2	20.000	10.000	0.206	0.497	0.176	0.493
3	30.000	10.000	0.205	0.665	0.199	0.667
4	40.000	10.000	0.254	0.822	0.214	0.792
5	50.000	10.000	0.269	0.872	0.228	0.875
6	60.000	10.000	0.249	0.914	0.230	0.925
7	10.000	20.000	0.226	0.464	0.224	0.484
8	20.000	20.000	0.308	0.764	0.295	0.783
9	30.000	20.000	0.327	0.937	0.340	0.923
10	40.000	20.000	0.358	0.969	0.359	0.975
11	50.000	20.000	0.334	0.993	0.374	0.992
12	60.000	20.000	0.401	0.996	0.391	0.998
13	10.000	30.000	0.306	0.667	0.307	0.653
14	20.000	30.000	0.402	0.914	0.412	0.921
15	30.000	30.000	0.445	0.988	0.460	0.985
16	40.000	30.000	0.518	0.999	0.497	0.998
17	50.000	30.000	0.490	1.000	0.515	1.000
18	60.000	30.000	0.525	1.000	0.533	1.000
19	10.000	40.000	0.376	0.754	0.388	0.773
20	20.000	40.000	0.525	0.967	0.513	0.973
21	30.000	40.000	0.581	0.998	0.574	0.998
22	40.000	40.000	0.621	0.999	0.611	1.000
23	50.000	40.000	0.611	1.000	0.623	1.000
24	60.000	40.000	0.621	1.000	0.648	1.000
25	10.000	50.000	0.474	0.864	0.462	0.857
26	20.000	50.000	0.591	0.988	0.601	0.991
27	30.000	50.000	0.642	1.000	0.665	1.000
28	40.000	50.000	0.700	1.000	0.702	1.000
29	50.000	50.000	0.719	1.000	0.721	1.000
30	60.000	50.000	0.701	1.000	0.737	1.000

Here the interesting thing is that if we look at 'zpow1' or 'spow1', then the power values obtained for equal-sized designs (for example 10 schools with 60 students, 20 schools with 30 students and 30 schools with 20 students) are approximately equal at 0.92 (note numbers of students and schools are stored as 'N-level 1' and 'N-level 2', respectively). This is not the case for the intercepts, where the power goes up from around 0.24 for 10 schools with 60 students, to around 0.4 for 30 schools with 20 students. This is because in a random intercept model, the clustering is only affecting the overall response and not the relationship with predictor variables. It appears here that a sample size somewhere between 400 and 500, regardless of clustering, will result in a power of 0.8; this is smaller than in Section 2.2.1, but this will be mainly due to the increase in the gender estimate we are using (0.262 instead of 0.234). To illustrate, if we consider the one-level calculation with the new gender estimate and total variability, we see that indeed the estimated sample size would be between 400 and 500, since

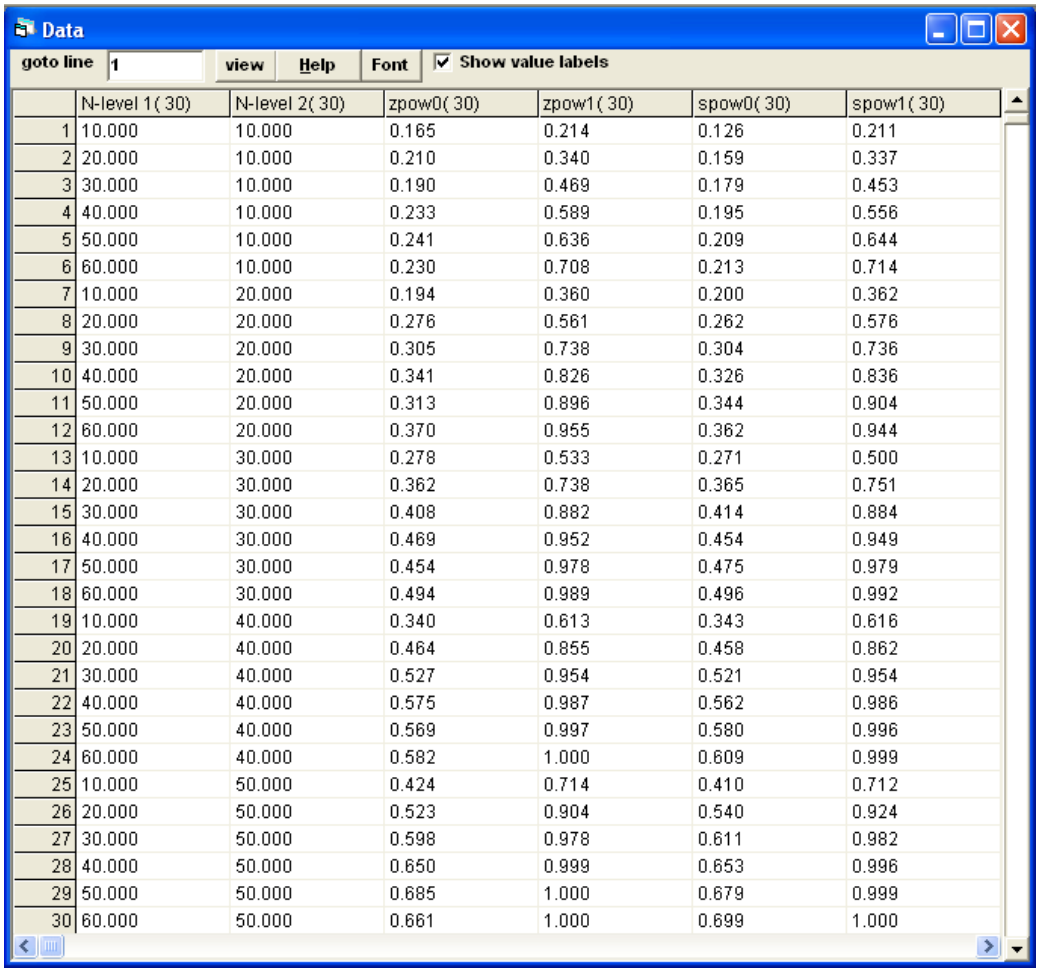
$$\gamma = 2.802 SE(\gamma)$$
$$\rightarrow 0.262 = 2.802 \times \sqrt{\sigma^2 / 0.4n + \sigma^2 / 0.6n}$$
$$\rightarrow 0.262 = 2.802 \times \sqrt{1/0.24n}$$
$$\rightarrow n = (2.802/0.262)^2 \times 1/0.24 = 476.6$$

This method of calculating the sample size is, of course, not appropriate here, and it transpires that when we fix the number of schools to 50 then a power of 0.8 is achieved somewhere between 8 and 9 pupils per school, which is smaller than the 477 obtained here. However, what we are illustrating is the fact that it is not *necessarily* true that accounting for a clustered design, as in a variance components model, automatically requires a larger sample size.

If we now consider the effect of changing the variability of the predictor so that it is split between the 2 levels, we will need to rerun MLPowSim and change the following lines:

The variance of the predictor x1 at level 1: **0.12**
The variance of the predictor x1 at level 2: **0.12**

The rest of the inputs will be as before. Running this in MLwiN gives the following:



Data

goto line 1 | view | Help | Font | Show value labels

	N-level 1(30)	N-level 2(30)	zpow0(30)	zpow1(30)	spow0(30)	spow1(30)
1	10.000	10.000	0.165	0.214	0.126	0.211
2	20.000	10.000	0.210	0.340	0.159	0.337
3	30.000	10.000	0.190	0.469	0.179	0.453
4	40.000	10.000	0.233	0.589	0.195	0.556
5	50.000	10.000	0.241	0.636	0.209	0.644
6	60.000	10.000	0.230	0.708	0.213	0.714
7	10.000	20.000	0.194	0.360	0.200	0.362
8	20.000	20.000	0.276	0.561	0.262	0.576
9	30.000	20.000	0.305	0.738	0.304	0.736
10	40.000	20.000	0.341	0.826	0.326	0.836
11	50.000	20.000	0.313	0.896	0.344	0.904
12	60.000	20.000	0.370	0.955	0.362	0.944
13	10.000	30.000	0.278	0.533	0.271	0.500
14	20.000	30.000	0.362	0.738	0.365	0.751
15	30.000	30.000	0.408	0.882	0.414	0.884
16	40.000	30.000	0.469	0.952	0.454	0.949
17	50.000	30.000	0.454	0.978	0.475	0.979
18	60.000	30.000	0.494	0.989	0.496	0.992
19	10.000	40.000	0.340	0.613	0.343	0.616
20	20.000	40.000	0.464	0.855	0.458	0.862
21	30.000	40.000	0.527	0.954	0.521	0.954
22	40.000	40.000	0.575	0.987	0.562	0.986
23	50.000	40.000	0.569	0.997	0.580	0.996
24	60.000	40.000	0.582	1.000	0.609	0.999
25	10.000	50.000	0.424	0.714	0.410	0.712
26	20.000	50.000	0.523	0.904	0.540	0.924
27	30.000	50.000	0.598	0.978	0.611	0.982
28	40.000	50.000	0.650	0.999	0.653	0.996
29	50.000	50.000	0.685	1.000	0.679	0.999
30	60.000	50.000	0.661	1.000	0.699	1.000

Here we see (by looking at ‘zpow1’) that increasing the number of schools for a fixed sample size increases power. For example, 10 schools each with 20 pupils has a power of 0.34, whilst 20 schools each with 10 pupils has a power of 0.36. The effect in this example is rather small but what is more impressive is the effect on the overall sample size required. We now see that to get a power of 0.8, we would need nearly 800 pupils, as opposed to the estimate of between 400 and 500 we found when we didn’t account for the variability between the gender ratios in schools.

We will now confirm these findings with PINT.

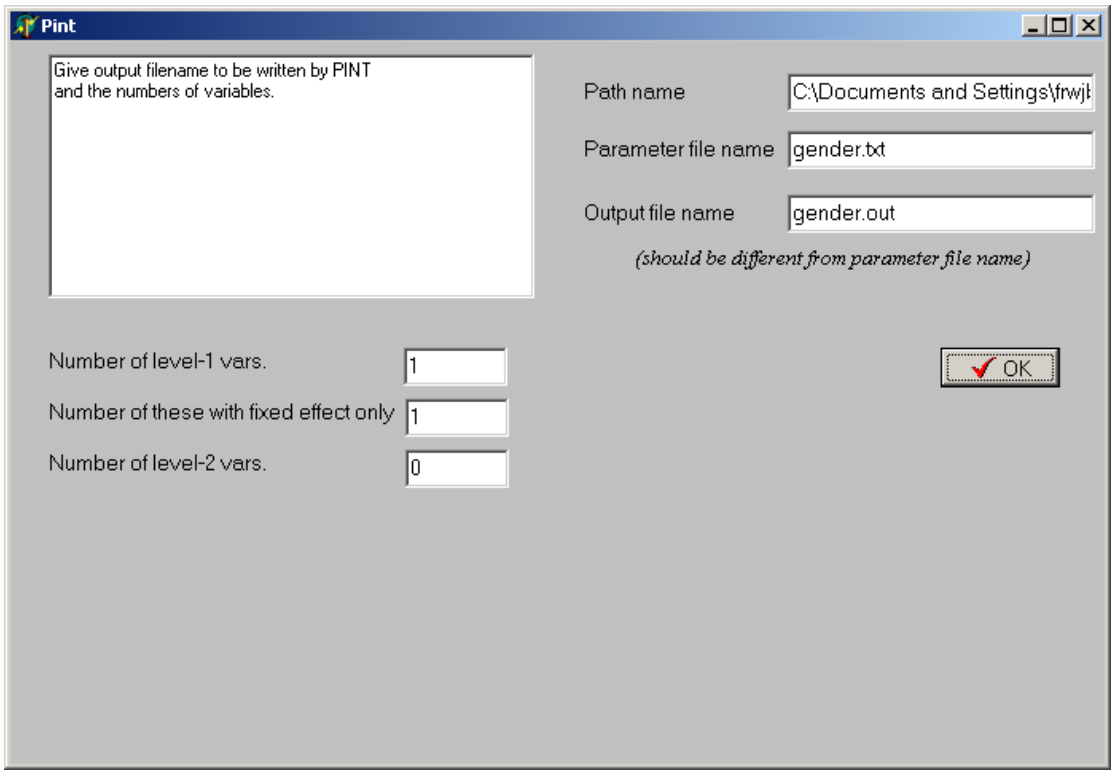
PINT requires a text file as input, containing all the information about the design we are interested in. For the example that contains all the variability in gender at level 1 we need to create a text file as follows:

```
1     1     0
10    -10     60
10     50
0.839
0.161
0.24
0.0
0.6
```

Here we have, in order:

1 for the number of level 1 predictors (in this case gender);
1 for the number of level 1 predictors that are not also random effects;
0 for the number of level 2 predictors;
10 for the smallest number of level 1 units per level 2 unit;
-10 for the step size at level 1;
60 for the largest number of level 1 units per level 2 unit;
10 for the smallest number of level 2 units;
50 for the largest number of level 2 units (note a step size of 2 is chosen here automatically);
0.839 for the level 1 variance;
0.161 for the level 2 variance;
0.24 for the level 1 variance associated with the predictor (gender);
0 for the level 2 variance associated with the predictor (gender);
0.6 for the mean of the gender predictor.

As PINT only calculates the standard errors, the fixed effect estimates are not required as inputs. Loading up PINT (version 2.11) we are first asked for the input file in a dialogue box, and then are greeted by a screen as follows:



Clicking on the OK button will result in many windows appearing, each asking the user to confirm (or change) the inputs. If you click on OK at each prompt, PINT will run and store the output in a file named *gender.out* (assuming you have named the input text file *gender.txt*, as we have).

The file *gender.out* contains a large amount of background information on the input settings before giving a table of standard error estimates. We show this for every combination with the number of clusters as a multiple of 10 to save some space:

```
The following table contains the standard errors (s.e.):
Fixed:   s.e. of regr. coeff.s of level-1 variables with a fixed
effect only.
Const:   s.e. of the intercept.
```

Sample sizes			Standard errors	
N*n	N	n	Fixed	Const
100	10	10	0.18697	0.19255
200	20	10	0.13221	0.13615
300	30	10	0.10795	0.11117
400	40	10	0.09349	0.09627
500	50	10	0.08362	0.08611
200	10	20	0.13221	0.16306
400	20	20	0.09349	0.11530
600	30	20	0.07633	0.09414
800	40	20	0.06610	0.08153
1000	50	20	0.05913	0.07292
300	10	30	0.10795	0.15196
600	20	30	0.07633	0.10745
900	30	30	0.06232	0.08773
1200	40	30	0.05397	0.07598
1500	50	30	0.04828	0.06796
400	10	40	0.09349	0.14610
800	20	40	0.06610	0.10330
1200	30	40	0.05397	0.08435
1600	40	40	0.04674	0.07305
2000	50	40	0.04181	0.06534
500	10	50	0.08362	0.14246
1000	20	50	0.05913	0.10073
1500	30	50	0.04828	0.08225
2000	40	50	0.04181	0.07123
2500	50	50	0.03739	0.06371
600	10	60	0.07633	0.13999
1200	20	60	0.05397	0.09898
1800	30	60	0.04407	0.08082
2400	40	60	0.03817	0.06999
3000	50	60	0.03414	0.06260

We can now use these output standard errors to convert into an equivalent power. We have to do this by hand as this is not done explicitly by the PINT software.

We earlier had the formula

$$\frac{\gamma}{SE(\gamma)} = Z_{1-\alpha/2} + Z_{1-\beta}$$

$$\rightarrow Z_{1-\beta} = \frac{\gamma}{SE(\gamma)} - Z_{1-\alpha/2}$$

for our example we have

$$Z_{1-\beta} = \frac{0.262}{SE(\gamma)} - 1.96$$

and so for each of the standard errors given in the 4th column of the above outcome we can use the above formula and look up the power in the normal tables. For a power of 0.8 we find we require a standard error of 0.0935, or less, in this example. Looking at the PINT column we see that this value would occur at around 400 pupils in total,

as we observed in MLPowSim. We can also see in the PINT output that, for all designs with exactly 400 pupils, the same standard error and hence the same power is obtained for the gender predictor. This was suggested earlier, and MLPowSim appears to give this result (with some Monte Carlo error), but the PINT approximate standard errors are identical for each scenario.

We can also look at the second scenario where we have the variance of the gender predictor split between the two levels.
The PINT input file is now as follows:

```
1     1     0
10   -10    60
10    50
0.839
0.161
0.12
0.12
0.6
```

If we run this input file in PINT, we can again look at the output standard errors:

```
The following table contains the standard errors (s.e.):
Fixed:   s.e. of regr. coeff.s of level-1 variables with a fixed
effect only.
Const:   s.e. of the intercept.


    Sample sizes      Standard errors

    N*n      N      n     Fixed   Const
    100     10     10   0.22820 0.20794
    200     20     10   0.16136 0.14703
    300     30     10   0.13175 0.12005
    400     40     10   0.11410 0.10397
    500     50     10   0.10205 0.09299
    200     10     20   0.17021 0.17528
    400     20     20   0.12035 0.12394
    600     30     20   0.09827 0.10120
    800     40     20   0.08510 0.08764
   1000     50     20   0.07612 0.07839
    300     10     30   0.14248 0.16188
    600     20     30   0.10075 0.11447
    900     30     30   0.08226 0.09346
   1200     40     30   0.07124 0.08094
   1500     50     30   0.06372 0.07239
    400     10     40   0.12519 0.15440
    800     20     40   0.08852 0.10918
   1200     30     40   0.07228 0.08914
   1600     40     40   0.06260 0.07720
   2000     50     40   0.05599 0.06905
    500     10     50   0.11304 0.14959
   1000     20     50   0.07993 0.10578
   1500     30     50   0.06526 0.08637
   2000     40     50   0.05652 0.07480
   2500     50     50   0.05055 0.06690
    600     10     60   0.10388 0.14623
```

```
1200    20    60    0.07345 0.10340
1800    30    60    0.05997 0.08443
2400    40    60    0.05194 0.07311
3000    50    60    0.04646 0.06540
```

Here we see that – as with MLPowSim – the standard errors, and hence power associated with the sample sizes, does depend on the design, and for equivalent total numbers of pupils the greater the number of schools the smaller the standard error and the larger the power. Looking for a standard error of 0.0935 or smaller we see that this occurs when we have 40 pupils in 20 schools, 20 pupils in 40 schools, and so on, as we found with MLPowSim.

We will occasionally compare our results from MLPowSim with those from PINT in later examples, but as this is a book about MLPowSim our coverage of PINT will be brief. If the reader requires more information regarding PINT, there is a user's guide available from http://stat.gamma.rug.nl/snijders/ which provides further details.

2.3.4 Higher level predictor variables

Continuing with our topic of the effect of gender on exam score, we saw in the last example that differential sex ratios between schools had an impact on our sample size calculation. In fact we saw an ICC for gender of 0.5: i.e. 50% of the variability between "pupil's gender" is due to schools. This is partly due to the large numbers of single sex schools in the tutorial dataset. In the MLwiN User's Manual they study another hypothesis concerning the effect of single sex school attendance, as it appears that such pupils do better, in general, than pupils in a mixed school.

Here we will test a version of this hypothesis to demonstrate how to use MLPowSim with predictors at the cluster (school) level. In the tutorial dataset there is a categorical variable *school gender* which takes 3 values: mixed schools, boys' schools and girls' schools. As the current version of MLPowSim only deals with continuous and binary variables, and in fact the effects of boys' schools and girls' schools are similar in magnitude, we will create a version of this predictor that purely differentiates between mixed and single-sex schools. Note that in Chapter 5, we will revisit this as an example of how to modify the macros produced by MLPowSim to deal with categorical predictors at higher levels.

We fitted a model with this predictor to the tutorial dataset and the result was estimates of -0.101 for the intercept (mixed schools) and 0.193 for the single-sex schools predictor. The model had estimates of 0.159 and 0.848 for level 2 and residual (level 1) variances, respectively. Of the 65 schools in the dataset, we have 30 single sex schools, but to express the variable as a level 2 predictor we (currently) have to convert this to a continuous variable with mean 30/65 = 0.462, and variance (0.462)*(1-0.462) = 0.249.

We will use these numbers to set up an MLPowSim scenario. For illustration, we will assume a constant 40 pupils per school, and then vary the number of schools.
After choosing a balanced 2-level model, and the usual numbers of simulations, and the usual random seed and significance level, we enter the following inputs when prompted:

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**
How many explanatory variables do you want to include in your model? **1**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **2**
Assuming normality, please input its parameters here:
The mean of the predictor x1: **0.462**
The variance of the predictor x1 at level 1: **0**
The variance of the predictor x1 at level 2: **0.249**
Do you want the coefficient associated with explanatory variable x1 to be random (1=YES 0=NO) ? **0**

Sample size set up

Please input the smallest number of units for the second level: **10**
Please input the largest number of units for the second level: **200**
Please input the step size for the second level: **10**
Please input the smallest number of units for the first level per second level: **40**
Please input the largest number of units for the first level per second level: **40**
Please input the step size for the first level per second level: **10**

Parameter estimates

Please input estimate of beta_0: **-0.101**
Please input estimate of beta_1: **0.193**
Please input estimate of sigma^2_u: **0.159**
Please input estimate of sigma^2_e: **0.848**

Files to perform power analysis for the 2 level nested model with the following sample criterion have been created
Sample size in the first level starts at 10 and finishes at 200 with the step size 10
Sample size in the second level starts at 40 and finishes at 40 with the step size 10
1000 simulations for each sample size combination will be performed

Press any key to continue…

If we run the macro code produced in MLwiN, we will get the following output in the View/Edit Data window:

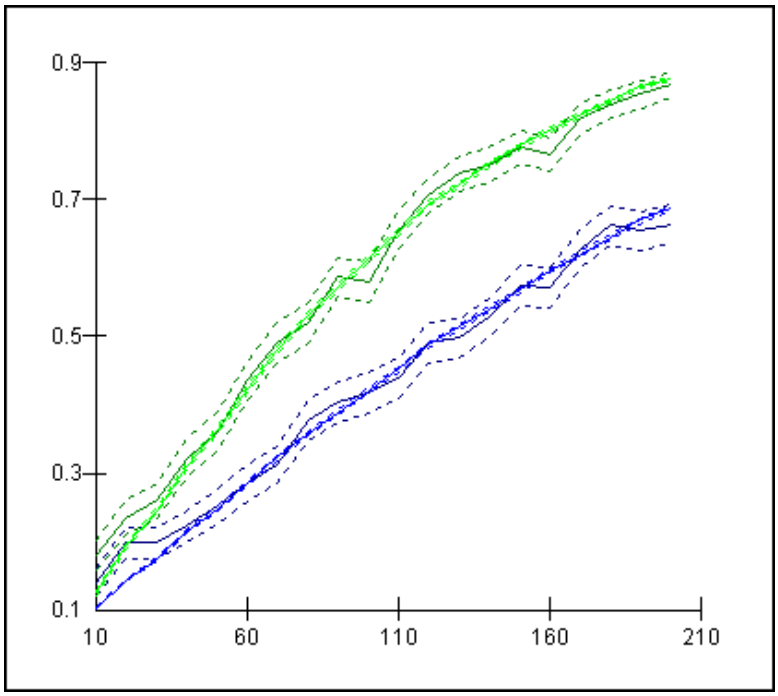
Data

goto line 1 | view | Help | Font | Show value labels

	N-level 1(20)	N-level 2(20)	zpow0(20)	zpow1(20)	spow0(20)	spow1(20)
1	40.000	10.000	0.123	0.164	0.084	0.107
2	40.000	20.000	0.183	0.222	0.126	0.178
3	40.000	30.000	0.183	0.249	0.160	0.233
4	40.000	40.000	0.208	0.313	0.201	0.300
5	40.000	50.000	0.240	0.355	0.236	0.357
6	40.000	60.000	0.275	0.432	0.274	0.420
7	40.000	70.000	0.304	0.491	0.314	0.478
8	40.000	80.000	0.371	0.522	0.352	0.532
9	40.000	90.000	0.400	0.591	0.383	0.576
10	40.000	100.000	0.414	0.583	0.417	0.619
11	40.000	110.000	0.436	0.663	0.449	0.660
12	40.000	120.000	0.489	0.715	0.486	0.703
13	40.000	130.000	0.497	0.749	0.514	0.732
14	40.000	140.000	0.528	0.762	0.541	0.764
15	40.000	150.000	0.578	0.789	0.571	0.791
16	40.000	160.000	0.574	0.779	0.600	0.817
17	40.000	170.000	0.635	0.834	0.626	0.839
18	40.000	180.000	0.670	0.856	0.652	0.861
19	40.000	190.000	0.662	0.871	0.678	0.882
20	40.000	200.000	0.672	0.886	0.697	0.895

Here we see that we need around 160 schools of size 40 to detect a single sex school effect which is more schools than are present in the real tutorial dataset! This is not very surprising, since in the real dataset the average pupils per school is larger, and the effect of single sex schools only has a *p*-value of 0.033 on a 1-sided test.

So far, we have not mentioned graphs in our discussion of multilevel models. As described in Section 1.4.3, to plot the power curves we need to execute the graphing macro file *graphs.txt* in MLwiN, and then view the resulting plot via **Customised graph(s)** from the **Graphs** menu. This will produce the following:



Note, by default the *graphs.txt* macro plots separate curves for each parameter, and estimation method, against column c210 ('N-level 2': the number of schools). This means that if we vary the number of pupils and the number of schools we will get a messy graph, but in this case, as we have fixed the number of pupils as 40 per school, this is not the case. Once again, we observe that the brighter curves, plotting results from the SE method, are much smoother than the 0/1 method.

We can compare our results with PINT. On this occasion, since the parameter estimate is 0.193, we are looking for a standard error of 0.0689 for a power of 0.8.

We will use the following input file:

```
 0     0     1
 40    -10    40
 10    150
 0.848
 0.159
  0.249
  0.462
```

which results in the following output file:

```
Sample sizes      Standard errors

    N*n      N      n    Const   Group
    400     10     40   0.18294 0.26902
    800     20     40   0.12936 0.19022
   1200     30     40   0.10562 0.15532
   1600     40     40   0.09147 0.13451
   2000     50     40   0.08181 0.12031
   2400     60     40   0.07468 0.10983
   2800     70     40   0.06914 0.10168
   3200     80     40   0.06468 0.09511
   3600     90     40   0.06098 0.08967
   4000    100     40   0.05785 0.08507
   4400    110     40   0.05516 0.08111
   4800    120     40   0.05281 0.07766
   5200    130     40   0.05074 0.07461
   5600    140     40   0.04889 0.07190
   6000    150     40   0.04723 0.06946
   6400    160     40   0.04573 0.06725
   6800    170     40   0.04437 0.06525
   7200    180     40   0.04312 0.06341
   7600    190     40   0.04197 0.06172
   8000    200     40   0.04091 0.06015
```

Here we see that around 160 schools results in the required reduction in standard error, as we found with MLPowSim.

2.3.5 A model with 3 predictors

So far we have looked at predictors in isolation, but as we saw in Section 2.2 for single level models, if we are interested in testing many hypotheses we might need to consider a model with many predictor variables. For the final model considered in this section we will look at three predictor variables: gender, school gender, and the London Reading Test (LRT) score. We have discussed the first two in this section already, and encountered the LRT when considering single level models (e.g. Section 2.2.2). Our hypotheses here will concern the effect of gender and school gender when accounting for intake ability, and conversely the effect of intake ability when accounting for gender and school gender.

If we fit a variance components model to the tutorial dataset with these three predictor variables, we will get the following:

$$\text{normexam}_{ij} \sim \text{N}(XB, \Omega)$$

$$\text{normexam}_{ij} = \beta_{0ij}\text{cons} + 0.166(0.033)\text{girl}_{ij} + 0.165(0.076)\text{single sex}_{j} + 0.560(0.012)\text{standlrt}_{ij}$$

$$\beta_{0ij} = -0.167(0.054) + u_{0j} + e_{0ij}$$

$$\begin{bmatrix} u_{0j} \end{bmatrix} \sim \text{N}(0, \Omega_u) \; : \; \Omega_u = \begin{bmatrix} 0.081(0.016) \end{bmatrix}$$

$$\begin{bmatrix} e_{0ij} \end{bmatrix} \sim \text{N}(0, \Omega_e) \; : \; \Omega_e = \begin{bmatrix} 0.562(0.013) \end{bmatrix}$$

$$-2*\textit{loglikelihood(IGLS Deviance)} = 9325.449(4059 \text{ of } 4059 \text{ cases in use})$$

Here we see for the real data that there are significant effects for all three predictor variables. As we discovered earlier for one-level models, the relationship of the response with LRT is particularly strong, and we need very small sample sizes to find a significant effect. In order to get accurate sample size estimates we require information about the variability (at both levels) and correlation between the predictors. To estimate these from the real data we could look at school means of the three predictors, and their variability and correlations. We could also look at fitting a multilevel multivariate model for the two predictors, gender and LRT, to get the within covariance matrix. In the inputs that follow, we will take estimates obtained from such an approach. Note that this will result in an assumed multivariate normal distribution for the predictors, which is an approximation for the binary variables. In Chapter 5 we discuss what may be a better approach of dealing with the school gender and gender predictors.

After choosing a balanced 2-level model, and the usual numbers of simulations, and the usual random seed and significance level, we enter the following inputs when prompted:

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**

Do you want to have a random intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**
How many explanatory variables do you want to include in your model? **3**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **3**
Assuming multivariate normality, please input its parameters here:
The mean of the predictor x1: **0.6**
The mean of the predictor x2: **0.462**
The mean of the predictor x3: **0**
The variance matrix of the predictors at level 1
The element [1,1] : **0.120**
The element [2,1] : **0**
The element [2,2] : **0**
The element [3,1] : **0.020**
The element [3,2] : **0**
The element [3,3] : **0.902**
The variance matrix of the predictors at level 2
The element [1,1] : **0.125**
The element [2,1] : **0.045**
The element [2,2] : **0.249**
The element [3,1] : **0.013**
The element [3,2] : **-0.006**
The element [3,3] : **0.116**
Do you want the coefficient associated with explanatory variable x1 to be random (1=YES 0=NO) ? **0**
Do you want the coefficient associated with explanatory variable x2 to be random (1=YES 0=NO) ? **0**
Do you want the coefficient associated with explanatory variable x3 to be random (1=YES 0=NO) ? **0**

Sample size set up

Please input the smallest number of units for the second level: **10**
Please input the largest number of units for the second level: **150**
Please input the step size for the second level: **10**
Please input the smallest number of units for the first level per second level: **40**
Please input the largest number of units for the first level per second level: **40**
Please input the step size for the first level per second level: **10**

Parameter estimates

Please input estimate of beta_0: **-0.167**
Please input estimate of beta_1: **0.166**
Please input estimate of beta_2: **0.165**
Please input estimate of beta_3: **0.560**
Please input estimate of sigma^2_u: **0.081**
Please input estimate of sigma^2_e: **0.562**

Files to perform power analysis for the 2 level nested model with the following sample criterion have been created
Sample size in the first level starts at 10 and finishes at 150 with the step size 10
Sample size in the second level starts at 40 and finishes at 40 with the step size 10
1000 simulations for each sample size combination will be performed

Press any key to continue…

This will create the macros needed to perform this simulation exercise in MLwiN. To run these macros takes a little longer than the earlier examples (around 7.5 minutes). If we run the macros and look at the **View/Edit Data** window with the following five columns chosen (i.e. only the number of schools and the powers from the SE method), we have:

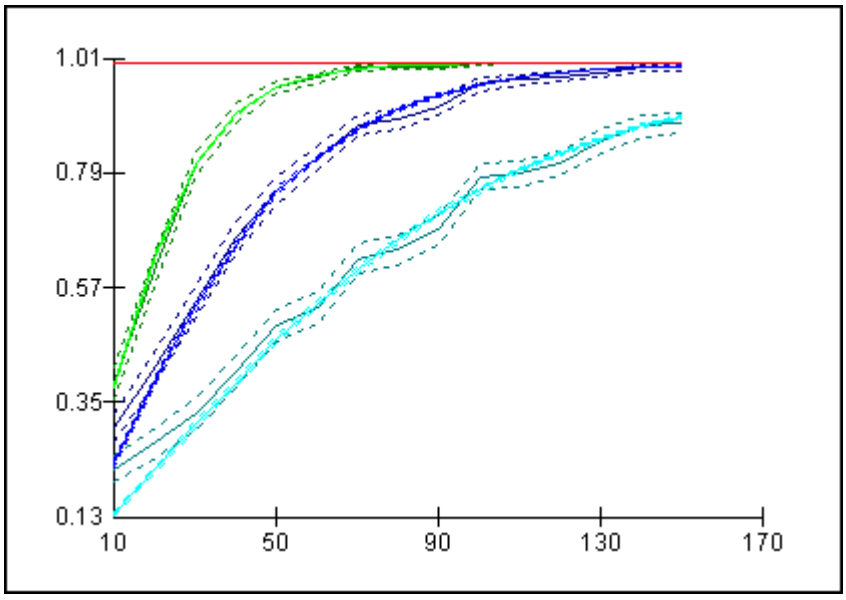
Data

goto line 1 view Help Font Show value labels

	N-level 2(15)	spow0(15)	spow1(15)	spow2(15)	spow3(15)
1	10.000	0.232	0.383	0.136	1.000
2	20.000	0.399	0.637	0.225	1.000
3	30.000	0.535	0.808	0.309	1.000
4	40.000	0.653	0.903	0.388	1.000
5	50.000	0.755	0.954	0.472	1.000
6	60.000	0.821	0.979	0.541	1.000
7	70.000	0.875	0.990	0.606	1.000
8	80.000	0.912	0.996	0.661	1.000
9	90.000	0.939	0.998	0.714	1.000
10	100.000	0.960	0.999	0.758	1.000
11	110.000	0.973	1.000	0.797	1.000
12	120.000	0.982	1.000	0.828	1.000
13	130.000	0.988	1.000	0.856	1.000
14	140.000	0.992	1.000	0.882	1.000
15	150.000	0.995	1.000	0.898	1.000

So here we see that to gain a power of 0.8 we need less than 10 schools for the LRT predictor ('spow3'), around 30 for the gender predictor ('spow1'), and between 110 and 120 for the school gender predictor ('spow2').

Again we can plot the power curves associated with the three predictors and the intercept, with the following results:



Here we see the intercept in dark blue, the gender effect in green, the school gender effect in cyan and the LRT predictor in red.

The PINT input code for this model is as follows:

```
2    2    1
```

```
40   -10    40
10   150
0.562
0.081
0.120
0.020 0.902
0.249
0.045 0.125
-0.006 0.013 0.116
0.6 0.0
0.462
```

which results in the following output:

```
Sample sizes      Standard errors

    N*n      N      n    Fixed   Fixed   Const   Group
    400     10     40   0.10136 0.03917 0.14280 0.19624
    800     20     40   0.07168 0.02770 0.10097 0.13876
   1200     30     40   0.05852 0.02262 0.08244 0.11330
   1600     40     40   0.05068 0.01959 0.07140 0.09812
   2000     50     40   0.04533 0.01752 0.06386 0.08776
   2400     60     40   0.04138 0.01599 0.05830 0.08012
   2800     70     40   0.03831 0.01481 0.05397 0.07417
   3200     80     40   0.03584 0.01385 0.05049 0.06938
   3600     90     40   0.03379 0.01306 0.04760 0.06541
   4000    100     40   0.03205 0.01239 0.04516 0.06206
   4400    110     40   0.03056 0.01181 0.04306 0.05917
   4800    120     40   0.02926 0.01131 0.04122 0.05665
   5200    130     40   0.02811 0.01086 0.03960 0.05443
   5600    140     40   0.02709 0.01047 0.03816 0.05245
   6000    150     40   0.02617 0.01011 0.03687 0.05067
```

Here the 4th column corresponds to gender, the 5th to LRT and the last to school gender. As we have different parameter estimates for each variable, for powers of 0.8 we require standard errors of 0.059, 0.200 and 0.059, respectively. Looking at the columns we see that these occur at around 30 schools for gender, with less than 10 schools for LRT and between 110 and 120 schools for school gender which agrees exactly with the results from MLPowSim!

Once you have figured out how to specify your model in PINT, and how to perform the post output translation from parameter estimates and standard errors to powers, it is clear that PINT is quicker than the simulation approach, but it is restricted to 2-level balanced models and to normal responses, neither of which restrictions exist with MLPowSim. We will briefly consider one of these restrictions in the next section.

2.3.6 The effect of balance

One of the features that PINT, in particular, relies on when constructing sample size calculations is that the nested design is balanced. Here we mean that we have the same number of level 1 units within each level 2 unit. This would seem a sensible strategy to adopt when collecting data, as there isn't usually a reason to pick more

level 1 units from specific clusters. In practice, though, things don't always pan out that way: for example, in an education setting, some of the pupils chosen in the sample may be absent on the day of the test, resulting in non-responses. It's also possible that, for some reason, a structured approach is adopted: for example, for some schools more pupils may be chosen than for other schools – perhaps certain school types are rarer and so we might wish to over-sample pupils from such schools, for instance. We will illustrate both these possibilities using the example we examined in Section 2.3.3, in which we compared boys' and girls' performance. There we saw that to have a power of 0.8 of detecting a positive effect on attainment for girls, we needed a sample size of nearly 800, assuming that the proportion of girls varied between schools. We will now investigate the impact of pupil non-response and structured sampling on this figure.

2.3.6.1 Pupil non-response

Here we will need to make several assumptions, firstly that non-response is at random and does not depend on (i) the exam response (ii) the gender of the pupils and (iii) the school they attend. We will also assume that the parameter estimates we used earlier (0.161 for the intercept, 0.262 for the gender predictor, and of variabilities 0.161 at level 2, and 0.839 at level 1) still hold. We might think that some of these assumptions could be incorrect, in particular the lack of a relationship between non-response and potential exam response. If so, we could adjust our simulation in some respect to account for this. For example, it's possible that the effect of greater numbers of low achievers dropping out might reduce variability in the response, might increase the intercept, and might reduce the gender effect, since more of the low achievers are boys and so more boys might be less likely to respond. However, for present purposes let us assume that the parameter estimates cited above are for the population who *did* respond and continue. We will now assume that we expect around 20% of pupils not to respond in the study.

The MLPowSim inputs are similar to those in Section 2.3.3, but are given in full here:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **3**
Please input the random number seed: **1**
Please input the significance level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**
How many explanatory variables do you want to include in your model? **1**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **2**
Assuming normality, please input its parameters here:
The mean of the predictor x1: **0.6**
The variance of the predictor x1 at level 1: **0.12**
The variance of the predictor x1 at level 2: **0.12**
Do you want the coefficient associated with explanatory variable x1 to be random (1=YES 0=NO) ? **0**

Sample size set up

Please input the smallest number of units for the second level: **10**
Please input the largest number of units for the second level: **50**
Please input the step size for the second level: **10**
Please choose one of the following scenarios for unbalance:
1: Binomial with the fixed trial and probability of non-response for first level nested in second
2: Fixed sample with your preference
Scenario type: **1**
Please enter your probability of non-response: **0.2**
Please input the smallest number of units for the first level per second level: **10**
Please input the largest number of units for the first level per second level: **60**
Please input the step size for the first level per second level: **10**

Parameter estimates

Please input estimate of beta_0: **-0.161**
Please input estimate of beta_1: **0.262**
Please input estimate of sigma^2_u: **0.161**
Please input estimate of sigma^2_e: **0.839**

Files to perform power analysis for the 2 level unbalanced nested model with the following sample criterion have been created
Sample size in the first level starts at 10 and finishes at 60 with the step size 10
Sample size in the second level starts at 10 and finishes at 50 with the step size 10
1000 simulations for each sample size combination will be performed

Press any key to continue…

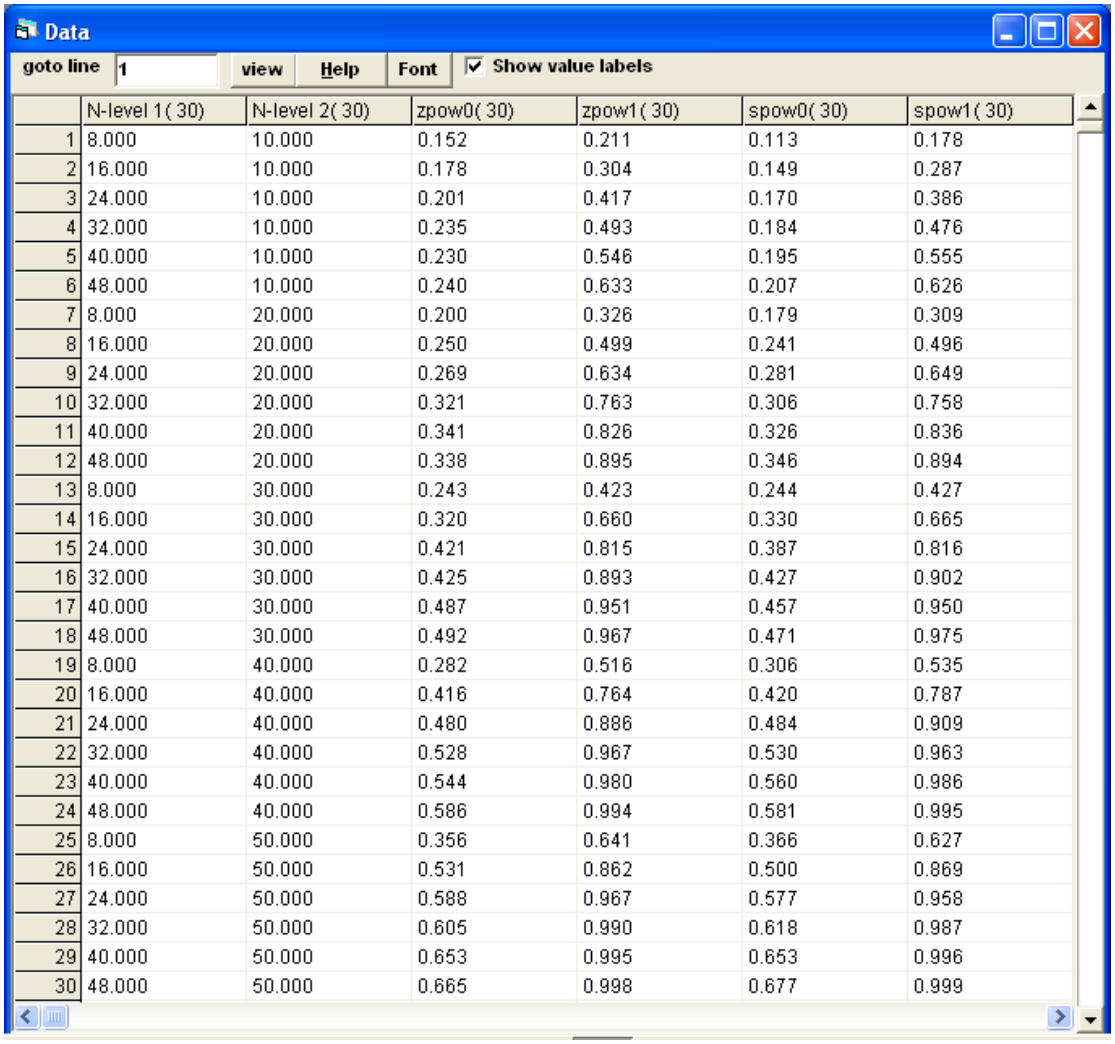
We can now run this scenario in MLwiN and look at the power estimates that it produces in the **View/Edit Data** window:

Data

goto line 1 | view | Help | Font | Show value labels

	N-level 1(30)	N-level 2(30)	zpow0(30)	zpow1(30)	spow0(30)	spow1(30)
1	10.000	10.000	0.155	0.204	0.113	0.179
2	20.000	10.000	0.186	0.315	0.149	0.289
3	30.000	10.000	0.176	0.363	0.168	0.386
4	40.000	10.000	0.232	0.462	0.187	0.478
5	50.000	10.000	0.209	0.541	0.195	0.554
6	60.000	10.000	0.236	0.617	0.206	0.627
7	10.000	20.000	0.199	0.307	0.180	0.311
8	20.000	20.000	0.246	0.497	0.240	0.500
9	30.000	20.000	0.299	0.647	0.284	0.649
10	40.000	20.000	0.310	0.760	0.307	0.757
11	50.000	20.000	0.341	0.821	0.328	0.838
12	60.000	20.000	0.345	0.896	0.342	0.895
13	10.000	30.000	0.242	0.434	0.245	0.430
14	20.000	30.000	0.374	0.655	0.331	0.666
15	30.000	30.000	0.376	0.816	0.388	0.814
16	40.000	30.000	0.428	0.892	0.421	0.901
17	50.000	30.000	0.488	0.948	0.455	0.950
18	60.000	30.000	0.496	0.977	0.472	0.975
19	10.000	40.000	0.326	0.568	0.305	0.536
20	20.000	40.000	0.423	0.779	0.422	0.788
21	30.000	40.000	0.484	0.900	0.484	0.909
22	40.000	40.000	0.525	0.956	0.528	0.964
23	50.000	40.000	0.556	0.986	0.562	0.986
24	60.000	40.000	0.570	0.995	0.588	0.995
25	10.000	50.000	0.348	0.629	0.365	0.625
26	20.000	50.000	0.480	0.865	0.499	0.869
27	30.000	50.000	0.566	0.958	0.571	0.957
28	40.000	50.000	0.642	0.984	0.617	0.987
29	50.000	50.000	0.625	0.999	0.653	0.996
30	60.000	50.000	0.673	0.998	0.678	0.999

Here we see that compared to the power estimates in Section 2.3.3, the values are reduced, as might be expected given the smaller actual sample size compared to the designed sample size. As we have a non-response probability of 0.2, we could consider the effect of looking at a sampling scheme with step sizes of 8 pupils per school as opposed to 10: i.e. 8, 16, 24, 32, 40 and 48 in a balanced model. If we do this by rerunning MLPowSim and MLwiN, we will get the following table of powers:



	N-level 1(30)	N-level 2(30)	zpow0(30)	zpow1(30)	spow0(30)	spow1(30)
1	8.000	10.000	0.152	0.211	0.113	0.178
2	16.000	10.000	0.178	0.304	0.149	0.287
3	24.000	10.000	0.201	0.417	0.170	0.386
4	32.000	10.000	0.235	0.493	0.184	0.476
5	40.000	10.000	0.230	0.546	0.195	0.555
6	48.000	10.000	0.240	0.633	0.207	0.626
7	8.000	20.000	0.200	0.326	0.179	0.309
8	16.000	20.000	0.250	0.499	0.241	0.496
9	24.000	20.000	0.269	0.634	0.281	0.649
10	32.000	20.000	0.321	0.763	0.306	0.758
11	40.000	20.000	0.341	0.826	0.326	0.836
12	48.000	20.000	0.338	0.895	0.346	0.894
13	8.000	30.000	0.243	0.423	0.244	0.427
14	16.000	30.000	0.320	0.660	0.330	0.665
15	24.000	30.000	0.421	0.815	0.387	0.816
16	32.000	30.000	0.425	0.893	0.427	0.902
17	40.000	30.000	0.487	0.951	0.457	0.950
18	48.000	30.000	0.492	0.967	0.471	0.975
19	8.000	40.000	0.282	0.516	0.306	0.535
20	16.000	40.000	0.416	0.764	0.420	0.787
21	24.000	40.000	0.480	0.886	0.484	0.909
22	32.000	40.000	0.528	0.967	0.530	0.963
23	40.000	40.000	0.544	0.980	0.560	0.986
24	48.000	40.000	0.586	0.994	0.581	0.995
25	8.000	50.000	0.356	0.641	0.366	0.627
26	16.000	50.000	0.531	0.862	0.500	0.869
27	24.000	50.000	0.588	0.967	0.577	0.958
28	32.000	50.000	0.605	0.990	0.618	0.987
29	40.000	50.000	0.653	0.995	0.653	0.996
30	48.000	50.000	0.665	0.998	0.677	0.999

Here we see that the results are very close to those from the non-response scenario. Of course, for this example we have chosen a non-response probability that corresponds in expectation to a whole number sample size per cluster, and it would have been quicker to use PINT to establish sample sizes. However, if the non-response probability had resulted in an average of 8.3 pupils per cluster, for instance, it would not have been possible to use PINT, although we could still have used PINT with sample sizes 8 per cluster and 9 per cluster, and then interpolated between the two.

2.3.6.2 Structured sampling

The other option available in MLPowSim is for the user to specify the number of clusters of each particular size. This might occur due to over-sampling specific clusters, or the user may simply wish to get estimates of power for specific datasets which are not balanced. We will consider the example in Section 2.3.6.1, and assume that 80% of clusters are of size 30, but the other 20% are of size 60. We will consider cases with 10, 20, 30, 40 and 50 schools.

The inputs will be almost the same as in Section 2.3.6.1, apart from where we specify the unbalanced structure, as follows:

Please choose one of the following scenarios for unbalance:
1: Binomial with the fixed trial and probability of non-response for first level nested in second
2: Fixed sample with your preference
Scenario type : **2**
Please choose how many distinct cluster sizes you want for second level units: **2**

Unbalanced set up inside the second level with 10 level 2 units
How many (from 1 to 10) groups do you want to be in the class 1? **8**
For class 1, please input the number of level 1 units: **30**
How many (from 2 to 2) groups do you want to be in the class 2? **2**
For class 2, please input the number of level 1 units: **60**

Unbalanced set up inside the second level with 20 level 2 units
How many (from 1 to 20) groups do you want to be in the class 1? **16**
For class 1, please input the number of level 1 units: **30**
How many (from 4 to 4) groups do you want to be in the class 2? **4**
For class 2, please input the number of level 1 units: **60**

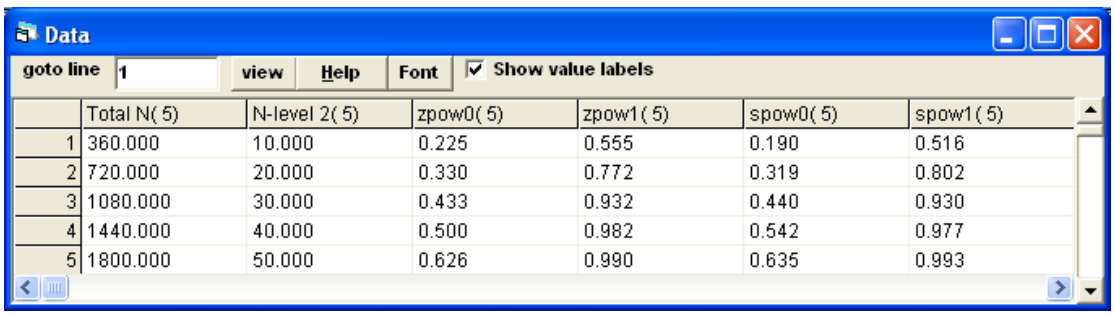
Unbalanced set up inside the second level with 30 level 2 units
How many (from 1 to 30) groups do you want to be in the class 1? **24**
For class 1, please input the number of level 1 units: **30**
How many (from 6 to 6) groups do you want to be in the class 2? **6**
For class 2, please input the number of level 1 units: **60**

Unbalanced set up inside the second level with 40 level 2 units
How many (from 1 to 40) groups do you want to be in the class 1? **32**
For class 1, please input the number of level 1 units: **30**
How many (from 8 to 8) groups do you want to be in the class 2? **8**
For class 2, please input the number of level 1 units: **60**

Unbalanced set up inside the second level with 50 level 2 units
How many (from 1 to 50) groups do you want to be in the class 1? **40**
For class 1, please input the number of level 1 units: **30**
How many (from 10 to 10) groups do you want to be in the class 2? **10**
For class 2, please input the number of level 1 units: **60**

The rest of the inputs are as before. As you can see, the procedure for inputting the model structure is relatively laborious, and we would not anticipate that this form of unbalanced design will be heavily-used in MLPowSim; however, the inputs only take a minute or two to type in, which is quicker than the macros take to run, so it is only a small overhead.

Running the resulting macros in MLwiN gives the following power estimates:



	Total N(5)	N-level 2(5)	zpow0(5)	zpow1(5)	spow0(5)	spow1(5)
1	360.000	10.000	0.225	0.555	0.190	0.516
2	720.000	20.000	0.330	0.772	0.319	0.802
3	1080.000	30.000	0.433	0.932	0.440	0.930
4	1440.000	40.000	0.500	0.982	0.542	0.977
5	1800.000	50.000	0.626	0.990	0.635	0.993

If we compare the powers produced here with those produced for the balanced design in Section 2.3.3, we can see that they lie somewhere between the powers for balanced

designs with 30 pupils per school and those with 40 pupils per school, as we might expect given our design has on average 36 pupils per school.

2.4 Random slopes/ Random coefficient models

Random intercept models are a special case of two-level model where the only relationship that is assumed different at the cluster level is the average effect or intercept in the model. The effect of predictors is assumed constant across clusters in a random intercept model. If we wish to allow for a different effect for a predictor in each cluster then we will fit a random slopes model, or random coefficients model. Note that the term 'slope' is generally reserved for continuous predictors where the coefficient associated with the predictor can be thought of as the slope of a predicted regression line. If such a regression were plotted for binary predictors, it would essentially join up the predictions for the two states of the predictor, and so 'random coefficient model' is a better term, meaning the effect of the binary predictor is different for different groups.

We could go through lots of examples of random coefficient models in this section, but we will limit ourselves to just one for brevity.

The tutorial dataset presents us with some problems when trying to find examples of random slopes models that follow on from our earlier investigations. Firstly, the gender predictor exhibits no significant between-school variability: i.e. the effect of gender doesn't vary across schools. This is possibly because many of the schools are single sex, and so can give no information on the effect of gender within them – in fact, the concept doesn't make sense in such schools. Secondly, the school gender predictor is a school-level predictor, and so cannot be treated as random at the school-level, and finally the LRT predictor is such a strong predictor that we will only need very small sample sizes regardless of any random slope.

We will therefore turn to a different example, again from an educational setting. Later on, we will investigate this example further when we look at cross-classified models. The example is used in the MLwiN User's Guide (Rasbash et al, 2004) to illustrate cross-classified modelling, and consists of exam scores for 3,435 secondary school pupils in Fife, Scotland. The response used is an attainment score for students at age 16, with the students nested within both primary school, and secondary school. For the purposes of our example, we will consider the primary school nesting which results in 3,435 pupils nested within 148 primary schools. We will again consider a gender predictor (*sex*), which in this case is also significant for the dataset, but also exhibits variability in effect between primary schools: i.e. the size of the effect of gender on attainment varies across schools.

The model fitted in MLwiN can be seen below:

$$\text{ATTAIN}_{ij} \sim \text{N}(XB,\ \Omega)$$
$$\text{ATTAIN}_{ij} = \beta_{0ij}\text{CONS} + \beta_{1j}\text{SEX}_{ij}$$
$$\beta_{0ij} = 5.370(0.116) + u_{0j} + e_{0ij}$$
$$\beta_{1j} = 0.495(0.107) + u_{1j}$$

$$\begin{bmatrix} u_{0j} \\ u_{1j} \end{bmatrix} \sim \text{N}(0,\ \Omega_u)\ :\ \Omega_u = \begin{bmatrix} 1.064(0.215) & \\ 0.109(0.140) & 0.180(0.166) \end{bmatrix}$$

$$\begin{bmatrix} e_{0ij} \end{bmatrix} \sim \text{N}(0,\ \Omega_e)\ :\ \Omega_e = \begin{bmatrix} 8.098(0.202) \end{bmatrix}$$

*-2*loglikelihood(IGLS Deviance)* = 17143.130(3435 of 3435 cases in use)

We will use these values as fixed effect estimates, and variance estimates, for the analysis that follows. We can also look at the variability in the predictor *sex,* assuming it is normally distributed. This can be done in MLwiN, producing:

$$\text{SEX}_{ij} \sim \text{N}(XB,\ \Omega)$$
$$\text{SEX}_{ij} = \beta_{0ij}\text{CONS}$$
$$\beta_{0ij} = 0.494(0.009) + u_{0j} + e_{0ij}$$

$$\begin{bmatrix} u_{0j} \end{bmatrix} \sim \text{N}(0,\ \Omega_u)\ :\ \Omega_u = \begin{bmatrix} 0.000(0.000) \end{bmatrix}$$

$$\begin{bmatrix} e_{0ij} \end{bmatrix} \sim \text{N}(0,\ \Omega_e)\ :\ \Omega_e = \begin{bmatrix} 0.250(0.006) \end{bmatrix}$$

*-2*loglikelihood(IGLS Deviance)* = 4985.648(3435 of 3435 cases in use)

So we see that MLwiN estimates no between-school variability in the ratio of boys to girls. Given this, we will assume a binomial distribution for the predictor with probability 0.494 of each pupil being a girl. We have on average 23 pupils per primary school, and so we will investigate sample sizes of 5, 10, 15, 20 and 25 within school, and numbers of schools ranging from 20 to 160, in steps of 20.

The inputs to MLPowSim are as follows:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**
Please choose model type
1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **2**
Please input the random number seed: **1**
Please input the significance level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**
How many explanatory variables do you want to include in your model? **1**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **1**
Please input probability of a 1 for x1 : **0.494**
Do you want the coefficient associated with explanatory variable x1 to be random (1=YES 0=NO) ? **1**

Sample size set up

Please input the smallest number of units for the second level: **20**
Please input the largest number of units for the second level: **100**
Please input the step size for the second level: **20**
Please input the smallest number of units for the first level per second level: **5**
Please input the largest number of units for the first level per second level: **25**
Please input the step size for the first level per second level: **5**

Parameter estimates

Please input estimate of beta_0: **5.370**
Please input estimate of beta_1: **0.495**
There is more than one random effect in your model and so you need to enter variance/covariance matrix.
Please input lower triangular entries (3 elements):
entry (1,1) is : **1.064**
entry (2,1) is : **0.109**
entry (2,2) is : **0.180**
Please input estimate of sigma^2_e: **8.098**

Files to perform power analysis for the 2 level nested model with the following sample criterion have been created
Sample size in the first level starts at 5 and finishes at 25 with the step size 5
Sample size in the second level starts at 20 and finishes at 100 with the step size 20
1000 simulations for each sample size combination will be performed

Press any key to continue…

This will set up the model. If we now run the macros in MLwiN, and focus on the columns for the gender predictor, we see the following:

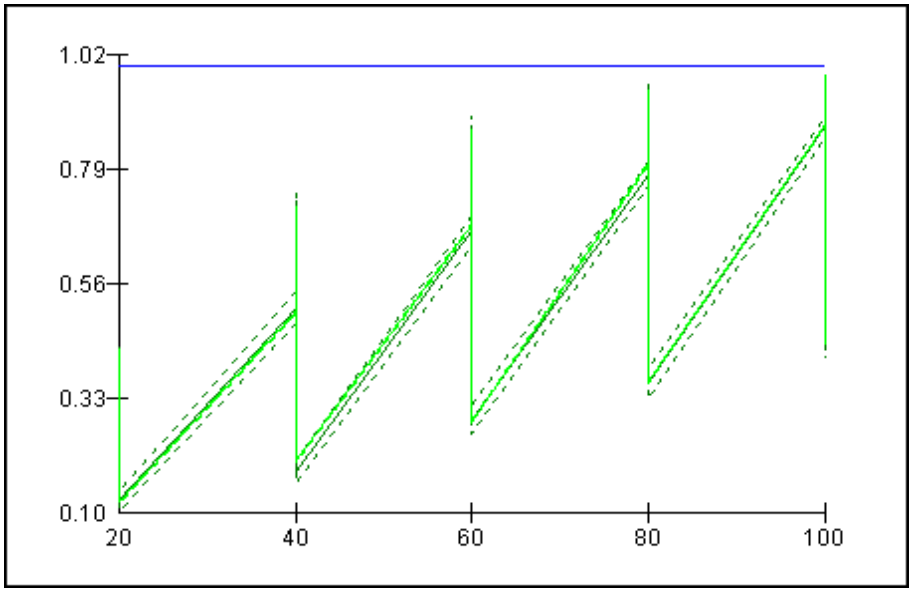
Data

goto line 1 | view | Help | Font | Show value labels

	N-level 1(25)	N-level 2(25)	zpow1(25)	spow1(25)
1	5.000	20.000	0.127	0.123
2	10.000	20.000	0.223	0.203
3	15.000	20.000	0.301	0.283
4	20.000	20.000	0.338	0.359
5	25.000	20.000	0.408	0.428
6	5.000	40.000	0.185	0.206
7	10.000	40.000	0.369	0.364
8	15.000	40.000	0.514	0.505
9	20.000	40.000	0.627	0.620
10	25.000	40.000	0.717	0.716
11	5.000	60.000	0.287	0.284
12	10.000	60.000	0.516	0.508
13	15.000	60.000	0.667	0.680
14	20.000	60.000	0.788	0.795
15	25.000	60.000	0.879	0.872
16	5.000	80.000	0.363	0.364
17	10.000	80.000	0.652	0.633
18	15.000	80.000	0.782	0.804
19	20.000	80.000	0.876	0.896
20	25.000	80.000	0.948	0.948
21	5.000	100.000	0.443	0.440
22	10.000	100.000	0.745	0.731
23	15.000	100.000	0.878	0.881
24	20.000	100.000	0.959	0.951
25	25.000	100.000	0.974	0.980

We see here that a power of greater than 0.8 is achieved by 25 pupils in 60 schools, 20 pupils in 80 schools, and 15 pupils in 100 schools. The power for 10 pupils in 100 schools is greater than that for 25 pupils in 40 schools, and so for the same total pupil number it is better to have more clusters with less pupils per cluster.

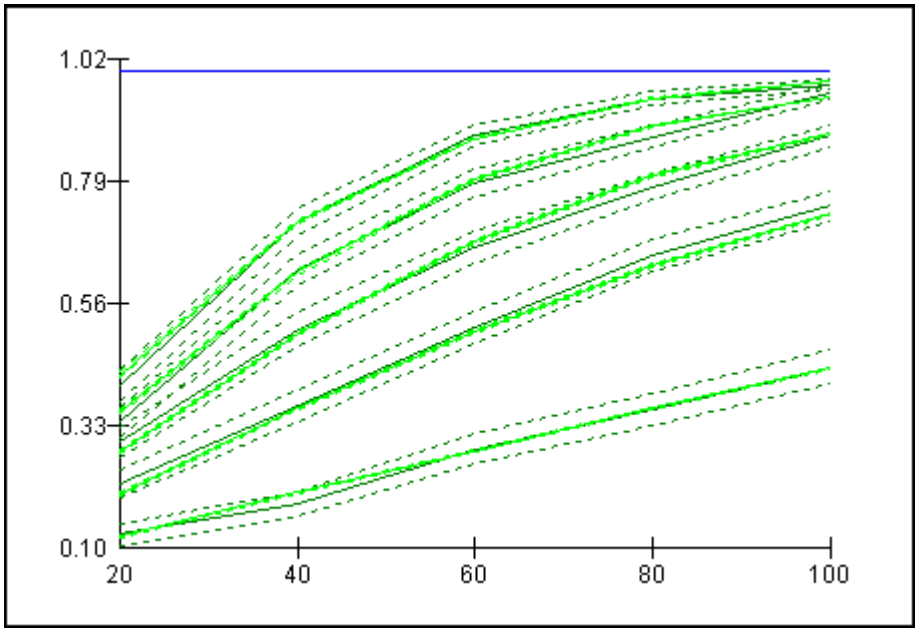
To plot the curves, we can execute the macro file *graphs.txt* (see Section 1.4.3); this produces the following graphs (via **Customised graph(s)** from the **Graphs** menu):



This graph is not correct because the grouping of pupils within schools has not been accounted for. To account for this we need to do the following:

In the **Customised graph** window select **ds#1** (may already be selected)
Now choose column **C209** from the **group** pull down list.
Next select **ds#2** by clicking on the c212 in the **Y** list
Again choose column **C209** from the **group** pull down list
Next select **ds#3** by clicking on the c231 in the **Y** list
Again choose column **C209** from the **group** pull down list
Finally select **ds#4** by clicking on the c232 in the **Y** list
Again choose column **C209** from the group pull down list
Now click on the **Apply** button to redraw graphs.

The graphs will now look as follows:



Here we have separate sets of lines for (from the bottom) 5 pupils per school, 10 pupils per school, and so on, up to 25 pupils per school.

We can compare results with those from a fitted model with no random slopes. A random intercepts model for the actual data has the following estimates:

$$\text{ATTAIN}_{ij} \sim \text{N}(XB,\ \Omega)$$
$$\text{ATTAIN}_{ij} = \beta_{0ij}\text{CONS} + 0.503(0.099)\text{SEX}_{ij}$$
$$\beta_{0ij} = 5.368(0.120) + u_{0j} + e_{0ij}$$

$$\begin{bmatrix} u_{0j} \end{bmatrix} \sim \text{N}(0,\ \Omega_u) \ :\ \Omega_u = \begin{bmatrix} 1.203(0.198) \end{bmatrix}$$

$$\begin{bmatrix} e_{0ij} \end{bmatrix} \sim \text{N}(0,\ \Omega_e) \ :\ \Omega_e = \begin{bmatrix} 8.144(0.200) \end{bmatrix}$$

*-2*loglikelihood(IGLS Deviance)* = 17146.150(3435 of 3435 cases in use)

If we use these estimates to set up a simulation study in MLPowSim, we will get the results shown below in MLwiN. We can see that the designs with a power greater than 0.8 are 20 pupils in 60 schools, 15 pupils in 80 schools, and between 10 and 15 pupils in 100 schools. The power of the equivalent designs appears to reduce when we account for the random slopes, as we might expect. It also appears that having more schools, each with fewer pupils but maintaining the total pupil number, tends to be associated with reduced power. This is somewhat contrary to what one might expect, and may be due to the binary predictor having more chance of being constant in small clusters.

Data

goto line 1 | view | Help | Font | Show value labels

	N-level 1(25)	N-level 2(25)	zpow1(25)	spow1(25)
1	5.000	20.000	0.137	0.134
2	10.000	20.000	0.236	0.228
3	15.000	20.000	0.337	0.320
4	20.000	20.000	0.386	0.410
5	25.000	20.000	0.473	0.494
6	5.000	40.000	0.214	0.224
7	10.000	40.000	0.403	0.404
8	15.000	40.000	0.566	0.560
9	20.000	40.000	0.679	0.688
10	25.000	40.000	0.750	0.784
11	5.000	60.000	0.293	0.310
12	10.000	60.000	0.566	0.555
13	15.000	60.000	0.742	0.735
14	20.000	60.000	0.859	0.850
15	25.000	60.000	0.914	0.919
16	5.000	80.000	0.422	0.393
17	10.000	80.000	0.686	0.679
18	15.000	80.000	0.866	0.846
19	20.000	80.000	0.937	0.933
20	25.000	80.000	0.980	0.973
21	5.000	100.000	0.492	0.472
22	10.000	100.000	0.785	0.772
23	15.000	100.000	0.905	0.916
24	20.000	100.000	0.974	0.972
25	25.000	100.000	0.993	0.991

It is possible to fit random coefficient models in the PINT package. However, as a result of making the mathematics behind the approximate standard errors easier to calculate, PINT has some restrictions. In particular, all predictors treated as random coefficients must have mean zero. This makes sense for some predictors, where centering is probably a sensible modelling option, however for categorical predictors, e.g. gender, a centered gender indicator is rather a strange concept!

As we only have one predictor, then centering it will only change our estimate of the intercept, which we are not interested in, and which PINT does not require. It will also change the between-intercept variance and covariance at level 2, but we can re-evaluate these on the real data and then run PINT with the following input code:

```
1     0     0
5    -5    25
20    100
8.098
1.215
0.198 0.180
0.249964
```

The fixed effect estimate for gender is 0.495, which means we would like a standard error smaller than 0.495/2.802 = 0.177. PINT gives standard errors for all combinations of pupils and schools, with a step size for both of 5, so from the output file we can extract the appropriate sample sizes, as follows:

```
Sample sizes      Standard errors

    N*n      N      n     Const   Random
   1050     70     15   0.15833 0.18283
   1125     75     15   0.15296 0.17663
   1200     80     15   0.14811 0.17102
   1275     85     15   0.14369 0.16591
   1100     55     20   0.17162 0.18090
   1200     60     20   0.16431 0.17320
   1300     65     20   0.15787 0.16640
   1400     70     20   0.15212 0.16035
   1125     45     25   0.18493 0.18110
   1250     50     25   0.17544 0.17181
   1375     55     25   0.16727 0.16381
   1500     60     25   0.16015 0.15684
```

Here we see that for only 15 pupils per school we would need 75 schools, for 20 pupils per school we would need 60, and for 25 pupils per school we would need 50, which roughly corresponds to the results in MLPowSim, although any minor differences may be due to the approximation used in PINT, or to Monte Carlo standard errors in MLPowSim, or even the fact that in MLPowSim we assumed that the predictor was binomially-distributed rather than a normal approximation.

2.5 Three-level random effect models

2.5.1 Balanced 3-level models – The ILEA dataset

Here we continue with an education theme, and use as our example the ILEA dataset dating from 1985-1987, and consisting of exam results at 16 for three years of London secondary school children (see Nuttall et al., 1989). The subsample of the data that we have used to derive the effect sizes is large: 15,632 pupils from 304 cohorts in 139 schools (note some schools did not participate in all 3 years of the study). We therefore have a three-level structure with pupils nested within cohorts, nested within schools.

The response of interest is the total exam score based on grades achieved in all subjects summed together. This response takes values from 1 to 70. We look at two predictor variables: gender, and the proportion of pupils in the cohort eligible for free school meals (FSM). Both these predictors are very significant with this large sample size, but we are interested in whether (i) a smaller sampling scheme would have resulted in sufficient power, or more importantly (ii) if we were to attempt a similar data collection exercise today, using smaller samples (assuming broadly similar effects exist), what sample sizes would result in similar power?

Here we will use the estimates produced by this large dataset as a guide for what we might expect in our data collection exercise. The fixed effect estimates from the whole data are 21.535 for the intercept, 2.839 for the gender effect, and -6.039 for the FSM effect. We will therefore use the values 21.5, 3 and -6 in our simulations as estimated effect sizes: i.e. girls tend to do 3 grades better in total over their collection of exams than boys, while the difference between a school with no pupils eligible to FSM, and one with *all* FSM pupils, is 6 grades in total across each pupil's collection of exam results.

The variability is estimated as 12.174, 2.5 and 142.635, for between schools, between cohorts within schools, and residual variability, respectively. We will therefore use 12, 2.5 and 140 here. The gender predictor has mean 0.523 and variances 0.138, 0.001 and 0.116, respectively: so slightly more girls than boys, with slightly more variability between schools than within schools. However, we will assume for our study an average 50/50 split, and equal variance between schools and within cohorts (residual variability) i.e. variances of 0.125, 0, and 0.125, respectively. There doesn't appear to be a significant relationship between %FSM and gender, and the average proportion of FSM per cohort is 0.423, with variability split as 0.017 between schools and 0.09 between cohorts. So, for the purposes of our illustration, we will use the values 0.4 for the mean and 0.02, 0.01 and 0 for the variances, respectively, for %FSM and independence between the 2 predictors. In terms of sample size we will assume a similar 3-year study design, and so we will have 3 cohorts per school, and we will vary the numbers of schools (between 10 and 40), and pupils per cohort sampled (between 10 and 50).

The inputs for MLPowSim will then be as follows:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **4**
Please input the random number seed: **1**
Please input the significance level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept associated with the second level in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept associated with the third level in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**
How many explanatory variables do you want to include in your model? **2**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **2**
Assuming normality, please input its parameters here:
The mean of the predictor x1: **0.5**
The variance of the predictor x1 at level 1: **0.125**
The variance of the predictor x1 at level 2: **0**
The variance of the predictor x1 at level 3: **0.125**
Please choose a type for the predictor x2 (1=Binary 2=Continuous): **2**
Assuming normality, please input its parameters here:
The mean of the predictor x2: **0.4**
The variance of the predictor x1 at level 1: **0**
The variance of the predictor x1 at level 2: **0.01**
The variance of the predictor x1 at level 3: **0.02**

Do you want the coefficient associated with explanatory variable x1 to be random at level two (1=YES 0=NO) ? **0**
Do you want the coefficient associated with explanatory variable x2 to be random at level two (1=YES 0=NO) ? **0**
Do you want the coefficient associated with explanatory variable x1 to be random at level three (1=YES 0=NO) ? **0**
Do you want the coefficient associated with explanatory variable x2 to be random at level three (1=YES 0=NO) ? **0**

Sample size set up

Please input the smallest number of units for the third level: **10**
Please input the largest number of units for the third level: **40**
Please input the step size for the third level: **10**
Please input the smallest number of units for the second level per third level: **3**
Please input the largest number of units for the second level per third level: **3**

Please input the step size for the second level per third level: **1**
Please input the smallest number of units for the first level per second level: **10**
Please input the largest number of units for the first level per second level: **50**
Please input the step size for the first level per second level: **10**

Parameter estimates

Please input estimate of beta_0: **21.5**
Please input estimate of beta_1: **3**
Please input estimate of beta_2: **-6**
Please input estimate of the level 3 variance (sigma^2_v): **12**
Please input estimate of the level 2 variance (sigma^2_u): **2.5**
Please input estimate of sigma^2_e: **140**

Files to perform power analysis for the 3 level nested model with the following sample criterion have been created
Sample size in the first level starts at 10 and finishes at 50 with the step size 10
Sample size in the second level starts at 3 and finishes at 3 with the step size 1
Sample size in the third level starts at 10 and finishes at 30 with the step size 10
1000 simulations for each sample size combination will be performed

Press any key to continue…

We can run the macros produced in MLwiN in the usual way. Since we are only interested in the two predictors, and not the intercept, if we select the columns containing the sample size at each level, and the columns containing the power estimates for the two predictors (via the **View/Edit Data** window), we will see the following:

Data

goto line 1 | view | Help | Font | Show value labels

	N-level 3(20)	N-level 1(20)	N-level 2(20)	zpow1(20)	zpow2(20)	spow1(20)	spow2(20)
1	10.000	10.000	3.000	0.445	0.213	0.424	0.164
2	10.000	20.000	3.000	0.660	0.257	0.661	0.216
3	10.000	30.000	3.000	0.798	0.307	0.812	0.256
4	10.000	40.000	3.000	0.900	0.349	0.901	0.291
5	10.000	50.000	3.000	0.946	0.326	0.949	0.306
6	20.000	10.000	3.000	0.702	0.280	0.692	0.280
7	20.000	20.000	3.000	0.920	0.410	0.914	0.377
8	20.000	30.000	3.000	0.975	0.423	0.979	0.438
9	20.000	40.000	3.000	0.992	0.479	0.995	0.487
10	20.000	50.000	3.000	1.000	0.533	0.999	0.526
11	30.000	10.000	3.000	0.831	0.411	0.853	0.386
12	30.000	20.000	3.000	0.980	0.528	0.982	0.517
13	30.000	30.000	3.000	0.998	0.610	0.998	0.597
14	30.000	40.000	3.000	0.998	0.636	1.000	0.651
15	30.000	50.000	3.000	1.000	0.690	1.000	0.692
16	40.000	10.000	3.000	0.929	0.508	0.934	0.487
17	40.000	20.000	3.000	0.991	0.647	0.997	0.636
18	40.000	30.000	3.000	1.000	0.719	1.000	0.719
19	40.000	40.000	3.000	1.000	0.781	1.000	0.776
20	40.000	50.000	3.000	1.000	0.827	1.000	0.811

Here we see that for the gender predictor ('zpow1' & 'spow1') we do not need a particularly big design, with 10 schools ('N-level 3') with 3 cohorts of 30 pupils ('N-level 1'), or 20 schools with 3 cohorts between 10 and 20 both producing powers of around 0.8. However, for the proportion FSM predictor ('zpow2' & 'spow2'), which is a cohort-level predictor, we clearly need more schools, and we see that even with

30 schools with 50 pupils per cohort we do not reach a power of 0.8, whilst for 40 schools 50 pupils per cohort suffices to produce a power greater than 0.8.

MLPowSim is flexible enough to allow the numbers of units at all three levels to vary, and we have simply fixed the number of cohorts here to 3 as this represents our study design. As with 2-level modelling, MLPowSim can also allow any of the predictor variables to be treated random at higher levels for 3-level models as well, but we do not give examples of this here. We will, however, consider the options that exist for unbalanced 3-level models, and we turn to these in the following few sections.

2.5.2 Non-response at the first level in a 3-level design

We will consider here a scenario where individual pupils do not respond at random from our sample – for example, perhaps we constructed a sampling frame of students earlier in their schooling, and some students then moved school and so were not included in the final sample. We will use exactly the same inputs for parameter estimates as in Section 2.5.1, but will assume a non-response probability of 0.2, and will additionally consider 60 pupils per school to account, in part, for this non-response.

To investigate a non-balanced 3-level design we need to select option:

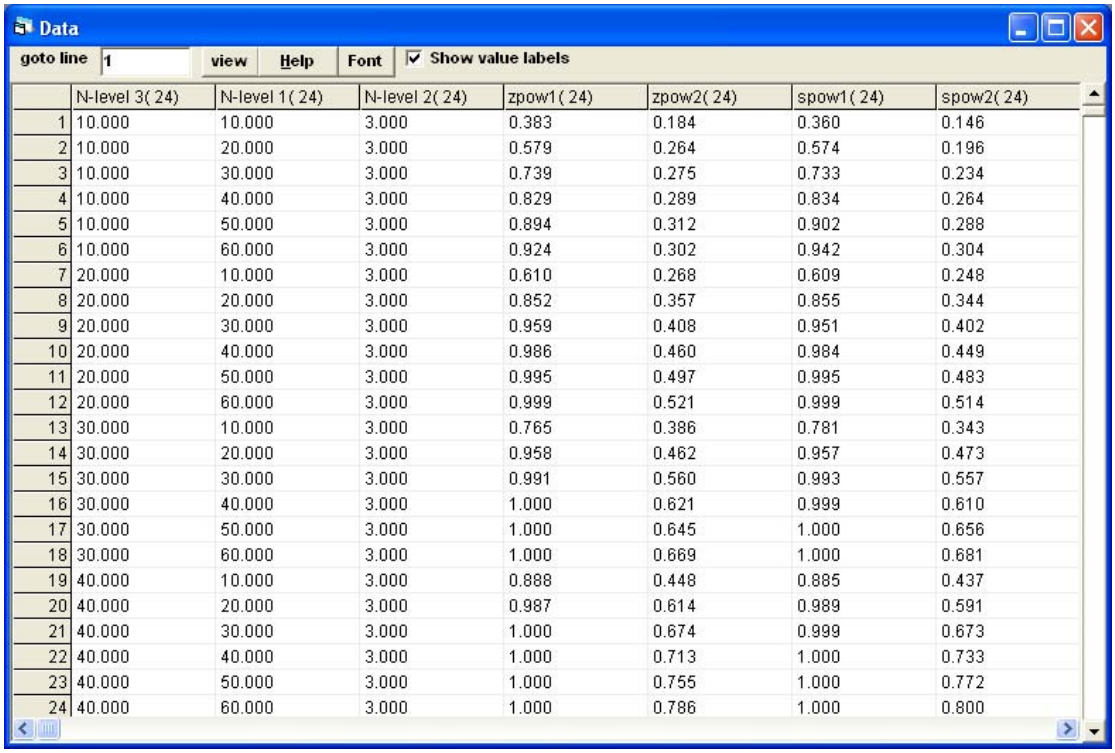
5 ('3-level unbalanced data nested model')

when prompted in MLPowSim, and then all our inputs are as for the balanced case until we reach the section on *Sample size set up*, where we enter the following:

```
                Sample size set up

Please input the smallest number of units for the third level: 10
Please input the largest number of units for the third level: 40
Please input the step size for the third level: 10
                  Unbalanced set up
Please choose one of the following scenarios for unbalanced sampling:
1: Non-response of level 1 units using a Binomial probability of non-response
2: Non-response of level 2 units using a Binomial probability of non-response
3: Fixed sample size in first level with your preference
Scenario type : 1
Please input the probability of non-response for the first level units: 0.2
Please input the smallest number of units for the second level per third level: 3
Please input the largest number of units for the second level per third level: 3
Please input the step size for the second level per third level: 1
Please input the smallest number of units for the  first level per second level: 10
Please input the largest number of units for the  first level per second level: 60
Please input the step size for the first level per second level: 10
```

The remaining inputs are as in Section 2.5.1. If we run the macros produced in MLwiN, we get the following in the **View/Edit Data** window:



Data

goto line 1 | view | Help | Font | Show value labels

	N-level 3(24)	N-level 1(24)	N-level 2(24)	zpow1(24)	zpow2(24)	spow1(24)	spow2(24)
1	10.000	10.000	3.000	0.383	0.184	0.360	0.146
2	10.000	20.000	3.000	0.579	0.264	0.574	0.196
3	10.000	30.000	3.000	0.739	0.275	0.733	0.234
4	10.000	40.000	3.000	0.829	0.289	0.834	0.264
5	10.000	50.000	3.000	0.894	0.312	0.902	0.288
6	10.000	60.000	3.000	0.924	0.302	0.942	0.304
7	20.000	10.000	3.000	0.610	0.268	0.609	0.248
8	20.000	20.000	3.000	0.852	0.357	0.855	0.344
9	20.000	30.000	3.000	0.959	0.408	0.951	0.402
10	20.000	40.000	3.000	0.986	0.460	0.984	0.449
11	20.000	50.000	3.000	0.995	0.497	0.995	0.483
12	20.000	60.000	3.000	0.999	0.521	0.999	0.514
13	30.000	10.000	3.000	0.765	0.386	0.781	0.343
14	30.000	20.000	3.000	0.958	0.462	0.957	0.473
15	30.000	30.000	3.000	0.991	0.560	0.993	0.557
16	30.000	40.000	3.000	1.000	0.621	0.999	0.610
17	30.000	50.000	3.000	1.000	0.645	1.000	0.656
18	30.000	60.000	3.000	1.000	0.669	1.000	0.681
19	40.000	10.000	3.000	0.888	0.448	0.885	0.437
20	40.000	20.000	3.000	0.987	0.614	0.989	0.591
21	40.000	30.000	3.000	1.000	0.674	0.999	0.673
22	40.000	40.000	3.000	1.000	0.713	1.000	0.733
23	40.000	50.000	3.000	1.000	0.755	1.000	0.772
24	40.000	60.000	3.000	1.000	0.786	1.000	0.800

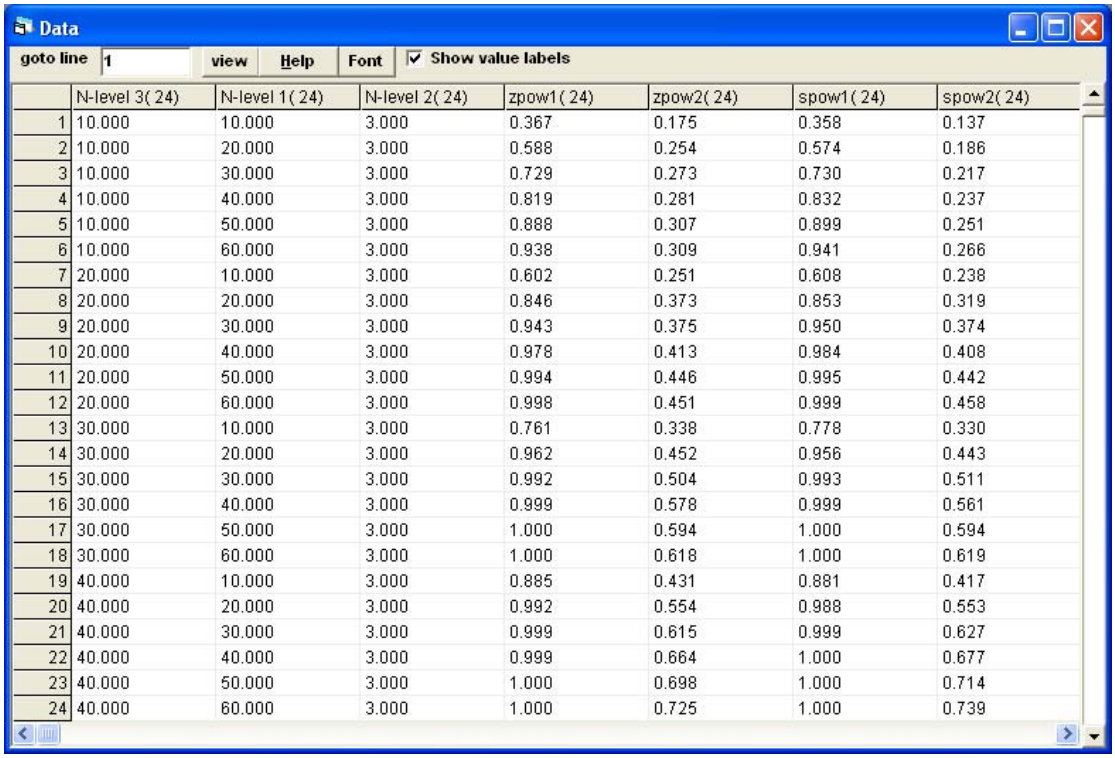
Unsurprisingly, we see that the power is lower when non-response occurs, as we found with the two-level models we considered earlier (Section 2.3.6.1). As one might expect, the power for designs with 50 pupils per school, and a 20% average non-response rate, are close to those observed with 40 pupils per school and no non-response. Next we will investigate the effect of whole cohort non-response.

2.5.3 Non-response at the second level in a 3-level design

In the actual ILEA dataset, the design is not balanced at the second level: some schools joined the study in the second cohort, some schools dropped out after the first cohort, and some schools even managed to miss the second cohort. 304 cohorts for 139 schools means that in the actual dataset 27% of the possible cohorts are missing. Here, however, we will stick to a 0.2 probability of a missing cohort, in line with Section 2.5.2. Again, we need to modify our inputs in MLPowSim, but this time there are only a few changes, as follows:

```
                    Unbalanced set up
Please choose one of the following scenarios for unbalanced sampling:
1: Non-response of level 1 units using a Binomial probability of non-response
2: Non-response of level 2 units using a Binomial probability of non-response
3: Fixed sample size in first level with your preference
Scenario type : 2
Please input the probability of non-response for the second level units: 0.2
```

If we run the resulting macros in MLwiN and view the **Data** window as before we will this time get the following results:



Data

goto line 1 | view | Help | Font | Show value labels

	N-level 3(24)	N-level 1(24)	N-level 2(24)	zpow1(24)	zpow2(24)	spow1(24)	spow2(24)
1	10.000	10.000	3.000	0.367	0.175	0.358	0.137
2	10.000	20.000	3.000	0.588	0.254	0.574	0.186
3	10.000	30.000	3.000	0.729	0.273	0.730	0.217
4	10.000	40.000	3.000	0.819	0.281	0.832	0.237
5	10.000	50.000	3.000	0.888	0.307	0.899	0.251
6	10.000	60.000	3.000	0.938	0.309	0.941	0.266
7	20.000	10.000	3.000	0.602	0.251	0.608	0.238
8	20.000	20.000	3.000	0.846	0.373	0.853	0.319
9	20.000	30.000	3.000	0.943	0.375	0.950	0.374
10	20.000	40.000	3.000	0.978	0.413	0.984	0.408
11	20.000	50.000	3.000	0.994	0.446	0.995	0.442
12	20.000	60.000	3.000	0.998	0.451	0.999	0.458
13	30.000	10.000	3.000	0.761	0.338	0.778	0.330
14	30.000	20.000	3.000	0.962	0.452	0.956	0.443
15	30.000	30.000	3.000	0.992	0.504	0.993	0.511
16	30.000	40.000	3.000	0.999	0.578	0.999	0.561
17	30.000	50.000	3.000	1.000	0.594	1.000	0.594
18	30.000	60.000	3.000	1.000	0.618	1.000	0.619
19	40.000	10.000	3.000	0.885	0.431	0.881	0.417
20	40.000	20.000	3.000	0.992	0.554	0.988	0.553
21	40.000	30.000	3.000	0.999	0.615	0.999	0.627
22	40.000	40.000	3.000	0.999	0.664	1.000	0.677
23	40.000	50.000	3.000	1.000	0.698	1.000	0.714
24	40.000	60.000	3.000	1.000	0.725	1.000	0.739

We have assumed an average 20% non-response rate as in Section 2.5.2 except at a different level of the data structure. This means that we should expect, on average, the same total number of pupils, so it is interesting to compare the relative effects on power of the two forms of non-response. If we look at the columns headed 'spow1' and 'spow2', and compare them with the equivalent columns in Section 2.5.2, we can gauge the effect on power for the two predictors: gender and proportion FSM. We see that there is very little to choose between the two forms of non-response for the gender predictor (a level 1 predictor which exhibits no between-cohort within-school variability), but for the proportion FSM predictor the cohort non-response scenario results in worse power. This makes sense, since this predictor is at the cohort-level and exhibits between-cohort variability, and so a cohort non-response scenario reduces both the total number of pupils and the total number of cohorts having an additional effect on power.

2.5.4 Individually chosen sample sizes at level 1

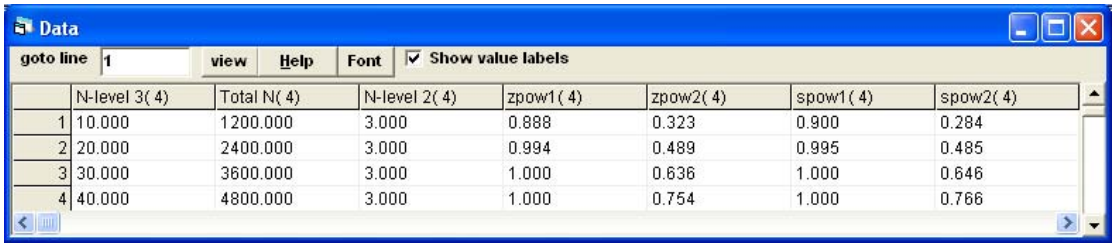
To complete our unbalanced options, we have the possibility of allowing different-sized clusters, as specified by the user. Here the assumption is that for each level 3 unit there will be the same number of level 2 units with the same structure in terms of cluster sizes: for instance, for the education example we might assume cluster sizes of 30, 40 and 50 pupils for the three cohorts within a school, but each school must then have the same structure. We will consider the ILEA example once again but assume, as discussed above, that the cluster sizes of each cohort increase, and so we have 3 cohorts of sizes 30, 40 and 50, respectively, for each school. The changes to the inputs to MLPowSim only occur for the unbalanced set up, as follows:

Unbalanced set up

Please choose one of the following scenarios for unbalanced sampling:

1: Non-response of level 1 units using a Binomial probability of non-response
2: Non-response of level 2 units using a Binomial probability of non-response
3: Fixed sample size in first level with your preference
Scenario type : **3**
Please input the smallest number of units for the second level per third level: **3**
Please input the largest number of units for the second level per third level: **3**
Please input the step size for the second level per third level: **1**
Please choose how many distinct classes you want the second level to have: **3**
Unbalanced set up inside the second level with 3 level 2 units
How many (from 1 to 3) level 2 units do you want to be in the class 1 ? **1**
For class 1, please input the number of level 1 units: **30**
How many (from 1 to 2) level 2 units do you want to be in the class 2 ? **1**
For class 2, please input the number of level 1 units: **40**
For class 3, please input the number of level 1 units: **50**

The remainder of the inputs are as previously given. Once the macros have been run in MLwiN, the outputs for this analysis are as follows:



	N-level 3(4)	Total N(4)	N-level 2(4)	zpow1(4)	zpow2(4)	spow1(4)	spow2(4)
1	10.000	1200.000	3.000	0.888	0.323	0.900	0.284
2	20.000	2400.000	3.000	0.994	0.489	0.995	0.485
3	30.000	3600.000	3.000	1.000	0.636	1.000	0.646
4	40.000	4800.000	3.000	1.000	0.754	1.000	0.766

The power estimates produced are only slightly smaller than those produced by equivalent designs, but with 40 pupils in each of the 3 cohorts per school.

2.6 Cross-classified Models

For the cross-classified models we will once again consider the educational example we encountered in Section 2.4, from Fife in Scotland (taken from the MLwiN User's Guide (Rasbash et al, 2004)). The dataset consists of records for 3,435 children from 19 secondary schools, and the response of interest is their exam attainment at age 16. For each child, we have also recorded the primary school they attended prior to secondary school, of which there are 148 in our sample. The data structure is therefore crossed, and we hypothesise that attainment at 16 will be affected by both the primary and secondary schools that the children attended.

One difficulty with cross-classified models is their estimation. In MLwiN it is generally recommended that MCMC estimation be used. The IGLS/RIGLS algorithm can be adapted to fit cross-classified models but this is currently achieved via some macros that cast the cross-classified model as a constrained nested model. These macros work fine for a single model, however we have not yet incorporated such methods into MLPowSim, as fitting thousands of models in this framework is more difficult. The problem with using MCMC estimation is the increased burden of computational time, and in this case using R will be quicker. In R the function *lmer* does not appear to have problems with cross-classified models although they are generally more computationally-expensive to run than nested models. In this section, we will therefore provide information on running the models using R first and then one example of MCMC in MLwiN.

As with nested data, ideally we might like to collect balanced cross-classified data. In this section we will firstly consider balanced data, before moving on to potentially more realistic unbalanced data scenarios.

2.6.1 Balanced cross-classified models.

As further background to our example, the response we are interested in is an attainment score from 1 to 10 that represents the pupils' score on a school leaving exam. For simplicity, we assume this score is continuous and normally-distributed as fitted in the User's Guide (although in reality an ordered categorical model might be more appropriate).

We will then fit a simple variance components model that assumes that the exam score for a particular pupil includes an overall population mean, an effect for the primary school they attended, an effect for the secondary school they attended, and a residual for that particular pupil. The average score in the actual data is 5.5, and so we form a null hypothesis (for illustration) that the average score is 5 versus an alternative that the average is higher than 5. For simplicity, we subtract 5 from all scores – as a result, we now have a null hypothesis that the average score is 0 – and we input an effect size (for the intercept) of 0.5. We give similar variances to those which appeared in the actual data, and use values of 0.4 for secondary school, 1.2 for primary school, and 8 for residual variability.

As we are assuming balanced data we will try to mimic a little the actual data collected. Given there were 148 primary schools and 19 secondary schools making potentially nearly 3,000 combinations this would be a little over 1 pupil per combination. We however see that in reality the data is fairly sparse with only 303 of the pairings of primary and secondary school actually occurring, with on average 11 pupils per combination. We will compromise by having 3 pupils per combination and trying between 20 and 100 primary schools (first cross-classified factor) and 10 and 30 secondary schools (second cross-classified factor). Here we give instructions for fitting this model in R, since this is quicker than the MCMC methods in MLwiN. The inputs for MLPowSim are as follows:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **0**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **6**
Please input the random number seed: **1**
Please input the significance level for testing the parameters: **0.025**

Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - REML, 1 - ML] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept associated with the first XC factor in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept associated with the second XC factor in your model (1=YES 0=NO)? **1**

Predictor(s) input

Do you want to include any explanatory variables in your model (1=YES 0=NO)? **0**

Sample size set up (balance)

Please input the smallest number of units for the first cross-classified factor: **20**
Please input the largest number of units for the first cross-classified factor: **100**
Please input the step size for the first cross-classified factor: **20**
Please input the smallest number of units for the second cross-classified factor: **10**
Please input the largest number of units for the second cross-classified factor: **30**
Please input the step size for the second cross-classified factor: **10**
Please input the smallest number of replications per XC cell : **3**
Please input the largest number of replications per XC cell : **3**
Please input the step size for the number of replications : **1**

Parameter estimates

Fixed effects input
Please input estimate of beta_0: **0.5**

Random effects input
Please input estimate of the variance of first factor (sigma^2_u): **1.2**
Please input estimate of the variance of second factor (sigma^2_v): **0.4**
Please input estimate of sigma^2_e: **8**

Final sample size check
The first XC factor: start=20 end=100 step size=20
The second XC factor: start=10 end=30 step size=10
The first level (replication): start=3 end=3 step size=1

Do you want to continue (YES=1 , NO=0)? **1**
Do you want to have the CI for the power in your output (YES=1 , NO=0)? **1**

After running MLPowSim we need to start up R and read in and run the file *powersimu.r* (see Section 1.5) which contains all the inputs for running the simulations. The simulations will take close to an hour to run in R, and at the end we get the following results if we ask to see the stored data frame *output* by typing *output* at the command prompt:

```
> output
  #XC2 #XC1 #repeat  zLb0  zpb0  zUb0  sLb0  spb0  sUb0
1   10   20       3 0.328 0.358 0.388 0.330 0.335 0.340
2   10   40       3 0.419 0.450 0.481 0.459 0.466 0.473
3   10   60       3 0.520 0.551 0.582 0.533 0.541 0.548
```

4	10	80	3	0.574	0.604	0.634	0.578	0.586	0.595
5	10	100	3	0.582	0.612	0.642	0.605	0.614	0.624
6	20	20	3	0.388	0.419	0.450	0.409	0.414	0.420
7	20	40	3	0.537	0.568	0.599	0.592	0.597	0.602
8	20	60	3	0.663	0.692	0.721	0.690	0.695	0.700
9	20	80	3	0.716	0.743	0.770	0.749	0.754	0.759
10	20	100	3	0.780	0.805	0.830	0.793	0.798	0.803
11	30	20	3	0.457	0.488	0.519	0.451	0.457	0.463
12	30	40	3	0.633	0.662	0.691	0.655	0.660	0.665
13	30	60	3	0.739	0.765	0.791	0.768	0.772	0.776
14	30	80	3	0.803	0.826	0.849	0.834	0.837	0.841
15	30	100	3	0.840	0.861	0.882	0.872	0.875	0.879

We can see from these results that designs with 20 secondary schools and 100 primary schools or 30 secondary schools and 80 primary schools result in a power of approximately 0.8 or greater. It is interesting that these designs have 6,000 and 7,200 pupils, respectively, whilst the actual dataset has only 3,435 pupils. This is in part due to the replication of pupils within a particular pairing of primary school and secondary school. If in fact we remove this replication, and instead have only 1 pupil for each combination, we get a far smaller dataset and the following power calculations:

#XC2	#XC1	#repeat	zLb0	zpb0	zUb0	sLb0	spb0	sUb0
20	80	1	0.683	0.711	0.739	0.707	0.713	0.719
20	100	1	0.717	0.744	0.771	0.756	0.761	0.767
20	120	1	0.754	0.780	0.806	0.792	0.797	0.803
20	140	1	0.786	0.810	0.834	0.813	0.818	0.824
30	80	1	0.784	0.808	0.832	0.804	0.808	0.812
30	100	1	0.830	0.852	0.874	0.853	0.857	0.860
30	120	1	0.860	0.880	0.900	0.878	0.882	0.885
30	140	1	0.884	0.902	0.920	0.905	0.908	0.911

Here we see that the power values are not reduced much and for 20 secondary schools and 140 primary schools, and for 30 secondary schools and 80 primary schools, we have a power of greater than 0.8 with total sample sizes of 2,800 and 2,400 pupils, respectively. What this is demonstrating is that sampling additional pupils from new schools increases power far more than sampling further pupils from the same schools. This backs up the results for the simpler nested models that we looked at earlier.

The prospect of collecting balanced data in practice for this problem is non-existent as logistically we could not take groups of 3 pupils from each primary school and send a group to every secondary school. For one thing we would need 60 pupils from each primary school for 20 secondary schools, which is unlikely given many primary schools will only have around 30 pupils in total. We will now look at various possible unbalanced data designs, some of which are feasible in this situation and some of which we include for completeness.

2.6.2 Non-response of single observations.

We begin by considering the simplest possible cause of lack of balance, the possibility that some pupils do not respond. Here we will investigate a fairly extreme situation where we anticipate that 50% of the pupils will not respond. We have chosen this level of non-response because, in our example of two crossed higher level classifications, each with a reasonable amount of variability attached to it, we find small amounts of dropout do not have a great impact on the power. This links in with the fact that in the last section when we reduced the number of pupils per combination from 3 to 1, we saw only small changes in power. A dropout rate of 50% will also result in some primary school/secondary school combinations having complete dropout.

The MLPowSim input for this situation is as follows:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **0**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **7**
Please input the random number seed: **1**
Please input the significance level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - REML, 1 - ML] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept associated with the first XC factor in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept associated with the second XC factor in your model (1=YES 0=NO)? **1**

Predictor(s) input

Do you want to include any explanatory variables in your model (1=YES 0=NO)? **0**

Random slope set up

Sample size set up (unbalanced)

Please choose one of the following scenarios for unbalanced sampling:
1: Non-response of level 1 units using a Binomial probability of non-response
2: Non-response of combinations of crossed factors using a Binomial probability of non-response
3: Fixed sized samples for each XC1 unit with probabilities for XC2 identifiers
4: Fixed total sample with each observation sampled from a
contingency table of probabilities for each combination of XC1 and XC2

Scenario type : **1**

Please input the probability of non-response : **0.5**
Please input the smallest number of units for the first cross-classified factor: **20**
Please input the largest number of units for the first cross-classified factor: **100**
Please input the step size for the first cross-classified factor: **20**
Please input the smallest number of units for the second cross-classified factor: **10**
Please input the largest number of units for the second cross-classified factor: **30**
Please input the step size for the second cross-classified factor: **10**
Please input the smallest number of replications per XC cell : **3**
Please input the largest number of replications per XC cell : **3**
Please input the step size for the number of replications : **1**

Parameter estimates

Fixed effects input
Please input estimate of beta_0: **0.5**

Random effects input
Please input estimate of the variance of first factor (sigma^2_u): **1.2**
Please input estimate of the variance of second factor (sigma^2_v): **0.4**
Please input estimate of sigma^2_e: **8**

Final sample size check
The first XC factor: start=20 end=100 step size=20
The second XC factor: start=10 end=30 step size=10
The first level (replication): start=3 end=3 step size=1

Do you want to continue (YES=1 , NO=0)? **1**
Do you want to have the CI for the power in your output (YES=1 , NO=0)? **1**

Having answered all the questions we next run the R package, and after waiting again for around an hour we will get the following output:

>output

	#XC2	#XC1	#1-level	zLb0	zpb0	zUb0	sLb0	spb0	sUb0
1	10	20	3	0.308	0.337	0.366	0.307	0.312	0.318
2	10	40	3	0.422	0.453	0.484	0.428	0.435	0.443
3	10	60	3	0.466	0.497	0.528	0.503	0.511	0.519
4	10	80	3	0.507	0.538	0.569	0.547	0.555	0.564
5	10	100	3	0.542	0.573	0.604	0.591	0.600	0.610
6	20	20	3	0.375	0.405	0.435	0.386	0.391	0.397
7	20	40	3	0.518	0.549	0.580	0.566	0.571	0.576
8	20	60	3	0.637	0.666	0.695	0.668	0.673	0.678
9	20	80	3	0.713	0.740	0.767	0.728	0.734	0.739
10	20	100	3	0.728	0.755	0.782	0.774	0.780	0.785
11	30	20	3	0.415	0.446	0.477	0.430	0.437	0.443
12	30	40	3	0.611	0.641	0.671	0.639	0.644	0.649
13	30	60	3	0.711	0.738	0.765	0.751	0.755	0.760
14	30	80	3	0.792	0.816	0.840	0.817	0.820	0.824
15	30	100	3	0.840	0.861	0.882	0.863	0.866	0.869

Here we see that the power has reduced, in comparison to the data without dropout, as we might expect; we now need *at least* 30 secondary schools and 80 primary schools to get a power of 0.8.

2.6.3 Dropout of whole groups

The other method of dropout that can be used in MLPowSim to create unbalanced designs involves the complete dropout of specific combinations of primary and secondary school. Here we will have two possibilities for each combination of primary and secondary school: either (i) the combination is in the dataset and so 3 pupils are sampled or (ii) the combination is not in the dataset and so no pupils are sampled. The user is required to input the probability of possibility (ii) and the inputs are identical to the case of single person dropout, aside from selecting sampling option 2 rather than 1 as detailed below:

Sample size set up (unbalanced)

Please choose one of the following scenarios for unbalanced sampling:
1: Non-response of level 1 units using a Binomial probability of non-response
2: Non-response of combinations of crossed factors using a Binomial probability of non-response
3: Fixed sized samples for each XC1 unit with probabilities for XC2 identifiers
4: Fixed total sample with each observation sampled from a
contingency table of probabilities for each combination of XC1 and XC2

Scenario type : **2**

Please input the probability of non-response : **0.5**

Upon running the R code we get the following output:

```
> output
   #XC2 #XC1 #1-level  zLb0  zpb0  zUb0  sLb0  spb0  sUb0
 1   10   20       3 0.297 0.326 0.355 0.300 0.305 0.311
 2   10   40       3 0.412 0.443 0.474 0.425 0.432 0.439
 3   10   60       3 0.467 0.498 0.529 0.494 0.502 0.510
 4   10   80       3 0.512 0.543 0.574 0.546 0.555 0.564
 5   10  100       3 0.539 0.570 0.601 0.584 0.593 0.603
 6   20   20       3 0.368 0.398 0.428 0.388 0.394 0.399
 7   20   40       3 0.537 0.568 0.599 0.561 0.567 0.573
 8   20   60       3 0.631 0.660 0.689 0.663 0.668 0.673
 9   20   80       3 0.697 0.725 0.753 0.730 0.735 0.741
10   20  100       3 0.748 0.774 0.800 0.774 0.779 0.785
11   30   20       3 0.403 0.434 0.465 0.429 0.434 0.440
12   30   40       3 0.608 0.638 0.668 0.633 0.638 0.644
13   30   60       3 0.719 0.746 0.773 0.745 0.750 0.754
14   30   80       3 0.808 0.831 0.854 0.819 0.823 0.827
15   30  100       3 0.817 0.840 0.863 0.859 0.862 0.866
```

Here we again see that the power is reduced compared to the case in which there were no dropouts, however there is very little to choose between this and the other (pupil level) dropout scenario. This may be because of the small number of replications, or even because when we remove a primary and secondary school combination we still have other information on each of the two schools involved through other pairings.

2.6.4 Unbalanced designs – sampling from a pupil lookup table.

The two dropout options for producing unbalanced designs make sense when it is easy to sample from every combination of the two factors. In reality, however, the majority of pupils in a particular primary school will all attend the same secondary school, and the real design is close to a nested one, with primary schools nested within secondary schools. In fact, if we count the number of pupils not attending the most popular secondary for a particular primary school, we find that only 288 pupils do not fit a nested structure. In order to more closely mimic the actual data structure we could use the actual data as a guide for the pattern of schools. Here we tally up the numbers of pupils in each combination of primary and secondary school and simulate data with probabilities proportional to the numbers of pupils present for each combination.

We will look first at simply choosing pupils at random from the set of all pupils (this is option 4 in the list of (unbalanced) scenarios in MLPowSim). Essentially we are using the 3,435 pupils to give probabilities of each combination of primary and secondary school, and so if no pupils in the real data went to a particular combination, then in the simulated datasets no pupils would be observed either. The school labels are purely used to describe the structure of the data and the school effects from the actual data are not used. In the simulations, only the variances of the primary and secondary schools are used to generate new school effects for the simulated schools.

To run this option we need a file that contains the numbers of pupils observed for each combination, and this is provided as '*fife.txt'* which contains a row for each primary school. We will consider sampling between 200 and 4,000 pupils, and the inputs for MLPowSim are as follows:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **0**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **7**
Please input the random number seed: **1**
Please input the significance level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - REML, 1 - ML] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept associated with the first XC factor in your model (1=YES 0=NO)? **1**

Do you want to have a random intercept associated with the second XC factor in your model (1=YES 0=NO)? **1**

Predictor(s) input

Do you want to include any explanatory variables in your model (1=YES 0=NO)? **0**

Sample size set up (unbalanced)

Please choose one of the following scenarios for unbalanced sampling:
1: Non-response of level 1 units using a Binomial probability of non-response
2: Non-response of combinations of crossed factors using a Binomial probability of non-response
3: Fixed sized samples for each XC1 unit with probabilities for XC2 identifiers
4: Fixed total sample with each observation sampled from a
contingency table of probabilities for each combination of XC1 and XC2

Scenario type : **4**

Please input the filename (text file) including sample sizes of cells for XC1 crossed with XC2 : **fife.txt**
Please input the unit numbers of XC1 (numbers of row in fife.txt file): **148**
Please input the unit numbers of XC2 (numbers of column in fife.txt file): **19**
Please input the smallest number of total units: **200**
Please input the largest number of total units: **4000**
Please input the step size for the total units: **200**

Parameter estimates

Fixed effects input
Please input estimate of beta_0: **0.5**

Random effects input
Please input estimate of the variance of first factor (sigma^2_u): **1.2**
Please input estimate of the variance of second factor (sigma^2_v): **0.4**
Please input estimate of sigma^2_e: **8**

Final sample size check
The first and second XC samples are row and column numbers in fife.txt file as follows:
Row=148 column=19
The first level (replication) sample is fixed as 1.
Total sample range for XCs combination: start=200 end=4000 step size=200

Do you want to continue (YES=1 , NO=0)? **1**
Do you want to have the CI for the power in your output (YES=1 , NO=0)? **1**

If we run the file produced in R (which again will take an hour or so), we will get the following estimates stored in the data frame *output*:

```
> output
  #XC2 #XC1 #Tsample  zLb0  zpb0  zUb0  sLb0  spb0  sUb0
1   19  148      200 0.388 0.419 0.450 0.429 0.435 0.442
2   19  148      400 0.575 0.605 0.635 0.573 0.581 0.589
3   19  148      600 0.605 0.635 0.665 0.650 0.658 0.666
4   19  148      800 0.646 0.675 0.704 0.691 0.699 0.708
5   19  148     1000 0.689 0.717 0.745 0.708 0.716 0.725
6   19  148     1200 0.693 0.721 0.749 0.731 0.740 0.748
7   19  148     1400 0.725 0.752 0.779 0.747 0.755 0.762
8   19  148     1600 0.728 0.755 0.782 0.757 0.764 0.772
```

9	19	148	1800	0.728	0.755	0.782	0.760	0.768	0.775
10	19	148	2000	0.722	0.749	0.776	0.763	0.771	0.779
11	19	148	2200	0.725	0.752	0.779	0.777	0.785	0.792
12	19	148	2400	0.745	0.771	0.797	0.780	0.788	0.795
13	19	148	2600	0.744	0.770	0.796	0.779	0.786	0.793
14	19	148	2800	0.742	0.768	0.794	0.782	0.789	0.796
15	19	148	3000	0.746	0.772	0.798	0.783	0.790	0.798
16	19	148	3200	0.752	0.778	0.804	0.788	0.795	0.803
17	19	148	3400	0.748	0.774	0.800	0.790	0.797	0.804
18	19	148	3600	0.740	0.766	0.792	0.798	0.805	0.812
19	19	148	3800	0.760	0.785	0.810	0.796	0.803	0.810
20	19	148	4000	0.768	0.793	0.818	0.800	0.807	0.814

What is interesting here is that the power increases very quickly for the small sample sizes but then tends to plateau having reached roughly 0.8 after around 3,000 pupils. Increases in sample sizes when sample size is smaller will generally increase both the number of pupils and the numbers of schools. However, having reached 3,000 pupils, most simulated datasets will include virtually all the primary schools, and so further increasing the number of pupils will not have as much of an impact. Note that some primary schools only have 1 or 2 pupils in the real data, and so even with 3,000 pupils there is a good chance they will not appear in a simulated dataset.

2.6.5 Unbalanced designs – sampling from lookup tables for each primary/secondary school.

The final possible way to generate unbalanced data in MLPowSim (option 3) is perhaps the most realistic in the case of our example. Often, when one collects data, the design is based on one factor, for example the primary schools or the secondary schools, with the other factor recorded but not controlled. For example, we might decide we wish to collect educational data from pupils in secondary school, and having decided to take a balanced sample from each secondary school, we also record the primary school that each attended. We could also consider the alternative situation of setting up a study while pupils are in primary school and hence selecting a fixed size sample from each primary school. We then follow these pupils as they go through the education system noting also their choice of secondary school. We will consider this situation first and consider following between 2 and 20 pupils in each primary school.

The (later) inputs to MLPowSim are as follows:

Sample size set up (unbalanced)

Please choose one of the following scenarios for unbalanced sampling:
1: Non-response of level 1 units using a Binomial probability of non-response
2: Non-response of combinations of crossed factors using a Binomial probability of non-response
3: Fixed sized samples for each XC1 unit with probabilities for XC2 identifiers
4: Fixed total sample with each observation sampled from a
contingency table of probabilities for each combination of XC1 and XC2

Scenario type : **3**

Please input the filename (text file) including sample sizes of cells for XC1 crossed with XC2 : **fife.txt**

Please input the unit numbers of XC1 (numbers of row in fife.txt file): **148**
Please input the unit numbers of XC2 (numbers of column in fife.txt file): **19**
Please input the smallest number of units per first cross-classified factor unit: **2**
Please input the largest number of units per first cross-classified factor unit: **20**
Please input the step size per first cross-classified factor unit: **1**

Parameter estimates

Fixed effects input
Please input estimate of beta_0: **0.5**

Random effects input
Please input estimate of the variance of first factor (sigma^2_u): **1.2**
Please input estimate of the variance of second factor (sigma^2_v): **0.4**
Please input estimate of sigma^2_e: **8**

Final sample size check

The first and second XC samples are row and column numbers in fife.txt file as follows:
Row=148 column=19
The first level (replication) sample is fixed as 1.
Total sample range for XCs combination: start=2 end=20 step size=1

The first XC factor: start=10 end=50 step size=10
The second XC factor: start=10 end=30 step size=10
The first level (replication): start=5 end=5 step size=1

Do you want to continue (YES=1 , NO=0)? **1**
Do you want to have the CI for the power in your output (YES=1 , NO=0)? **1**

If we run the output file in R we will get the following output:

```
>output
   #XC2 #XC1 #Tninrow  zLb0  zpb0  zUb0  sLb0  spb0  sUb0
 1   19   148       2 0.527 0.558 0.589 0.558 0.567 0.575
 2   19   148       3 0.600 0.630 0.660 0.637 0.646 0.654
 3   19   148       4 0.636 0.665 0.694 0.683 0.692 0.700
 4   19   148       5 0.683 0.711 0.739 0.716 0.724 0.733
 5   19   148       6 0.683 0.711 0.739 0.730 0.739 0.747
 6   19   148       7 0.728 0.755 0.782 0.745 0.754 0.763
 7   19   148       8 0.738 0.764 0.790 0.756 0.764 0.772
 8   19   148       9 0.724 0.751 0.778 0.764 0.772 0.780
 9   19   148      10 0.726 0.753 0.780 0.773 0.781 0.789
10   19   148      11 0.736 0.762 0.788 0.775 0.783 0.791
11   19   148      12 0.730 0.757 0.784 0.780 0.788 0.796
12   19   148      13 0.762 0.787 0.812 0.786 0.793 0.801
13   19   148      14 0.724 0.751 0.778 0.792 0.800 0.807
14   19   148      15 0.747 0.773 0.799 0.792 0.800 0.808
15   19   148      16 0.768 0.793 0.818 0.804 0.811 0.818
16   19   148      17 0.755 0.781 0.807 0.797 0.804 0.812
17   19   148      18 0.753 0.779 0.805 0.799 0.807 0.814
18   19   148      19 0.758 0.784 0.810 0.803 0.810 0.818
19   19   148      20 0.766 0.791 0.816 0.803 0.811 0.818
```

Here we see that, even for small sample sizes, the power is quite big, and again plateaus out at the desired level of 0.8 by about 14 pupils per primary school – 2,072 pupils in total. Sampling further pupils has very little impact on the power. It is interesting here that the standard error method tends to give a larger power estimate than the 0/1 method.

We can also consider sampling fixed numbers of pupils per secondary school. To do this we require a file with secondary schools as rows, and primary schools as columns, and such a file is available as *fife2.txt*. The inputs are as above apart from the following:

Please input the filename (text file) including sample sizes of cells for XC1 crossed with XC2 :
fife2.txt
Please input the unit numbers of XC1 (numbers of row in fife.txt file): **19**
Please input the unit numbers of XC2 (numbers of column in fife.txt file): **148**
Please input the smallest number of units per first cross-classified factor unit: **5**
Please input the largest number of units per first cross-classified factor unit: **200**
Please input the step size per first cross-classified factor unit: **5**

This will produce the following output in R:

	#XC2	#XC1	#Tninrow	zLb0	zpb0	zUb0	sLb0	spb0	sUb0
1	148	19	5	0.281	0.310	0.339	0.287	0.291	0.295
2	148	19	10	0.403	0.434	0.465	0.429	0.435	0.442
3	148	19	15	0.502	0.533	0.564	0.518	0.525	0.532
4	148	19	20	0.546	0.577	0.608	0.584	0.591	0.599
5	148	19	25	0.586	0.616	0.646	0.620	0.628	0.636
6	148	19	30	0.619	0.649	0.679	0.650	0.658	0.666
7	148	19	35	0.647	0.676	0.705	0.678	0.686	0.694
8	148	19	40	0.654	0.683	0.712	0.693	0.701	0.709
9	148	19	45	0.673	0.701	0.729	0.698	0.706	0.714
10	148	19	50	0.659	0.688	0.717	0.716	0.723	0.731
11	148	19	55	0.692	0.720	0.748	0.724	0.732	0.739
12	148	19	60	0.702	0.730	0.758	0.727	0.735	0.743
13	148	19	65	0.697	0.725	0.753	0.729	0.737	0.745
14	148	19	70	0.692	0.720	0.748	0.739	0.747	0.755
15	148	19	75	0.706	0.733	0.760	0.745	0.753	0.761
16	148	19	80	0.716	0.743	0.770	0.749	0.757	0.765
17	148	19	85	0.721	0.748	0.775	0.754	0.761	0.769
18	148	19	90	0.719	0.746	0.773	0.756	0.763	0.771
19	148	19	95	0.729	0.756	0.783	0.763	0.770	0.778
20	148	19	100	0.732	0.759	0.786	0.759	0.767	0.775
21	148	19	105	0.722	0.749	0.776	0.769	0.776	0.783
22	148	19	110	0.725	0.752	0.779	0.773	0.781	0.788
23	148	19	115	0.730	0.757	0.784	0.773	0.780	0.788
24	148	19	120	0.756	0.782	0.808	0.773	0.781	0.788
25	148	19	125	0.724	0.751	0.778	0.777	0.784	0.791
26	148	19	130	0.749	0.775	0.801	0.788	0.795	0.802
27	148	19	135	0.749	0.775	0.801	0.781	0.788	0.796
28	148	19	140	0.757	0.783	0.809	0.787	0.794	0.801
29	148	19	145	0.730	0.757	0.784	0.782	0.789	0.796

30	148	19	150	0.752 0.778 0.804 0.788 0.795 0.802
31	148	19	155	0.772 0.797 0.822 0.787 0.794 0.801
32	148	19	160	0.748 0.774 0.800 0.791 0.798 0.805
33	148	19	165	0.762 0.787 0.812 0.790 0.798 0.805
34	148	19	170	0.786 0.810 0.834 0.789 0.796 0.803
35	148	19	175	0.768 0.793 0.818 0.787 0.794 0.801
36	148	19	180	0.755 0.781 0.807 0.799 0.806 0.813
37	148	19	185	0.754 0.780 0.806 0.792 0.799 0.806
38	148	19	190	0.766 0.791 0.816 0.788 0.794 0.801
39	148	19	195	0.753 0.779 0.805 0.798 0.805 0.812
40	148	19	200	0.767 0.792 0.817 0.802 0.809 0.816

Here we see that although the power increases quickly with increasing pupils per school, it then plateaus off. We therefore need something of the order of 170 pupils per school (3,230 in total) to get a power of 0.8.

2.6.6 Using MCMC in MLwiN for cross-classified models.

The alternative to using R for the cross-classified models is to use MCMC in MLwiN. This is far more time-consuming, and so here we just repeat the balanced cross-classified modelling approach. With MCMC estimation we need to decide on a burn-in length and main run length for each simulation. In the case of our example, we have chosen the (rather arbitrary) values of 5,000 and 10,000 iterations, respectively. The following inputs are required in MLPowSim:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **6**
Please input the random number seed: **1**
Please input the significance level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Currently only MCMC estimation is available in MLPowSim for cross-classified models
Please input burnin length for each simulation : **5000**
Please input main run length for each simulation : **10000**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept associated with the first XC factor in your model (1=YES 0=NO)? **1**

Do you want to have a random intercept associated with the second XC factor in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **0**

Sample size set up

Please input the smallest number of units for the first cross-classified factor: **20**
Please input the largest number of units for the first cross-classified factor: **100**
Please input the step size for the first cross-classified factor: **20**
Please input the smallest number of units for the second cross-classified factor: **10**
Please input the largest number of units for the second cross-classified factor: **30**
Please input the step size for the second cross-classified factor: **10**
Please input the smallest number of replications per XC cell : **3**
Please input the largest number of replications per XC cell : **3**
Please input the step size for the number of replications : **1**

Parameter estimates

Fixed effects input
Please input estimate of beta_0: **0.5**

Random effects input
Please input estimate of the variance of the first classification: **1.2**
Please input estimate of the variance of the second classification: **0.4**
Please input estimate of sigma^2_e: **8**

Files to perform power analysis for the 3 level cross-classified model with the following sample criterion have been created
Power analysis for the model with the following sample criterion starts now. Please wait ...

Sample size in the first factor starts at 20 and finishes at 100 with the step size 20
Sample size in the second factor starts at 10 and finishes at 30 with the step size 10
Number of replications per cell starts at 3 and finishes at 3 with the step size 1
1000 simulations for each sample size combination will be performed

Press any key to continue…

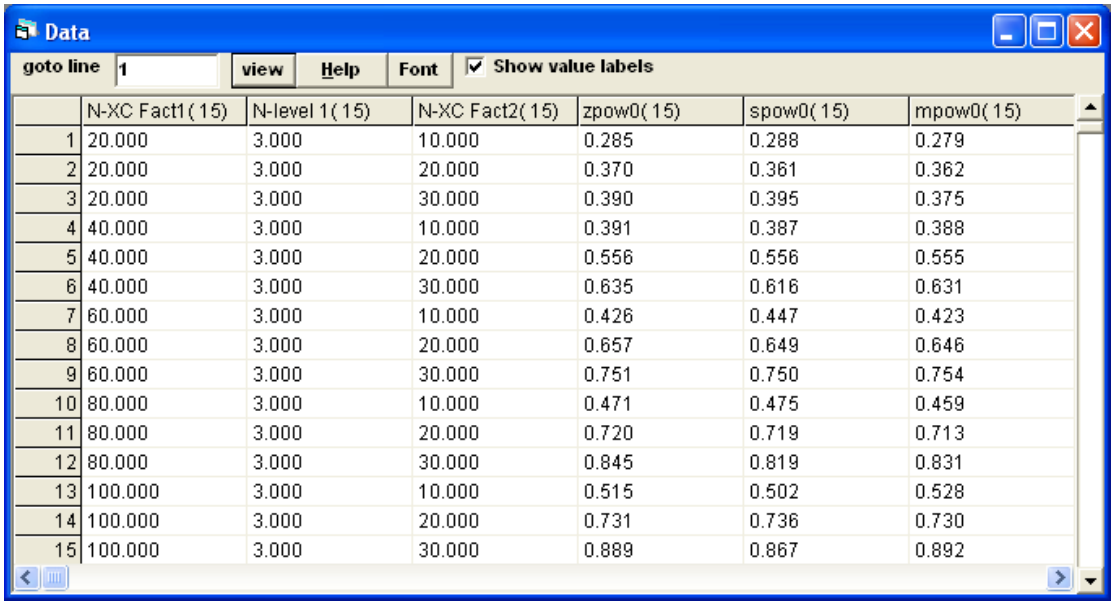
Having run MLPowSim we next need to run the macros produced in MLwiN. For this we will need to select the macro *simu.txt* and view the columns c208, c209, c210 c211, c231 and c421 in the **View/Edit Data** window (see Section 1.4). The simulations here took 36 hours on my machine and produced the following output:

Data

goto line 1 | view | Help | Font | Show value labels

	N-XC Fact1(15)	N-level 1(15)	N-XC Fact2(15)	zpow0(15)	spow0(15)	mpow0(15)
1	20.000	3.000	10.000	0.257	0.285	0.246
2	20.000	3.000	20.000	0.360	0.369	0.345
3	20.000	3.000	30.000	0.405	0.401	0.420
4	40.000	3.000	10.000	0.410	0.394	0.432
5	40.000	3.000	20.000	0.580	0.544	0.550
6	40.000	3.000	30.000	0.622	0.577	0.573
7	60.000	3.000	10.000	0.470	0.465	0.469
8	60.000	3.000	20.000	0.674	0.629	0.649
9	60.000	3.000	30.000	0.756	0.752	0.771
10	80.000	3.000	10.000	0.529	0.469	0.515
11	80.000	3.000	20.000	0.762	0.710	0.755
12	80.000	3.000	30.000	0.866	0.844	0.856
13	100.000	3.000	10.000	0.555	0.502	0.544
14	100.000	3.000	20.000	0.723	0.682	0.739
15	100.000	3.000	30.000	0.855	0.865	0.840
16	-	-	-	-	-	-

Here we see that we need to sample at least 80 primary schools and 30 secondary schools to gain a power of 0.8. We can see that the stability of the power estimates using MCMC with a burn-in of 5000 and a main run of 10,000 is not as good as that observed using R. For example all 3 power estimation methods suggest that a design with 80 primary schools and 20 secondary schools has more power than one with 100 primary schools and 20 secondary schools! This suggests that maybe 5,000 and 10,000 iterations are still not enough, and we need even more. Given that the above run took 36 hours this starts becoming infeasible, but for the purposes of comparison, below we present the results from 100,001 iterations:



	N-XC Fact1 (15)	N-level 1 (15)	N-XC Fact2 (15)	zpow0 (15)	spow0 (15)	mpow0 (15)
1	20.000	3.000	10.000	0.285	0.288	0.279
2	20.000	3.000	20.000	0.370	0.361	0.362
3	20.000	3.000	30.000	0.390	0.395	0.375
4	40.000	3.000	10.000	0.391	0.387	0.388
5	40.000	3.000	20.000	0.556	0.556	0.555
6	40.000	3.000	30.000	0.635	0.616	0.631
7	60.000	3.000	10.000	0.426	0.447	0.423
8	60.000	3.000	20.000	0.657	0.649	0.646
9	60.000	3.000	30.000	0.751	0.750	0.754
10	80.000	3.000	10.000	0.471	0.475	0.459
11	80.000	3.000	20.000	0.720	0.719	0.713
12	80.000	3.000	30.000	0.845	0.819	0.831
13	100.000	3.000	10.000	0.515	0.502	0.528
14	100.000	3.000	20.000	0.731	0.736	0.730
15	100.000	3.000	30.000	0.889	0.867	0.892

Here we see the power estimates are considerably more stable, increasing monotonically with sample size (Note that we actually ran the above analysis in several bits and pieced them together and so the power values you see will not be exactly identical to if you run them yourself)

The table below compares the power estimates we earlier derived via R (see Section 2.6.1) with those we have just obtained above (all the power estimates listed in the table are those derived from the standard error method):

			Estimation method (with stats package)	
N-XC Fact1	N-XC Fact2	N-level 1	MCMC (MLwiN)	ML (R)
20	10	3	0.288	0.335
20	20	3	0.361	0.414
20	30	3	0.395	0.457
40	10	3	0.387	0.466
40	20	3	0.556	0.597
40	30	3	0.616	0.660
60	10	3	0.447	0.541
60	20	3	0.649	0.695

60	30	3	0.750	0.772
80	10	3	0.475	0.586
80	20	3	0.719	0.754
80	30	3	0.819	0.837
100	10	3	0.502	0.614
100	20	3	0.736	0.798
100	30	3	0.867	0.875

It's apparent that, especially for smaller sample sizes, the power estimates from the MCMC method (run for 100,001 iterations) are smaller than those generated by R (using maximum likelihood estimation), but the estimates derived from each method become more similar as sample size increases. It has been shown (Browne and Draper, 2006) that ML estimation (via the IGLS) algorithm gives under-estimates for higher level variances in multilevel models when the number of higher level units is small. This underestimation will result in larger power estimates when the number of higher level units is small which may in part explain the differences in the above table.

3 Binary Response models

In the last chapter we dealt with models where the response variable is assumed to be continuous and to follow a normal distribution. In other situations we might have binary response data: for example, in educational research the response might be whether or not a student passes an exam, in health many studies have success of a treatment or mortality as a response variable, and so on. As with continuous responses, binary responses can also exhibit dependence through clustering: for example, more students will pass the exam in a good school than in a poorer school, and so the results of different pupils from the same school are likely to be more correlated than the results of pupils chosen at random. In this chapter, we begin by looking at the common methods of devising power calculations for simple binary response models before linking models together in a unified framework, and also adding-in multilevel structure.

3.1 Simple binary response models – comparing data with a fixed proportion.

In this chapter our dataset of interest involves the use of contraceptives by women in Bangladesh: an example dataset used in the MLwiN User's Guide (Rasbash et al, 2004). We will therefore have a binary response which represents whether or not a woman uses any form of contraceptive. The simplest possible model is then a single proportion model, where we disregard possible predictor variables and simply assume there is an underlying proportion of women who use contraceptives: i.e. for each woman there is a probability π of using contraceptives. We may then want to compare this unknown proportion against some fixed value, for example we might like to know

how many women we would need to sample to be able to state that the proportion of women using contraceptives is greater or less than ½ .

The approach that is commonly used for getting approximate sample sizes in this simple scenario is to make a normal assumption to the Binomial distribution, and then test the hypothesis as we would with the simple single means model described earlier.

The normal approximation to the Binomial assumes that a sample proportion p is normally-distributed with mean π and variance $\pi(1-\pi)/n$, which is approximated by $p(1-p)/n$ where n here represents the chosen sample size. This approximation is best when the underlying π is close to 0.5 and the sample size is large.

So let us suppose that we believe the proportion of women that use contraceptives is 0.4, and we wish to estimate how many women we need to sample to have a power of 0.8 of saying that the proportion is less than 0.5. The formula for calculating the sample size is as follows (assuming a two-sided test):

$$n \geq \left[\frac{\Phi^{-1}(0.8)\sqrt{\pi(1-\pi)} + \Phi^{-1}(0.975)\sqrt{\pi_0(1-\pi_0)}}{\pi - \pi_0} \right]^2 = \left[\frac{0.842\sqrt{0.4(1-0.4)} + 1.96\sqrt{0.5(1-0.5)}}{0.4-0.5} \right]^2$$

Here as we see π_0 is the probability under the null hypothesis (0.5) whilst π is the believed value (0.4). Solving for n we get $n \geq 193.9$ thus we would need a sample size of at least 194.

As we see a little later, this model can be cast into a standard modelling formulation – namely that of generalized linear models. When we considered continuous responses then the simple means model was a special case of the general linear modelling framework, but in the binary response case the simple proportion model is not quite a special case as it involves a different normal approximation as will become clear in Section 3.3.

3.2 Comparing two proportions.

The other commonly-considered simple model is used when we wish to establish whether the proportion of positive responses are different for two populations. For example, in our dataset we have a descriptive indicator of the area where the women live (either urban or rural). We might then like to see whether women use contraceptives more in urban or rural areas. Our null hypothesis in this case is that women are equally likely to use contraceptives in both areas, whereas we might hypothesise the alternative that women in urban areas are more likely to use contraceptives. Here we will use normal approximations again, so that under the null hypothesis we assume all women come from an approximate Normal distribution with some mean π and variance $\pi(1-\pi)/n$. Under the alternative hypothesis, the women come from different populations and have approximate Normal distributions with means π_U and π_R with corresponding variances $\pi_U(1-\pi_U)/n_u$ and $\pi_R(1-\pi_R)/n_R$ where $n = n_u + n_R$.

Now we choose n_u and n_R as part of our sampling strategy, and our options are to sample the same number of each, or to assume some fixed ratio for the two categories

based on the perceived population sizes. If the same sample size is assumed to be the same for each group, then the following formula holds:

$$n_u = n_R = \left(\frac{0.842\sqrt{\pi_u(1-\pi_u) + \pi_R(1-\pi_R)} + 1.96\sqrt{2\pi_0(1-\pi_0)}}{\pi_u - \pi_R} \right)^2$$

If we assume that π_U=0.5 and π_R=0.35 then π_0 = (0.5+0.35)/2 = 0.425. Solving, we find we need 170 women in each group and 340 women in total for a power of 0.8. In the Bangladesh dataset the ratio of urban to rural dwellers is 30%:70%; hence, to get a similar power, we will need 130 urban women and 302 rural dwellers, making 432 in total, which shows that a balanced number in each group is preferred as it reduces the overall sample size.

3.3 Logistic regression models

The two models described above – in which we compared an observed proportion to a fixed proportion, and also compared the proportions in two populations – are widely used in many applied areas, especially medical research. It is, however, difficult to extend this modelling framework to account for further categorical predictors and/or continuous predictors. Instead, we turn to generalized linear models and in particular logistic regression models. Here, we transform the underlying probability to a measure that can take values on the whole real line via a link function, and then fit a model to this transformed measure. As probabilities lie between 0 and 1 we need a function that maps values in the range [0,1] to values in the range (-∞,∞). The function has to be monotonic: i.e. with each probability mapping onto a different value; by convention, we expect 0 to map onto -∞ and 1 onto ∞. This suggests that inverse cumulative distribution functions (CDFs) are ideal candidates, and the most commonly-used function is the inverse CDF of the logistic distribution, resulting in a model known as a logistic regression. Please note that the inverse (standard) normal CDF is also commonly-used, resulting in probit regression.

We can write a logistic regression model as follows:

$$y_i \sim Bernouilli(\pi_i)$$

$$\log\left(\frac{\pi_i}{1-\pi_i} \right) = X_i\beta$$

Here the logit function of π_i is modelled by predictors X_i and corresponding coefficients β. The reason this function is modelled rather than simply π_i is that the product $X_i\beta$ (which is known as the linear predictor) can take any value, and so modelling π_i directly can result in predicted probabilities less than 0 and greater than 1!

Models similar to those we explored above, namely the single proportion and the comparison of two proportions, can be fitted in this framework by careful selection of predictor variables, as we discuss next.

3.3.1 A single proportion in the logistic regression framework

The simplest logistic regression model is created by including just an intercept in the linear predictor. This model basically fits a single proportion to a set of data and the coefficient β can be back-transformed to this underlying proportion π as follows:

$$\pi = \frac{e^{\beta}}{1+e^{\beta}}.$$

The estimate of π obtained via this transformation will be the same as the estimate obtained in the single proportion model: i.e. the number of successes out of the number of trials. The difference when fitting a logistic regression model is that the parameter β is estimated along with its standard error, and so we have the option of using a different normal approximation by assuming β is normally-distributed rather than π. In reality, neither of these quantities is truly normally-distributed, but making the assumption for β, rather than π, links in with further logistic regression models and leads to the use of Wald tests for testing significance.

We will now investigate how we can use MLPowSim to determine power for various sample sizes for this model, using the Bangladeshi dataset. As discussed earlier, we are trying to establish a sample size to detect that the actual usage of contraceptives is less than 50%, based on our belief that the actual usage is 40%. For a logistic regression model, the proportion 40% corresponds to a value of -0.4055 for β. We are fortunate that 50% corresponds to 0, and so we only need to test whether β is less than 0, which is the standard test in MLPowSim. Note: if you wanted to check whether the proportion is different from another value, you would need to modify the macros produced by MLPowSim to test whether the corresponding transformed value for β is in the intervals or not.

Here are the inputs required in MLPowSim to fit this model using MLwiN:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **1**
Please input the random number seed: **1**
Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **1**

Please input link function [0 – logit, 1 – probit, 2- cloglog] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **0**

Sample size set up

Please input the smallest sample size : **30**
Please input the largest sample size : **300**
Please input the step size: **30**

Parameter estimates

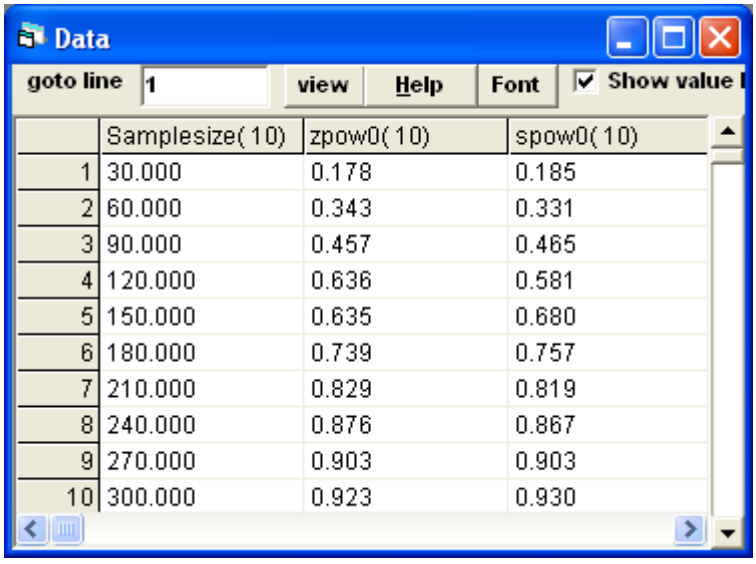
Please input estimate of beta_0: **-0.4055**

Files to perform power analysis for the 1 level model with the following sample criterion have been created
Sample size starts at 30 and finishes at 300 with the step size 30
1000 simulations for each sample size combination will be performed

Press any key to continue…

Note, that whilst our hypothesis is one-sided (i.e. we're predicting actual usage is less than 50%, rather than more), we have chosen a significance level of 0.025 rather than the more common 0.05. This is because it corresponds to a two-sided test of significance at level 0.05 which is the more commonly used hypothesis in practice.

Having set up the macros we can now run them in MLwiN. You will need to change the directories as before, so that the current directory is the directory that contains the macros (see Section 1.4). You may get an error message when you first attempt to execute the macros of the form "column length mismatch between DENOM and expl. variables." If so, click on OK on the error message box, and then click on Execute again. After the macros run, which can take a while, we will get the following output in the **View/Edit Data** window if we select columns c210, c211 and c231.



	Samplesize(10)	zpow0(10)	spow0(10)
1	30.000	0.178	0.185
2	60.000	0.343	0.331
3	90.000	0.457	0.465
4	120.000	0.636	0.581
5	150.000	0.635	0.680
6	180.000	0.739	0.757
7	210.000	0.829	0.819
8	240.000	0.876	0.867
9	270.000	0.903	0.903
10	300.000	0.923	0.930

Here we can see that to get a power of 0.8, a sample size of somewhere between 180 and 210 is required, with a linear interpolated estimated sample size of 201 from the standard error method. This is similar to the 194 suggested by the formulae in Section

3.1, but of course we would not expect identical values given that different normal approximations are used.

3.3.2 Comparing two proportions in the logistic regression framework

To fit a model that investigates the difference between two proportions in the logistic regression framework, we will need to include a second predictor in the linear predictor that identifies whether or not an individual woman is in the urban group. The model is then

$$y_i \sim Bernouilli(\pi_i)$$
$$\log\left(\frac{\pi_i}{1-\pi_i}\right) = \beta_0 + \beta_1 Urban_i$$

with β_0 representing the transformed proportion of contraception usage for rural women, and β_1 representing the (transformed) difference in proportion between urban and rural women. To conduct power calculations in MLPowSim for the specific case where we believe that 35% of rural women, and 50% of urban women, use contraceptives, we would use estimated effects of -0.619 for β_0 to correspond to 35%, and 0.619 for β_1, so that $\beta_0+\beta_1=0$ which corresponds to 50% of urban women. For the purposes of simulating samples of women, we will assume a binomial distribution for the urban indicator, with probability 0.3; if we are simply surveying women and recording their residence indicator, then this is a more realistic scenario than generating particular sample sizes in each category.

The inputs in MLPowSim are then as follows:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **1**
Please input the random number seed: **1**
Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **1**
Please input link function [0 – logit, 1 – probit, 2- cloglog] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**

Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**
How many explanatory variables do you want to include in your model? **1**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **1**
Please input probability of a 1 for x1 : **0.3**

Sample size set up

Please input the smallest sample size : **50**
Please input the largest sample size : **500**
Please input the step size: **25**

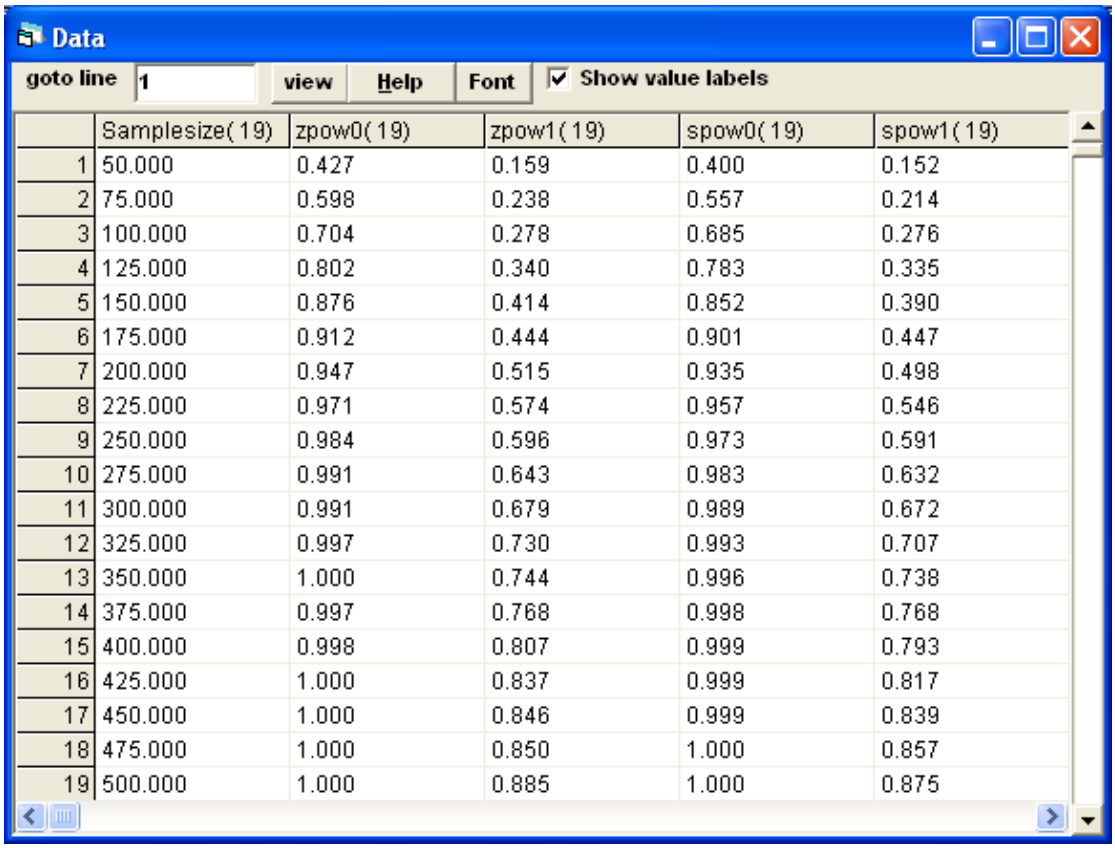
Parameter estimates

Please input estimate of beta_0: **-0.619**
Please input estimate of beta_1: **0.619**

Files to perform power analysis for the 1 level model with the following sample criterion have been created
Sample size starts at 50 and finishes at 500 with the step size 25
1000 simulations for each sample size combination will be performed

Press any key to continue…

After running the macros in MLwiN, and then selecting columns c210, c211, c212, c231 and c232, the **View/Edit Data** window should look as follows:



	Samplesize(19)	zpow0(19)	zpow1(19)	spow0(19)	spow1(19)
1	50.000	0.427	0.159	0.400	0.152
2	75.000	0.598	0.238	0.557	0.214
3	100.000	0.704	0.278	0.685	0.276
4	125.000	0.802	0.340	0.783	0.335
5	150.000	0.876	0.414	0.852	0.390
6	175.000	0.912	0.444	0.901	0.447
7	200.000	0.947	0.515	0.935	0.498
8	225.000	0.971	0.574	0.957	0.546
9	250.000	0.984	0.596	0.973	0.591
10	275.000	0.991	0.643	0.983	0.632
11	300.000	0.991	0.679	0.989	0.672
12	325.000	0.997	0.730	0.993	0.707
13	350.000	1.000	0.744	0.996	0.738
14	375.000	0.997	0.768	0.998	0.768
15	400.000	0.998	0.807	0.999	0.793
16	425.000	1.000	0.837	0.999	0.817
17	450.000	1.000	0.846	0.999	0.839
18	475.000	1.000	0.850	1.000	0.857
19	500.000	1.000	0.885	1.000	0.875

Here the columns headed ‘zpow0’ and ‘spow0’ give powers for β_0, which corresponds to testing that the probability that rural women use contraceptives is less than 0.5;

with around 125 women, this power reaches 0.8. The more interesting parameter is β_1, and we see that we need a sample of between 400 to 425 women to establish a difference between the probabilities of using contraceptives with a power of 0.8; this approximates the 432 that was calculated in Section 3.2 using the different normal approximation.

As with the normal response models in Section 2, we can perform power calculations for further categorical predictors and continuous predictors as well, but for brevity we do not give examples here, other than noting the inputs in MLPowSim will be very similar.

We will now move on to describe multilevel extensions of the binary response model.

3.4 Multilevel logistic regression models

If we return to our example dataset of Bangladeshi contraceptive use, we have now established how many women we need to survey to test two simple hypotheses with a certain power. The modelling so far has assumed that we can randomly sample women from the population; in practice, however, we are more likely to take samples from specific places, in which case we will have a structure of women nested within districts. It is likely that women from the same district will have similar probabilities of using contraceptives, and so we will not end up with an independent random sample. We can take this into account by fitting a random effect for district in our logistic regression model, as follows:

$$y_{ij} \sim Bernouilli(\pi_{ij})$$

$$\log\left(\frac{\pi_{ij}}{1-\pi_{ij}}\right) = \beta_0 + u_j, u_j \sim N(0, \sigma_u^2)$$

Here j indexes district, i indexes women within each district, β_0 is the overall average (transformed) proportion, and u_j represents district effects. From the real data we will again assume that our believed proportion is 0.4 which corresponds to a value of -0.4055 for β_0, and we will assume a variance of 0.25 for the clusters. The inputs in MLPowSim are then as follows:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **2**
Please input the random number seed: **1**

Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **1**
Please input link function [0 – logit, 1 – probit, 2- cloglog] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Please input Method [0 – MQL, 1 - PQL]: **0**
Please input order [1 – 1st, 2 – 2nd]: **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **0**

Sample size set up

Please input the smallest number of units for the second level: **10**
Please input the largest number of units for the second level: **50**
Please input the step size for the second level: **5**
Please input the smallest number of units for the first level per second level: **10**
Please input the largest number of units for the first level per second level: **10**
Please input the step size for the first level per second level: **1**

Parameter estimates

Please input estimate of beta_0: **-0.4055**
Please input estimate of sigma^2_u: **0.25**

Files to perform power analysis for the 2 level nested model with the following sample criterion have been created
Sample size in the first level starts at 10 and finishes at 10 with the step size 1
Sample size starts at 10 and finishes at 50 with the step size 5
1000 simulations for each sample size combination will be performed

Press any key to continue…

We have here decided to adopt a sampling scheme of 10 women from each district that is visited, and so the sample size that we are varying is the number of districts to visit. One thing to note here is that we have two additional questions with regard to the estimation method. For binary response multilevel models, MLwiN does not give maximum likelihood estimates, but instead gives quasi-likelihood estimates. There are two types of quasi-likelihood method available: marginal quasi-likelihood (MQL) and penalized quasi-likelihood (PQL). These methods use a Taylor series approximation and the order of this approximation can also be altered. Firstly we will show results for the simplest method: MQL 1.

If we look at columns c209, c210, c211 and c231 we see the following:

Data

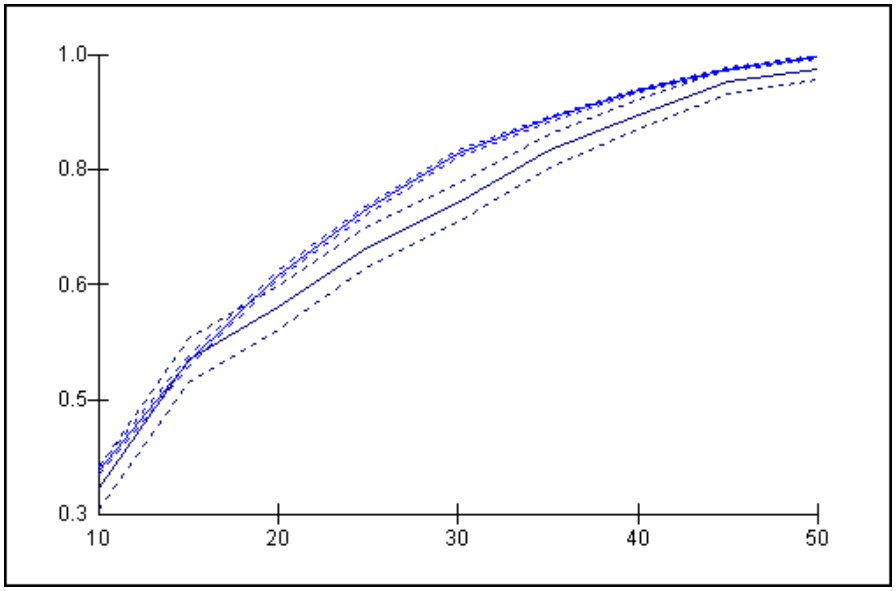
goto line 1 | view | Help | Font | Show value labels

	N-level 1(9)	N-level 2(9)	zpow0(9)	spow0(9)
1	10.000	10.000	0.356	0.382
2	10.000	15.000	0.535	0.533
3	10.000	20.000	0.608	0.654
4	10.000	25.000	0.693	0.745
5	10.000	30.000	0.754	0.822
6	10.000	35.000	0.826	0.870
7	10.000	40.000	0.877	0.910
8	10.000	45.000	0.922	0.939
9	10.000	50.000	0.940	0.957

Here we see that to get a power of 0.8, we will need to sample 30-35 districts, which translates to 300-350 women in total. This compares with only 201 women when we assume no district effects, which shows the importance of accounting for clustering in power calculations. One other thing to note is that the two methods of calculating the power give slightly different answers. This is better illustrated by graphs, which can be viewed by performing the following:

Select **Open Macro** from the **File** menu.
Select the macro file '*graphs.txt*' from the list and click on the **Open** button.
Click on the **Execute** button on the **macro** window.
Select **Customised Graph(s)** from the **Graphs** menu
Select **Apply** from the **Customised Graph** window.

The graphs that appear should look like this:



Here we see that the smoother SE method tends to give higher power values than the 0/1 method. In this case it is probably better to use the 0/1 method, because the SE

method only works well if the estimation method is unbiased, and it has been shown previously that 1st order MQL estimation tends to underestimate fixed effects (e.g. Goldstein and Rasbash, 1996), and hence their standard errors, thus inflating the power.

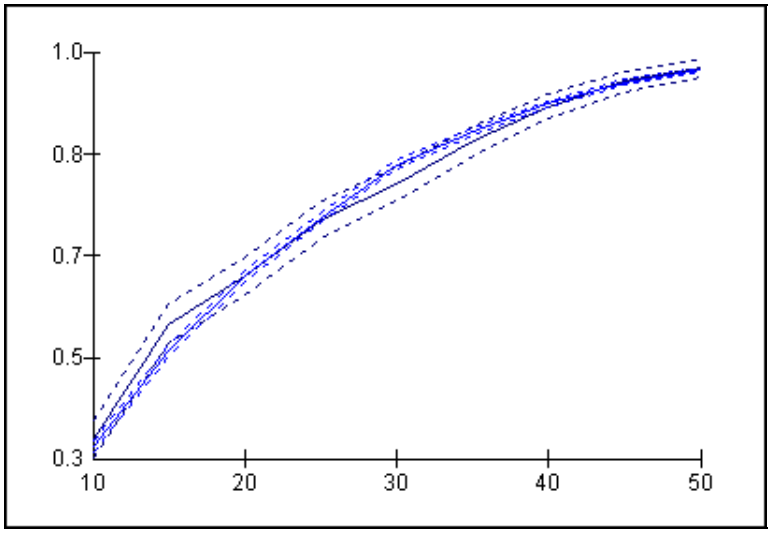
We will now look at 2nd order PQL estimation. To do this we again run MLPowSim, but this time answer **1**, when prompted, for PQL and **2** for 2nd order estimation. Once more, we run the resulting macros in MLwiN and look at columns C209, c210, c211 and c231 in the **View/Edit Data** window, where we see the following:

Data

goto line 1 | view | Help | Font | Show value labels

	N-level 1(9)	N-level 2(9)	zpow0(9)	spow0(9)
1	10.000	10.000	0.361	0.351
2	10.000	15.000	0.542	0.500
3	10.000	20.000	0.618	0.619
4	10.000	25.000	0.707	0.711
5	10.000	30.000	0.762	0.793
6	10.000	35.000	0.831	0.844
7	10.000	40.000	0.885	0.889
8	10.000	45.000	0.924	0.923
9	10.000	50.000	0.945	0.944

We can also look at the graphs for this estimation method by repeating the boxed instructions given above:



Here we see better agreement between the two methods of calculating power. This makes sense, since PQL is less biased than MQL, and the bias will only be noticeable in designs with very large cluster variability.

3.5 Multilevel logistic regression models in R

Power calculations for all the models outlined above can also be conducted using R, with generally little change in MLPowSim user input. For illustrative purposes, here we will outline power calculations for a multilevel logistic regression model in R. Compared to MLwiN, R has a different selection of possible estimation methods for binary response models. We will choose PQL in keeping with the example above, although it is also possible to use Laplace approximation methods, and Adaptive Gaussian Quadrature. The inputs in MLPowSim are as follows:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **0**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **2**
Please input the random number seed: **1**
Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **1**
Please input link function [0 – logit, 1 – probit, 2- cloglog] : **0**
Please input approximation method [0 - PQL, 1 - Laplace, 2 - AGQ] : **0**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept in your model (1=YES 0=NO)? **1**

Predictor(s) Input

Do you want to include any explanatory variables in your model (1=YES 0=NO)? **0**

Sample size set up

Please input the smallest number of units for the second level: **10**
Please input the largest number of units for the second level: **50**
Please input the step size for the second level: **5**
Please input the smallest number of units for the first level per second level: **10**
Please input the largest number of units for the first level per second level: **10**
Please input the step size for the first level per second level: **1**

Parameter estimates

Fixed Effects Input

Please input estimate of beta_0: **-0.4055**

Random Effects Input

Please input estimate of sigma^2_u: **0.25**

Final sample size check
The second level: start=10 end=50 step size=5
The first level: start=10 end=10 step size=1
Do you want to continue (YES=1 , NO=0)? **1**
Do you want to have the CI for the power in your output (YES=1 , NO=0)? **1**

Having responded to all the questions in MLPowSim, we now need to fire up the R package and run the macro file *powersimu.r* (see Section 1.5 for details on how to do this). Please note that R will take considerably longer than MLwiN to run this model, but will give you progress updates by letting you know each time 10 iterations are complete. Upon finishing all iterations, R will finish running the code, and the results will be stored in a file called *powerout.txt*. We can view the results by typing the name of the data frame (*output*) saved by the commands we have just executed in the R console:

```
> output
N       n       zLb0    zpb0    zUb0    sLb0    spb0    sUb0
10      10      0.319   0.349   0.379   0.342   0.35    0.358
15      10      0.422   0.453   0.484   0.491   0.499   0.508
20      10      0.573   0.603   0.633   0.601   0.61    0.62
25      10      0.673   0.701   0.729   0.701   0.709   0.718
30      10      0.75    0.776   0.802   0.769   0.777   0.784
35      10      0.803   0.826   0.849   0.832   0.838   0.844
40      10      0.835   0.857   0.879   0.875   0.88    0.885
45      10      0.891   0.909   0.927   0.914   0.918   0.922
50      10      0.926   0.941   0.956   0.942   0.945   0.948
```

Here we see that R gives powers of 0.826 and 0.838 for 35 districts, which compares favourably with powers of 0.831 and 0.844 from MLwiN.

MLPowSim can fit all the data structures covered in Chapter 2 using binary responses as well as normally distributed responses. For the sake of brevity we will not, however, give examples of unbalanced data structures, three level models and cross-classified models. Instead we move onto count data.

4 Count Data

We have now considered modelling both continuous and binary responses and calculating power calculations for such models. Clustered binary responses can also be considered as counts. If we assume we have collected pass/fail exam responses for children within a classroom, we would generally model the data as binary to allow the inclusion of predictor variables for the individual children, for example gender or birth date, to see if they influence whether the child passes. If, however, we have no pupil-level predictors, then we could model the proportion that pass using a (general) Binomial distribution with parameters n_i (the number of pupils in classroom i (that is known)) and p_i (the probability of passing for classroom i which we will model using classroom and school level predictors).

In MLPowSim we do not explicitly deal with general Binomial modelling as it is less common than the use of the Bernouilli (Binomial when n=1) distribution for binary data. It is also always possible to expand a single general Binomial response into a series of Bernouilli responses each with the same probability.

One can also think of the number of pupils passing the exam as a count response and model these individual counts using a different distribution designed for such responses, for example a Poisson distribution. We encounter two problems here: firstly, although the number passing is indeed a count, it has a finite upper limit – the number of pupils in the school. This means that through a Poisson model we will have a positive probability of more pupils passing than are present in the class. Secondly, if we model the counts without accounting for the class-size we will generally find the unsurprising result that larger classes have more pupils passing! We will discuss this further in later sections.

Other examples of count data are the number of heavy good vehicles (HGVs) passing a road junction in an hour and the number of cancer cases of a particular type in a population over a 10 year period. In the first example there will be a finite number of HGVs in the area, but the number is unknown, and also each HGV can pass the junction more than once during our survey period and so we would not consider this as a proportion. In the second example, we might be able to work out the population size for the population, however the incidence rate of most cancers is (thankfully) very small, and so the Poisson distribution is a good approximation for the Binomial in such cases.

4.1 Modelling rates

Both the illustrative examples of HGVs and cancer cases have one thing in common: the response is a count over a fixed time period. In reality, the Poisson distribution is generally used to model event rates: for example HGVs per hour. If the time periods for each measurement (or the population size, in the case of the cancer example we considered) are the same size, then there isn't a big distinction between rates and counts. If, however, the sizes associated with each response are different (which is often the case when dealing with populations) then there are methods to adjust for these different sizes via what is known as an *offset*. We will consider this further below, and in more detail in Section 4.4. There are standard formulae for sample size calculations for models comparing a single rate to a hypothesized value, and for comparing two rates. These formulae are very similar to those for continuous Normally-distributed data, but with both the variances and means replaced by the rates. Here we should recall that the Poisson distribution has one parameter, λ, and both the mean and variance of a Poisson (λ) distribution are λ. We will now describe a 1-level Poisson model to illustrate the case of two rates.

4.2 Comparison of two rates

We will here consider an example of traffic control. Let's assume we believe that a stretch of minor road experiences, on average, 10 HGVs per hour travelling along it during the peak period of 7am to 10am. Due to road works to another road, local

people believe that this will increase to 15 HGVs per hour during this period, and they want to petition the authorities to put safety measures in place whilst the roadworks are taking place. They want to know how many periods they would need to watch the road, counting HGVs, to show an increase in HGV traffic.

The standard formula for the sample size is

$$n \geq \frac{(Z_\beta + Z_{\alpha/2})^2(\lambda_a + \lambda_b)}{(\lambda_a - \lambda_b)^2} = \frac{(0.842 + 1.96)^2(15 + 10)}{(15 - 10)^2} = 7.85$$

where λ_b and λ_a are the expected rates before and after the road works start, and so 8 hours of watching both before and after (i.e. 16 hours in total) will suffice to gain a power of at least 0.8 of detecting a significant increase in traffic.

We will now show how this model can fit into a Poisson modelling framework.

4.3 Poisson log-linear regressions

For Poisson models we need to relate a rate (that has to be positive) to predictor variables in such a way that we do not predict rates that are negative. We do this by modelling the log of the rate as a linear function of predictor variables in what is known as a log-linear model and can be described as follows:

$$y_i \sim Poisson(\lambda_i)$$
$$\log(\lambda_i) = X_i\beta$$

Here the exponentials of the β coefficients represent multiplicative effects to the rate as we would predict λ_i as $\exp(X_i\beta)$.

We can fit a model with different rates for two groups as follows:

$$y_i \sim Poisson(\lambda_i)$$
$$\log(\lambda_i) = \beta_0 + \beta_1 After_i$$

Here $After_i$ is an indicator variable that takes value 1 if the hour was after the roadworks started and 0 if the hour was before the roadworks started. We now need to link the effect sizes β to the expected rates for the two periods. For the period before the road works we expect 10 HGVs per hour and so $\exp(\beta_0)=10$ so $\beta_0=\log_e(10)=2.303$. For the period after the road works we expect 15 HGVs and so $\exp(\beta_0+\beta_1)=15$, $\beta_0+\beta_1=\log_e(15)=2.708$ and so $\beta_1=2.708-2.303 = 0.405$.

To test for no increase we are interested in whether β_1 is greater than 0. We will now run MLPowSim to create the macros for MLwiN to perform the power calculation.

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **1**
Please input the random number seed: **1**
Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **2**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**
How many explanatory variables do you want to include in your model? **1**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **1**
Please input probability of a 1 for x1 : **0.5**

Sample size set up

Please input the smallest sample size : **4**
Please input the largest sample size : **40**
Please input the step size: **2**

Parameter estimates

Please input estimate of beta_0: **2.303**
Please input estimate of beta_1: **0.405**

Files to perform power analysis for the 1 level model with the following sample criterion have been created
Sample size starts at 2 and finishes at 40 with the step size 2
1000 simulations for each sample size combination will be performed

Press any key to continue…

It should be noted that here we are starting with two survey periods and working up to 40. Due to restrictions in how this is set up in MLPowSim, we have to give a probability that each period is before or after. This is NOT what we want here since, in the case of small samples especially, we would likely generate some simulated datasets where all periods are before, or all periods are after, the roadworks, and these would be useless for testing our hypothesis (i.e. that the rate of HGVs passing is greater after the roadworks have begun, than before). Consequently, we will need to slightly modify the macros produced. If we load up the file *setup.txt* in a text editor we can find the line that produces the predictor that indicates whether the period is before, or after. This line is as follows:

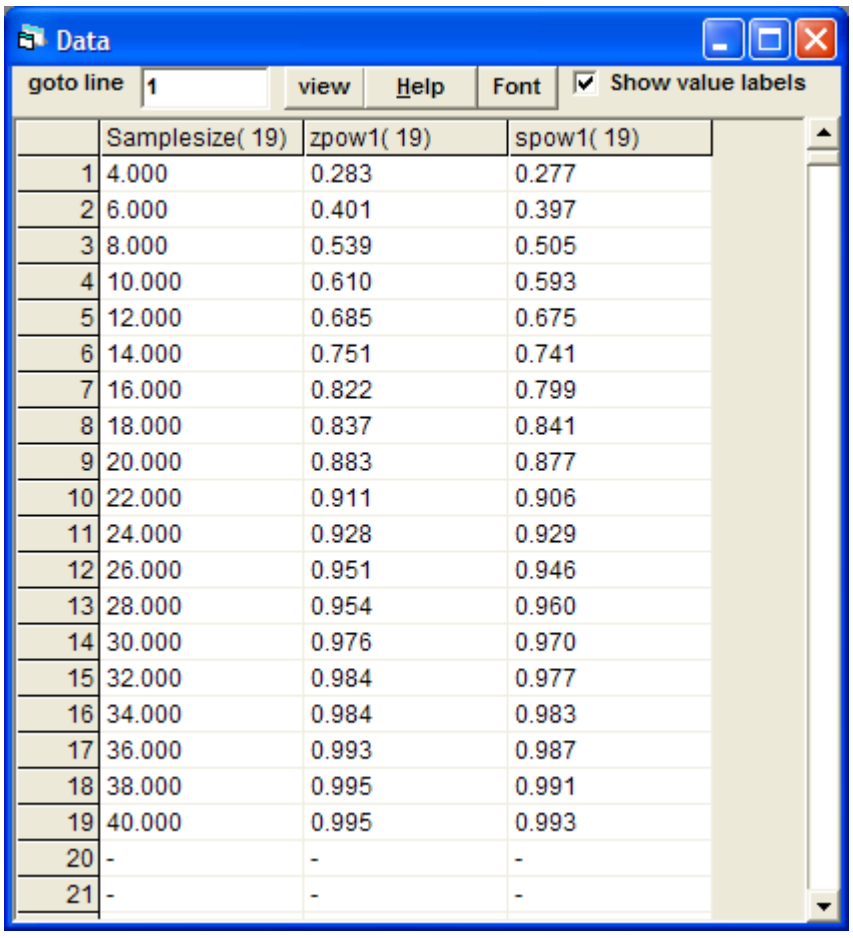
BRAN b23 c11 0.500000 1

We can remove this line and place the following three lines before the line LOOP b40 1 b41

```
CALC b24 = b23/2
CODE 2 1 b24 c11
CALC c11 = c11 – 1
```

Note that these lines firstly work out the number of pairs of survey periods, and then generate a predictor that labels the pairs and place this in c11. The CODE line uses the labels 1 and 2, and so to use the labels 0 and 1 to indicate before and after, we subtract 1 from c11. It is important after making these changes to ensure you save *setup.txt*.

If we now run the macro *simu.txt* in MLwiN, changing directory as usual, and open the View/Edit Data window to view columns c210, c212 and c232, to see the sample size and power estimates for the difference parameter β_1 from the two methods, we get the following:



	Samplesize(19)	zpow1(19)	spow1(19)
1	4.000	0.283	0.277
2	6.000	0.401	0.397
3	8.000	0.539	0.505
4	10.000	0.610	0.593
5	12.000	0.685	0.675
6	14.000	0.751	0.741
7	16.000	0.822	0.799
8	18.000	0.837	0.841
9	20.000	0.883	0.877
10	22.000	0.911	0.906
11	24.000	0.928	0.929
12	26.000	0.951	0.946
13	28.000	0.954	0.960
14	30.000	0.976	0.970
15	32.000	0.984	0.977
16	34.000	0.984	0.983
17	36.000	0.993	0.987
18	38.000	0.995	0.991
19	40.000	0.995	0.993
20	-	-	-
21	-	-	-

Here we see that a power of 0.8 is reached when we have roughly 16 observations, i.e. 8 in each group which agrees with the formulae given previously.

4.1.1 Using R

For 1-level Poisson models (and in fact for 1-level Binomial models) it turns out that using R is quicker than MLwiN as we can call a function designed specifically for fitting a 1-level model. If we initially select 0 for R when prompted in MLPowSim, we can enter the same inputs as above, although for R we will not be asked which estimation method we require. As above, we will again need to modify the code to create the balanced *x* predictor, and we do this by removing the following line in outputted file *powersimu.r* (NB we can inactivate this line of code by preceding it with ##, as shown below):

```
x[,2]<-rbinom(length,1,xprob[2])
```

and replacing it with the following:

```
##x[,2]<-rbinom(length,1,xprob[2])
zer <- rep(0,length/2)
one <- rep(1,length/2)
x[,2] <- c(zer,one)
```

If we run R, and then look at the output, we see the following estimates for the β_1 parameter (note here we don't show the estimates for β_0):

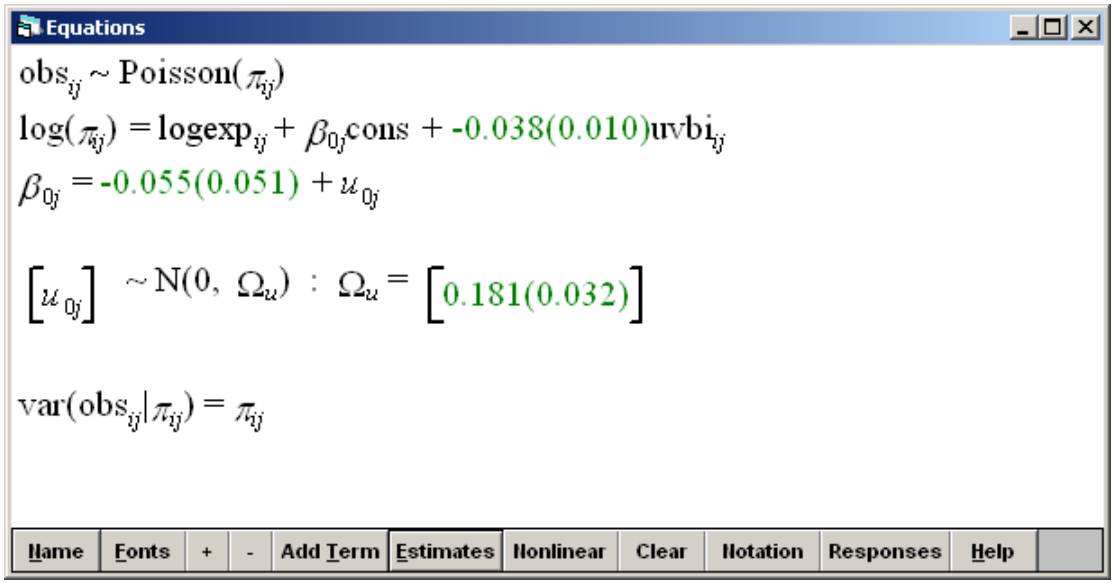
```
> output
    n     zLb1  zpb1  zUb1  sLb1  spb1  sUb1
 1  4    0.258 0.286 0.314 0.277 0.280 0.282
 2  6    0.383 0.414 0.445 0.394 0.397 0.399
 3  8    0.470 0.501 0.532 0.500 0.503 0.506
 4 10    0.548 0.579 0.610 0.595 0.598 0.601
 5 12    0.664 0.693 0.722 0.672 0.674 0.676
 6 14    0.729 0.756 0.783 0.739 0.741 0.744
 7 16    0.771 0.796 0.821 0.795 0.797 0.799
 8 18    0.824 0.846 0.868 0.841 0.842 0.844
 9 20    0.876 0.895 0.914 0.877 0.878 0.879
10 22    0.910 0.926 0.942 0.905 0.906 0.907
11 24    0.919 0.934 0.949 0.928 0.929 0.929
12 26    0.926 0.941 0.956 0.945 0.946 0.947
13 28    0.962 0.972 0.982 0.958 0.959 0.959
14 30    0.968 0.977 0.986 0.969 0.969 0.970
15 32    0.963 0.973 0.983 0.977 0.977 0.978
16 34    0.975 0.983 0.991 0.983 0.983 0.983
17 36    0.989 0.994 0.999 0.987 0.987 0.988
18 38    0.986 0.992 0.998 0.991 0.991 0.991
19 40    0.994 0.997 1.000 0.993 0.993 0.993
```

Here again we see that we need approximately 8 observations in each group to get a power of 0.8 as we saw both theoretically and using MLwiN.

4.4 Random effect Poisson regressions

We will here consider another example that appears in the MLwiN User's Guide (Rasbash et al, 2004). The melanoma mortality dataset (Langford, Bentham & McDonald, 1998) contains data on the number of male deaths due to malignant melanoma in various regions of the European community over a 10 year period. The dataset has three levels, with individual counts for counties nested within regions of 9 EC countries. For the purpose of our modelling example here, we will simply consider the two levels of counties nested within regions, and will consider the effect of UVB exposure on the rates of melanoma. UVB exposure is measured as the amount of UVB reaching the surface of the earth in each county, and this data is centred.

Running the two-level model in MLwiN (1st order MQL estimation) we get the following output:

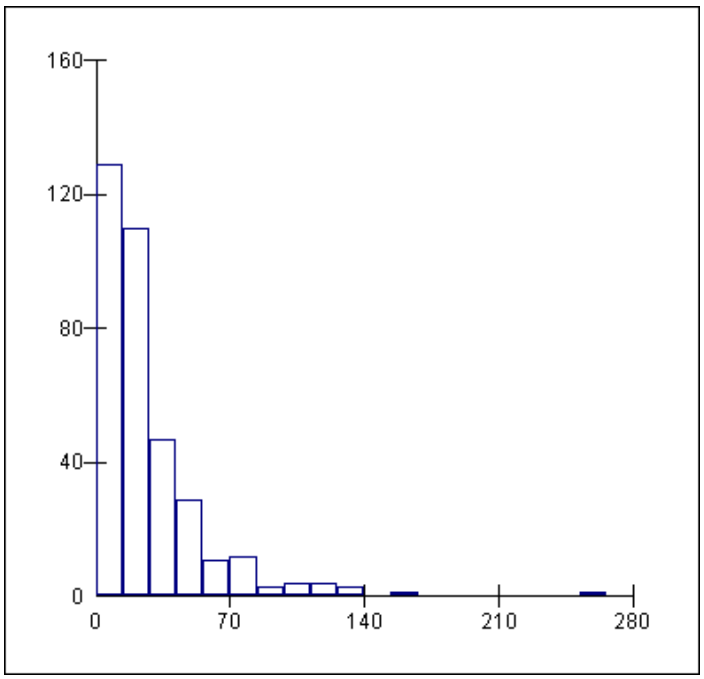


So we actually see (perhaps surprisingly) a negative effect of UVB exposure on the number of melanoma cases. Note that we are purely using this example to illustrate a certain type of model, but any reader interested in why this happens in this dataset should read the Langford et al. paper; our interest here is in performing a sample size calculation to determine how many counties in how many regions we would need to sample to find a significant effect. In the real dataset there are 354 counties in 78 regions, i.e. roughly 5 per region, so here we will consider varying the number of regions while maintaining a balanced design of 5 counties in each region.

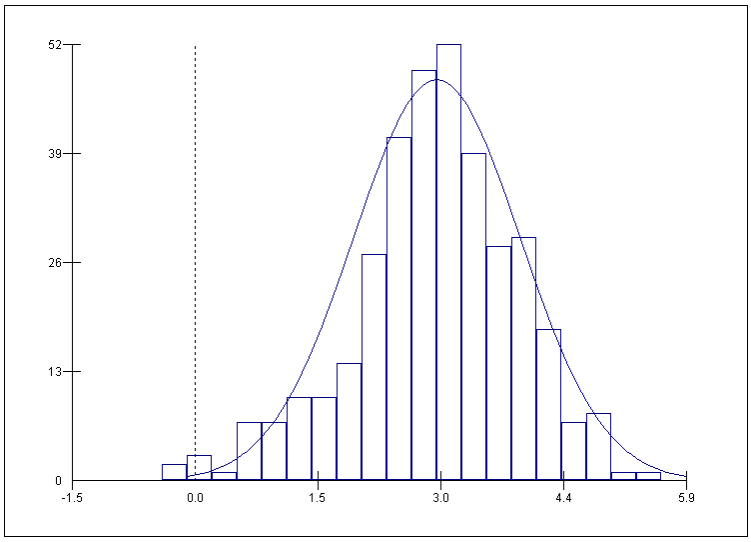
One thing to note in the above model is that the population size of counties varies, and so we are using an *offset* term to convert the number of cases to a rate response. In fact, as cancers are rare, rather than use the (logged) population size as an offset, expected numbers of cases are used instead. These are calculated by taking the total number of cases and working out how many cases we would expect in each county if there was an equal risk for each person (in fact, information on sex and age demographics in each region are usually used to calculate more accurate expected

counts). Therefore, in order to replicate the model for the sample size calculation, we will need to modify the standard macro generated by MLPowSim to include an offset term.

If we plot a histogram of the 354 expected counts, we get the following:



Basically, a fairly skewed distribution; taking logs of the data we get:



This is slightly longer-tailed than a normal distribution (compare the histogram with the curve in the figure above), however the normal is nevertheless a reasonable approximation. For each observation we will therefore generate a normally distributed offset from a Normal (2.9,1) distribution.

Firstly, however, we need to run MLPowSim to generate the macro code without the offset. To get information on the (centred) variable *uvbi* we first fit a 2-level model to see where the variance in this predictor lies:

$$\text{uvbi}_{ij} \sim \text{N}(XB,\ \Omega)$$
$$\text{uvbi}_{ij} = \beta_{0ij}\text{cons}$$
$$\beta_{0ij} = \text{-0.170(0.537)} + u_{0j} + e_{0ij}$$

$$\begin{bmatrix} u_{0j} \end{bmatrix} \sim \text{N}(0,\ \Omega_u)\ :\ \Omega_u = \begin{bmatrix} 22.395(3.584) \end{bmatrix}$$

$$\begin{bmatrix} e_{0ij} \end{bmatrix} \sim \text{N}(0,\ \Omega_e)\ :\ \Omega_e = \begin{bmatrix} 0.360(0.031) \end{bmatrix}$$

$$-2*\textit{loglikelihood(IGLS Deviance)} = 1069.796(354 \text{ of } 354 \text{ cases in use})$$

From this we will use 0 as the mean (as the data is centred) and 0.4 and 22.4 as the two levels of variability. These variances make sense as the UVB hitting the earth over a region is going to be fairly constant, while between regions it can vary a lot. The inputs to MLPowSim are therefore as follows:

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **2**
Please input the random number seed: **1**
Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **2**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Please input Method [0 - MQL, 1 - PQL] : **0**
Please input order [1 - 1st, 2 - 2nd] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**
How many explanatory variables do you want to include in your model? **1**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **2**
Assuming normality, please input its parameters here:
The mean of the predictor x1: **0**
The variance of the predictor x1 at level 1: **0.4**
The variance of the predictor x1 at level 2: **22.4**
Do you want the coefficient associated with explanatory variable x1 to be random (1=YES 0=NO) ? **0**

Sample size set up

Please input the smallest number of units for the second level: **20**
Please input the largest number of units for the second level: **80**
Please input the step size for the second level: **5**
Please input the smallest number of units for the first level per second level: **5**
Please input the largest number of units for the first level per second level: **5**
Please input the step size for the first level per second level: **1**

Parameter estimates

Please input estimate of beta_0: **-0.05**
Please input estimate of beta_1: **-0.04**
Please input estimate of sigma^2_u: **0.2**

Files to perform power analysis for the 2 level nested model with the following sample criterion have been created
Sample size in the first level starts at 5 and finishes at 5 with the step size 1
Sample size in the second level starts at 20 and finishes at 80 with the step size 5
1000 simulations for each sample size combination will be performed

Press any key to continue…

We now need to add some code to include the offset; this variable will be added into column c6. We make changes to the macro *setup.txt*, adding extra code around the line

LOOP b40 1 b41

as shown below (added lines in italics)

```
SET b13 = 3
DOFF 1 c6
LOOP b40 1 b41
  NRAN b23 c8
  CALC c6 = c8+2.9
  CALC 'offs' = c6
  NRAN b22 c590
```

Note that MLwiN will assign another column called 'offs' to contain the offsets and so it is important not only to say that there is an offset via the DOFF command but also to set the 'offs' column at each iteration.

We also need to add the offset into the simulations by changing

```
SIMU c5
```

to read (again, additional line in italics)

```
SIMU c5
CALC c5= c5+c6
```

so that the Poisson random numbers generated also include the offset. We then save the macro *setup.txt* and run the macro *simu.txt* in MLwiN. It should be noted that due

to problems in MLwiN's original Poisson random number generator with large rates that this model will only fit in the later Beta versions of MLwiN 1.10 (beta version 9, and later).

If we bring up the **View/Edit Data** window and select columns c209, c210, c212 and c232, which will be named *N-level 1*, *N-level 2*, *zpow1* and *spow1*, respectively, then once the macro has been run then we will see the following:

Data

goto line 1 | view | Help | Font | Show value labels

	N-level 1(13)	N-level 2(13)	zpow1(13)	spow1(13)
1	5.000	20.000	0.578	0.586
2	5.000	25.000	0.691	0.682
3	5.000	30.000	0.744	0.761
4	5.000	35.000	0.801	0.813
5	5.000	40.000	0.824	0.863
6	5.000	45.000	0.890	0.896
7	5.000	50.000	0.907	0.924
8	5.000	55.000	0.935	0.944
9	5.000	60.000	0.944	0.959
10	5.000	65.000	0.966	0.970
11	5.000	70.000	0.970	0.979
12	5.000	75.000	0.985	0.985
13	5.000	80.000	0.989	0.989
14	-	-	-	-

It is worth noting that for non-normal data the standard-error method doesn't work so well with estimation methods (like MQL1) that give biased estimates, however here we see reasonable agreement between the power estimates in *zpow1* and *spow1*, suggesting that this isn't such a problem for this Poisson model. The simulations suggest that only 35 regions should be enough to get the desired power of 0.8 when following cancer rates for a 10-year period. The user could also try fitting the models using PQL2, but we omit the details here.

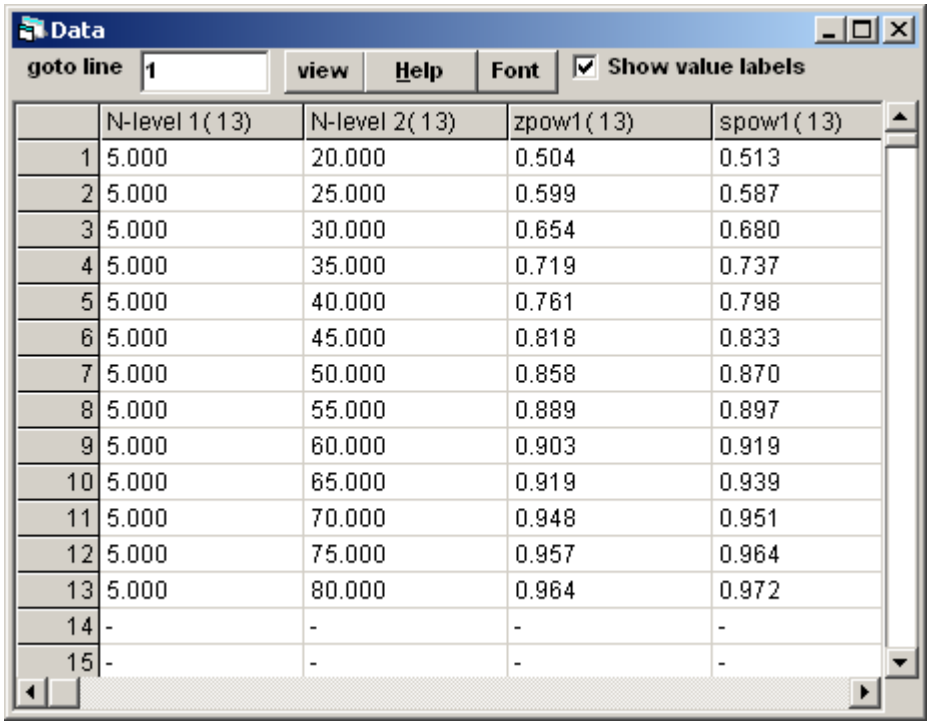
4.5 Further thoughts on Poisson data

In the examples in this chapter we have seen that it is possible to alter the output from MLPowSim to construct power calculations for models that do not naturally fit into the framework of those covered by the software. In the traffic example we saw how to construct a predictor variable that has a regular form rather than one that is generated from a specified probability distribution. In the melanoma example we saw how to include an offset in a Poisson model to deal with counts from different size populations. Disease mapping data, of which the melanoma dataset is an example, are often fitted with spatially-correlated random effects, either using multiple membership models or CAR models. Power calculations for these models are beyond the scope of the current version of MLPowSim but should be included (subject to funding) in later developments.

If we return to the melanoma dataset, it's worth noting that we can alter the sample size by changing more than just one aspect of the study design. Up to now, we have been looking at the effect of varying the number of counties for which data is collected (based on a 10-year collection period), however we could also look at varying the collection period length. We have seen that the modelling contains an offset that contains the (log of the) expected cases in a 10-year period. If we assume the probability of a case is uniform over that period, then we would expect half as many cases in a 5-year period. If we translate this into a distribution for the log of the expected counts we find that a Normal with a mean of 2.2, and a variance (once again) of 1, fits the bill. To fit such a model we simply need to modify one line in the macro *setup.txt* :

CALC c6 = c8+2.9 becomes CALC c6 = c8+2.2

We can then rerun the macros in MLwiN to get the following results:


Data

goto line 1 view Help Font Show value labels

	N-level 1(13)	N-level 2(13)	zpow1(13)	spow1(13)
1	5.000	20.000	0.504	0.513
2	5.000	25.000	0.599	0.587
3	5.000	30.000	0.654	0.680
4	5.000	35.000	0.719	0.737
5	5.000	40.000	0.761	0.798
6	5.000	45.000	0.818	0.833
7	5.000	50.000	0.858	0.870
8	5.000	55.000	0.889	0.897
9	5.000	60.000	0.903	0.919
10	5.000	65.000	0.919	0.939
11	5.000	70.000	0.948	0.951
12	5.000	75.000	0.957	0.964
13	5.000	80.000	0.964	0.972
14	-	-	-	-
15	-	-	-	-

Here we now require 45 regions to get a power of 0.8 (as opposed to 35 when we study the regions over 10 years). So we see that we can reduce the length of the study by increasing the number of regions and still get a similar power.

5 Code Details, Extensions and Further work

In this chapter we will firstly use an example to illustrate what the code generated by MLPowSim does, line by line. We will then employ this example to demonstrate how we might change the code to find power calculations for models that do not fit the standard framework. Finally, we will briefly discuss a further Bayesian method that creates power calculations using prior distributions for effect sizes, rather than point estimates (described in Wang and Gelfand, 2002).

5.1 An example using MLwiN

In this section, we will return to the tutorial example considered in Chapter 2. There we considered a variance components model with three predictors, but here we will ignore the London Reading Test (LRT) predictor, which needed a very small sample size due to its high correlation with the outcome. Instead, we will just focus on two gender-related predictors: pupil gender and school gender. The observed effects in the real dataset are different from those in the three predictor model since – when we do not include an intake measure – they represent effects of gender and school gender on raw attainment, rather than progress. Here we will use the actual estimates we obtained in the tutorial example, and we will give all the inputs for the model, so that we can see where the numbers come from when we look at the macros in detail.

Welcome to MLPowSim

Please input 0 to generate R code or 1 to generate MLwiN macros: **1**

Please choose model type

1. 1-level model
2. 2-level balanced data nested model
3. 2-level unbalanced data nested model
4. 3-level balanced data nested model
5. 3-level unbalanced data nested model
6. 3-classification balanced cross-classified model
7. 3-classification unbalanced cross-classified model

Model type : **2**
Please input the random number seed: **1**
Please input the significant level for testing the parameters: **0.025**
Please input number of simulations per setting: **1000**

Model setup

Please input response type [0 - Normal, 1- Bernouilli, 2- Poisson] : **0**
Please enter estimation method [0 - RIGLS, 1 - IGLS, 2 - MCMC] : **1**
Do you want to include the fixed intercept in your model (1=YES 0=NO)? **1**
Do you want to have a random intercept in your model (1=YES 0=NO)? **1**
Do you want to include any explanatory variables in your model (1=YES 0=NO)? **1**
How many explanatory variables do you want to include in your model? **2**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **3**
Assuming multivariate normality, please input its parameters here:
The mean of the predictor x1: **0.6**
The mean of the predictor x2: **0.462**
The variance matrix of the predictors at level 1
The element [1,1] : **0.120**
The element [2,1] : **0**
The element [2,2] : **0**
The variance matrix of the predictors at level 2
The element [1,1] : **0.125**
The element [2,1] : **0.045**
The element [2,2] : **0.249**
Do you want the coefficient associated with explanatory variable x1 to be random (1=YES 0=NO) ? **0**
Do you want the coefficient associated with explanatory variable x2 to be random (1=YES 0=NO) ? **0**

Sample size set up

Please input the smallest number of units for the second level: **20**
Please input the largest number of units for the second level: **300**
Please input the step size for the second level: **20**
Please input the smallest number of units for the first level per second level: **40**
Please input the largest number of units for the first level per second level: **40**
Please input the step size for the first level per second level: **10**

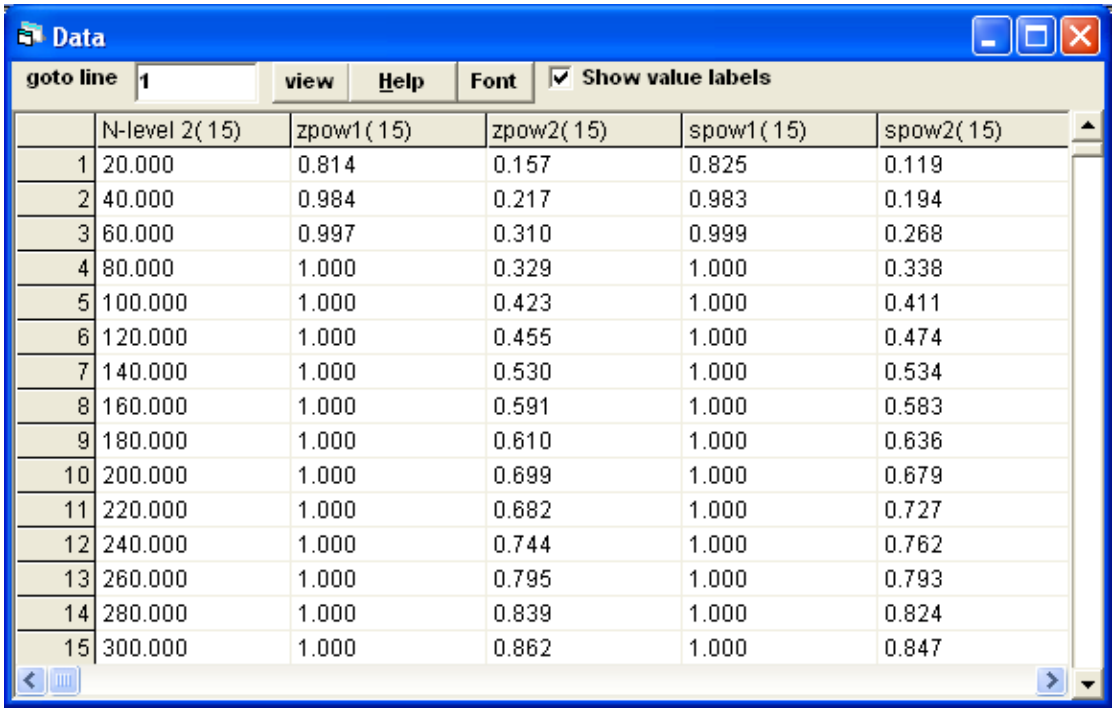
Parameter estimates

Please input estimate of beta_0: **-0.226**
Please input estimate of beta_1: **0.257**
Please input estimate of beta_2: **0.146**
Please input estimate of sigma^2_u: **0.156**
Please input estimate of sigma^2_e: **0.839**

Files to perform power analysis for the 2 level nested model with the following sample criterion have been created
Sample size in the first level starts at 20 and finishes at 300 with the step size 20
Sample size in the second level starts at 40 and finishes at 40 with the step size 10
1000 simulations for each sample size combination will be performed

Press any key to continue…

If we run the macros in MLwiN, and then highlight columns c210, c212, c213, c232 and c233 in the **View/Edit Data** window, we will see the following:



	N-level 2(15)	zpow1(15)	zpow2(15)	spow1(15)	spow2(15)
1	20.000	0.814	0.157	0.825	0.119
2	40.000	0.984	0.217	0.983	0.194
3	60.000	0.997	0.310	0.999	0.268
4	80.000	1.000	0.329	1.000	0.338
5	100.000	1.000	0.423	1.000	0.411
6	120.000	1.000	0.455	1.000	0.474
7	140.000	1.000	0.530	1.000	0.534
8	160.000	1.000	0.591	1.000	0.583
9	180.000	1.000	0.610	1.000	0.636
10	200.000	1.000	0.699	1.000	0.679
11	220.000	1.000	0.682	1.000	0.727
12	240.000	1.000	0.744	1.000	0.762
13	260.000	1.000	0.795	1.000	0.793
14	280.000	1.000	0.839	1.000	0.824
15	300.000	1.000	0.862	1.000	0.847

Here we see that the gender predictor needs very few (less than 20) schools to gain a power of 0.8 (*zpow1* & *spow1*), whilst the school gender predictor needs at least 260 schools to gain this power (*zpow2* & *spow2*). We will now examine, in detail, the corresponding macros:

5.1.1 The *simu.txt* macro

The *simu.txt* macro code for this example is as follows:

```
NOTE MLwiN macro code generated by MLPowSim
NOTE This is outer code to be run directly in MLwiN
NOTE You will also need simu2.txt, setup.txt and analyse.txt
SEED 1
ERASE C594-C598
NOTE setup the values of beta, sigma2u, sigma2e etc.
JOIN C598 -0.226000 C598
JOIN C598 0.257000 C598
JOIN C598 0.146000 C598
JOIN C596 0.156000 C596
JOIN C596 0.839000 C596
NOTE put MVN variances for predictors in model
JOIN c594 0.120000 c594
JOIN c594 0.000000 c594
JOIN c594 0.000000 c594
JOIN c595 0.125000 c595
JOIN c595 0.045000 c595
JOIN c595 0.249000 c595
NAME c209 "N-level 1"
NAME c210 "N-level 2"
NAME c211 "zpow0" c231 "spow0"
NAME c251 "zlow0" c291 "slow0"
NAME c271 "zupp0" c311 "supp0"
NAME c212 "zpow1" c232 "spow1"
NAME c252 "zlow1" c292 "slow1"
NAME c272 "zupp1" c312 "supp1"
NAME c213 "zpow2" c233 "spow2"
NAME c253 "zlow2" c293 "slow2"
NAME c273 "zupp2" c313 "supp2"
CALC b41 = 1000
LOOP b22 20 300 20
  OBEY simu2.txt
ENDL
```

MLwiN uses two storage devices: *columns*, which begin with the letter 'c' (but which can also be named), and which contain a vector of numbers, and *boxes*, which begin with the letter 'b', and contain single numbers.

The NOTE command in MLwiN allows us to provide comments, for our own reference as is done at the top of this file. The macro begins by setting the random number seed (SEED command) to the value inputted in MLPowSim. Then the columns c594-c598 are erased in case other macros have been run previously. The fixed effect estimates for the simulation are then stacked in column C598 using the JOIN command, as are the variance estimates in C596. Next the (lower diagonal) variance matrices for the two predictor variables are stacked in c594 and c595 for levels 1 and 2, respectively.

Then a number of columns are named to aid the viewer when inspecting the output. These contain the sample size at each level (*N-level 1* or *2*), and the power estimates (*pow*), together with upper (*upp*) and lower (*low*) intervals, for the intercept (*0*) and predictors (*1* and *2*) (for both standard error (*s*) and zero/one method (*z*)).

The number of simulations to be executed per setting (1000) is then stored in box b41. A loop is then run over the numbers of level 2 units, which at each pass through the loop are stored in box b22. Here the command LOOP b22 20 300 20 means looping starts from value 20 and steps through the loop in multiples of 20 until we reach 300. The OBEY command within the loop then calls another macro (*simu2.txt*) which will be run each time through the LOOP. Note that one feature of the MLwiN macro language is that only one LOOP can be present in each macro hence the need for additional macro files that are called via the OBEY command. We next look at the macro *simu2.txt*.

5.1.2 The *simu2.txt* macro

The *simu.txt* macro sets up looping through the desired numbers of highest level (in this case level 2) units. For one-level models, this macro will call straight through to the *setup* macro, whilst for three-level models there will be both a *simu2* and a *simu3* macro. In our case, the *simu2* macro allows looping through the numbers of level 1 units to be considered within the level 2 units, and the code, in *simu2*, looks like this:

```
NOTE MLwiN macro code generated by MLPowSim
NOTE This code simply covers second level of looping!
LOOP b21 40 40 10
  OBEY setup.txt
ENDL
```

Here b21 will store the number of level 1 units per level 2 unit, and since here we only consider 40, we have a loop running from 40 to 40 which will simply set b21 to 40 and be performed once. The file then calls the *setup* macro which does most of the work.

5.1.3 The *setup.txt* macro

As the name suggests, the *setup* macro sets up the data structures for the simulations, and runs the models. The code is as follows:

```
NOTE MLwiN macro code generated by MLPowSim
NOTE b21 - number of level per level 2, b22 - number of level 2
CALC b23 = b21*b22
ERASE c1011 c1012
GENErate 1 b23 c1
CODE b22 b21 1 c2
PUT b23 1 c4
PUT b23 1 c5
NAME c1 'l1id' c2 'l2id' c4 'cons' c5 'resp'
RESP c5
IDEN 2 c2
IDEN 1 c1
EXPL 1 c4
SETV 1 c4
SETV 2 c4
PUT b23 1 c11
```

```
ADDT c11
PUT b23 1 c12
ADDT c12
ERROR 0
BATCH 1
PREF 0
POST 0
LOOP b40 1 b41
  MRAN b22 c595 c601-c602
  REPE b21 c601 c621
  REPE b21 c602 c622
  MRAN b23 c594 c11-c12
  CALC c11 = 0.600000 + c11 +c621
  CALC c12 = 0.462000 + c12 +c622
  PICK 1 c598 b51
  EDIT 1 c1098 b51
  PICK 2 c598 b51
  EDIT 2 c1098 b51
  PICK 3 c598 b51
  EDIT 3 c1098 b51
  PICK 1 c596 b51
  EDIT 1 c1096 b51
  PICK 2 c596 b51
  EDIT 2 c1096 b51
  SIMU c5
  METH 1
  START
  JOIN c1098 c1096 c1011 c1011
  JOIN c1099 c1097 c1012 c1012
ENDL
OBEY analyse.txt
PAUSE 1
```

As can be seen, there is slightly more to this macro. The first CALC command puts the total number of pupils into box b23. The ERASE command empties some columns that will be used later. The command GENE 1 b23 c1 creates a column that contains the sequence of numbers from 1 to b23, representing the level 1 identifiers. Next, the CODE command will create a column of b21 repeats of the numbers between 1 and b22: i.e. will create a column of level 2 identifiers. The two PUT commands then create constant columns, one for the intercept and one for the response, which will later be replaced with a simulated response.

The NAME command labels the columns created, and the RESP command tells MLwiN that the response variable is stored in column c5. The IDEN commands give the columns that contain the level 2 and level 1 identifiers. The EXPL command sets the intercept as a predictor variable, and the two SETV commands then include residuals at level 1, and random intercepts at level 2, respectively.

The combinations of PUT and ADDT commands create columns for the two predictors (gender and school gender) which, before simulating, are simply given constant values, and adds these predictors into the model. The command ERROR 0 tells MLwiN to continue running the macro regardless of error messages, and the BATCH 1 command tells MLwiN that we are running in batch mode: i.e. from a macro.

The PREF 0 and POST 0 commands simply tell MLwiN that there are no pre or post files to be run, since we have a normal response model. Note that pre and post files are separate macros that MLwiN uses for other response types. We then LOOP through the b41 simulations for this setting (in this example b41 is 1000). The code inside the LOOP will create a simulated dataset, run the model, and then store the output as described below.

The first MRAN command generates b22 pairs of random (zero mean) multivariate normal-distributed variables in columns c601 and c602, using the (lower diagonal) variance matrix stored in c595: i.e. it creates the school-level parts of the two predictors. The two REPEat commands then match these school-level parts to the dataset in columns C621 and C622, respectively. The second MRAN command generates b23 pairs of random (zero mean) multivariate normal-distributed variables in columns c11 and c12, using the (lower diagonal) variance matrix stored in c594: i.e. it creates the student-level parts of the two predictors. The 2 CALC commands then create the whole predictor variables in c11 and c12, by adding their means to the student and school parts.

There are then a whole list of PICK and EDIT commands; these basically transfer the fixed effect and variance parameters for the simulation from their stored columns (c596 and c598) to the columns c1096 and c1098. These are special columns in MLwiN, containing the estimates for the variances and fixed effects (respectively) for the current fitted model. We copy the values in here so that we can run the SIMU command; this will create a response variable in C5 based on the values in c1096 and c1098, and the currently-set-up model.

We then have the METH 1 command which confirms that we are to use IGLS estimation, and the START command which fits the model to the current simulated data using IGLS. The two JOIN commands then take the estimates (fixed effects and variances) and variance of estimate matrices, respectively, for this simulation and place them into columns c1011 and c1012. It would be possible here to only store the fixed effects estimates and their variance matrix, since that is all we will use, but for completeness the variances are stored. The LOOP then ends with the ENDL command, and after the 1000 simulations are run the *analyse.txt* macro is called to create power estimates from the output.

The macro ends with a PAUSE 1 command which, for a split second, gives back control to the screen, and hence updates all the windows so that we can observe progress of the macro in the **Data** window. It is worth noting that if the macros have come up with a numerical error while model-fitting, which is possible for example when we have small sample sizes and random slopes models, then this error will be displayed when the PAUSE 1 command is reached; here, the effect of the error-suppressing ERROR 0 command will be nullified at this point. If you have this problem, it will be sensible to either increase the size of your smaller simulation designs, or remove the PAUSE 1 command so that MLwiN will perform all simulations before displaying the error message.

5.1.4 The *analyse.txt* macro

The *analyse.txt* macro takes the output from one set of simulations and calculates power estimates and confidence intervals for these estimates. The code is as follows:

```
NOTE MLwiN macro code generated by MLPowSim
CODE 5 1 b41 c30
CODE 9 1 b41 c31
SPLIT c1011 c30 c51-c55
SPLIT c1012 c31 c101-c109
NOTE calculate IGLS interval coverage
NED 0.975000 b42
JOIN c209 b21 c209
JOIN c210 b22 c210
CALC c101 = c101*(c101>0) - c101*(c101<0)
CALC c101 = sqrt(c101)
CALC c200= c51 + b42*c101
CALC c201= c200<0
AVER c201 b202 b203 b204
JOIN c211 b203 c211
CALC b204 = (b203)*(1-b203)/b41
CALC b205 = b203-b42*sqrt(b204)
JOIN c251 b205 c251
CALC b205 = b203+b42*sqrt(b204)
JOIN c271 b205 c271
CALC c103 = c103*(c103>0) - c103*(c103<0)
CALC c103 = sqrt(c103)
CALC c200= c52 - b42*c103
CALC c201= c200>0
AVER c201 b202 b203 b204
JOIN c212 b203 c212
CALC b204 = (b203)*(1-b203)/b41
CALC b205 = b203-b42*sqrt(b204)
JOIN c252 b205 c252
CALC b205 = b203+b42*sqrt(b204)
JOIN c272 b205 c272
CALC c106 = c106*(c106>0) - c106*(c106<0)
CALC c106 = sqrt(c106)
CALC c200= c53 - b42*c106
CALC c201= c200>0
AVER c201 b202 b203 b204
JOIN c213 b203 c213
CALC b204 = (b203)*(1-b203)/b41
CALC b205 = b203-b42*sqrt(b204)
JOIN c253 b205 c253
CALC b205 = b203+b42*sqrt(b204)
JOIN c273 b205 c273
NOTE calculate IGLS SE method
AVER c101 b202 b203 b204 b205
CALC b206= b203+b42*b205
CALC b207= b203-b42*b205
CALC b203=(-0.226000)/b203
CALC b203 = b203+b42
CALC b206=(-0.226000)/b206
CALC b206 = b206+b42
CALC b207=(-0.226000)/b207
CALC b207 = b207+b42
NPRO b203 b204
JOIN c231 b204 c231
```

```
NPRO b206 b204
JOIN c291 b204 c291
NPRO b207 b204
JOIN c311 b204 c311
AVER c103 b202 b203 b204 b205
CALC b206= b203+b42*b205
CALC b207= b203-b42*b205
CALC b203=0.257000/b203
CALC b203 = (-1)*b203+b42
CALC b206=0.257000/b206
CALC b206 = (-1)*b206+b42
CALC b207=0.257000/b207
CALC b207 = (-1)*b207+b42
NPRO b203 b204
JOIN c232 b204 c232
NPRO b206 b204
JOIN c292 b204 c292
NPRO b207 b204
JOIN c312 b204 c312
AVER c106 b202 b203 b204 b205
CALC b206= b203+b42*b205
CALC b207= b203-b42*b205
CALC b203=0.146000/b203
CALC b203 = (-1)*b203+b42
CALC b206=0.146000/b206
CALC b206 = (-1)*b206+b42
CALC b207=0.146000/b207
CALC b207 = (-1)*b207+b42
NPRO b203 b204
JOIN c233 b204 c233
NPRO b206 b204
JOIN c293 b204 c293
NPRO b207 b204
JOIN c313 b204 c313
```

Here there is a lot of repetition, since there are three fixed effect parameters to deal with. The first two CODE commands are to create indicator columns, so that the individual parameter estimates (in c1011) and their variances (in c1012) can be extracted. The two SPLIT commands perform this extraction, and put the estimates in columns beginning with c51, and their variance matrices in columns beginning with c101.

Next, the NED command finds the correct value from the normal distribution to represent the desired significance level; since we have set the significance level at 0.025, this is set at 0.975 (1-0.025). The following two JOIN commands store the numbers of level 1 and 2 units in c209 and c210, respectively for output purposes. We then have 4 CALC commands, followed by an AVER command and a JOIN command. The first CALC ensures the variances of the estimates are positive, the second CALC converts the variances to standard errors, whilst the third CALC then creates upper limits for the confidence intervals (as the predicted effect is negative) and stores them in c200. We then evaluate how many of these upper limits are themselves negative (i.e. we evaluate whether the confidence interval contains 0 or not): if an upper limit doesn't contain 0 then a value of 1 is stored in c201, whereas if it does contain 0 then a value of 0 is stored. The AVER command calculates the average of the 0/1 values, which is the 0/1 method of estimating power; this is then

stored in b203. Finally, the JOIN command adds this estimate to the column (in this case c211) which will contain the stacked list of powers for the various settings.

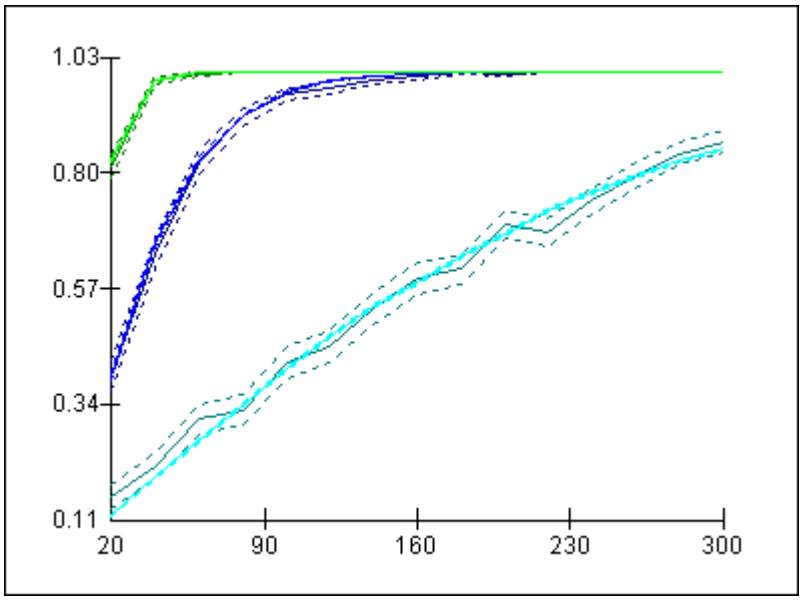
The next 5 lines calculate the standard error of this power estimate based on a Bernouilli assumption (in b204), and create lower and upper confidence intervals which are stored initially in b205 before being stacked in c251 and c271, respectively. The 11 lines for the intercept parameter are then repeated for the two predictors, with the lower limits being used, since the predicted effects are positive. This will take us to the NOTE command and finish the O/1 method.

For the SE method, we start by finding the average of the estimated standard errors. We begin with the intercepts, using C101, and store the result in b203, along with normally-distributed confidence limits stored in b206 and b207. The two lines CALC b203 = (-0.226000)/b203 and CALC b203 = b203+b42 then construct a value in b203 which, when converted to a normal probability, will give the power. Similar lines are given for the two confidence limits. The 3 pairs of NPRO and JOIN commands then calculate and stack the powers for the SE method in c231, with the lower limits in c291, and the upper limits in c311.

These 15 lines are all for the intercept parameter, and similar lines are then given for the two predictors, which takes us to the end of macro. The ending of the macro will result in a return to the *setup* macro, where we will run through the next scenario of pupil and school numbers, with the *analyse* macro being called once per scenario.

5.1.5 The *graph.txt* macro

The *graphs* macro is an additional macro which can assist the user in graphing their power calculations. It is called after the macros have run, and produces graphs like the ones shown below:



Basically, for each predictor and each method, three lines are drawn giving the mean power curve and confidence intervals. The macro is rather repetitive and so here we give just the code that produces the lines for the 0/1 method, and the intercept:

```
NOTE MLwiN macro code generated by MLPowSim
NOTE can be run after finishing execution to give graphs
GIND 1 1
GYCO c211
GXCO c210
GTYP 1
GCLR 1
CALC c251 = c211 - c251
GYER 1 c251
GYER 2 c251
GETY 1
```

The commands, in sequence, give the display and line number in GIND, and the columns to plot in GYCO and CXCO; GTYP 1 gives a line graph, and GCLR 1 gives colour 1 (dark blue). The CALC command constructs the difference between the mean and the upper limit to use as errors. Note that for the SE method, we do not have symmetric errors, and so there will be two CALC commands. The two GYER commands then state that the upper and lower errors are in C251. The GETY command sets error plotting to lines, as opposed to bars.

5.2 Modifying the example in MLwiN to include a multiple category predictor

Again, using the education-based example we employed in the preceding section, here we will look at how we might alter the code produced by MLPowSim to better represent the predictors in the model. Our modifications will need to take account of the following three factors:

(i) in reality, the school gender takes 3 values, representing mixed schools, girls' schools and boys' schools. We would typically fit this as a pair of indicator vectors that signify whether a school is a girls' school or not, and whether a school is a boys' school or not;

(ii) the gender predictor is strongly related to the school gender predictor, and if the school is single sex, then the gender predictor is determined for all the school's pupils;

(iii) the school gender predictor would normally be tested using a deviance test rather than separate Z tests for each category.

We will show how to modify the code to cater for each of these features, building up from the initial macros that can be generated by MLPowSim, which is where we start our discussion.

5.2.1 Initial macros

Although the code given previously is similar to our modelling situation, and we could in theory start from that, in practice it will be easier to start by assuming that we have two school gender predictors, representing girls' schools and boys' schools. It is also better to assume independence between the three predictors. To do this we need to change two parts of the macros we employed earlier. Firstly, when defining the predictors, we will have:

How many explanatory variables do you want to include in your model? **3**
Please choose a type for the predictor x1 (1=Binary 2=Continuous 3=all MVN): **1**
Please input probability of a 1 for x1 : **0.6**
Please choose a type for the predictor x2 (1=Binary 2=Continuous): **2**
Assuming normality, please input its parameters here:
The mean of the predictor x2: **0.15**
The variance of the predictor x2 at level 1: **0**
The variance of the predictor x2 at level 2: **0.13**
Please choose a type for the predictor x3 (1=Binary 2=Continuous): **2**
Assuming normality, please input its parameters here:
The mean of the predictor x3: **0.30**
The variance of the predictor x1 at level 1: **0**
The variance of the predictor x1 at level 2: **0.21**
Do you want the coefficient associated with explanatory variable x1 to be random (1=YES 0=NO) ? **0**
Do you want the coefficient associated with explanatory variable x2 to be random (1=YES 0=NO) ? **0**
Do you want the coefficient associated with explanatory variable x3 to be random (1=YES 0=NO) ? **0**

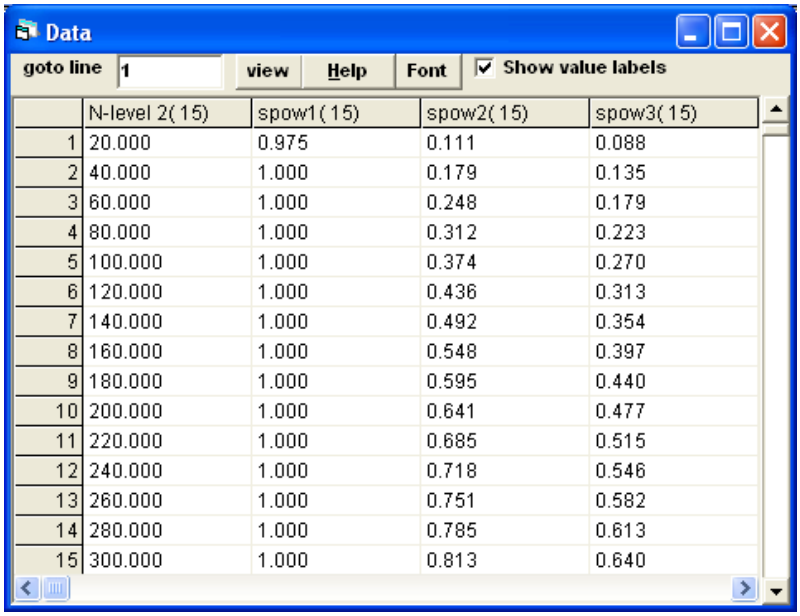
In the real data there are twice as many girls' schools than boys' schools, and we want to specify these as level 2 variables; this can only be done in MLPowSim if we assume the predictors are continuous, as we have specified in our input above.

Secondly, we need to alter the expected estimates to cater for the additional predictor, as follows:

Parameter estimates

Please input estimate of beta_0: **-0.228**
Please input estimate of beta_1: **0.262**
Please input estimate of beta_2: **0.191**
Please input estimate of beta_3: **0.123**
Please input estimate of sigma^2_u: **0.155**
Please input estimate of sigma^2_e: **0.839**

Here, most of the estimates have changed little from the model with a common single-sex school effect, however the 0.146 effect of single sex school has been split into a stronger (0.191) boys' school effect, and a slightly weaker (0.123) girls' school effect. To confirm that you have the correct macros running, they should give the following output in MLwiN:



	N-level 2(15)	spow1(15)	spow2(15)	spow3(15)
1	20.000	0.975	0.111	0.088
2	40.000	1.000	0.179	0.135
3	60.000	1.000	0.248	0.179
4	80.000	1.000	0.312	0.223
5	100.000	1.000	0.374	0.270
6	120.000	1.000	0.436	0.313
7	140.000	1.000	0.492	0.354
8	160.000	1.000	0.548	0.397
9	180.000	1.000	0.595	0.440
10	200.000	1.000	0.641	0.477
11	220.000	1.000	0.685	0.515
12	240.000	1.000	0.718	0.546
13	260.000	1.000	0.751	0.582
14	280.000	1.000	0.785	0.613
15	300.000	1.000	0.813	0.640

Here, we see results similar to those in Section 5.1, indicating that we need very few schools to detect a gender effect (*spow1*) but far more schools to detect school gender effects. We see that the girls' school effect (*spow3*) has less power than the boys' school effect (*spow2*); this is due, in the main, to the estimate for boys' schools being bigger in magnitude than the estimate for girls' schools.

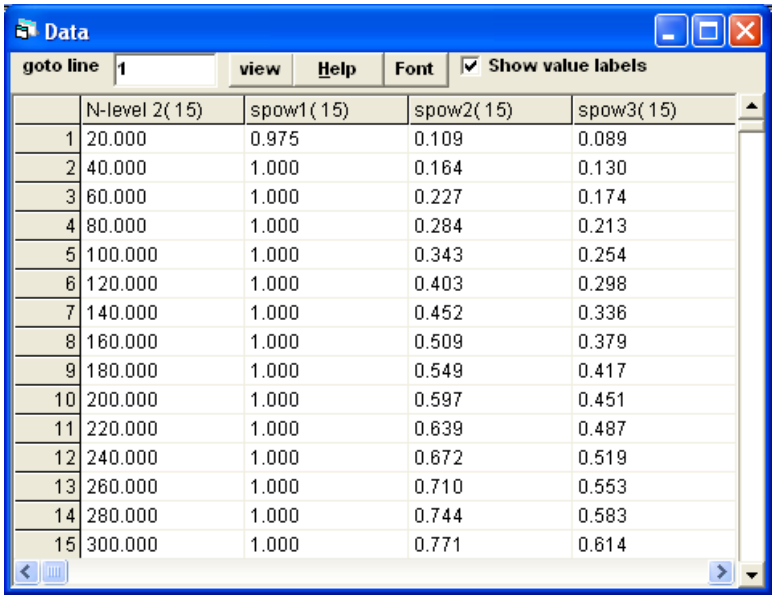
5.2.2 Creating a multiple category predictor

The results above are based on assuming two independent continuous level 2 predictors to represent the two single sex school categories. This is problematic, since the continuous predictors will have more information than the binary predictors, and so the power calculations may be overoptimistic. Here, we will alter the code in the macro *setup.txt* to convert these two continuous predictors to a multinomial variable that corresponds to two dummy variables. Below is the start of the inner loop code in *setup.txt* where added lines have been included in italics, and removed lines are superseded with a NOTE command (although in reality it might be easier to simply delete the commands):

```
LOOP b40 1 b41
  BRAN b23 c11 0.600000 1
  URAN b22 c589
  CALC c590 = c589< 0.15
  NOTE NRAN b22 c590
  NOTE CALC c590 = c590*0.360555
  NOTE REPE b21 c590 c591
  NOTE NRAN b23 c12
  NOTE CALC c12 = 0.150000 + c12*0.000000 + c591
  REPE b21 c590  c12
  NOTE NRAN b22 c590
  NOTE CALC c590 = c590*0.458258
  CALC c590 = (c589 > 0.15)&(c589 < 0.45)
  NOTE REPE b21 c590 c591
  NOTE NRAN b23 c13
  REPE b21 c590 c13
```

```
NOTE CALC c13 = 0.300000 + c13*0.000000 + c591
```

If we save these changes to *setup.txt* and rerun the macros we will get the following results:



	N-level 2(15)	spow1(15)	spow2(15)	spow3(15)
1	20.000	0.975	0.109	0.089
2	40.000	1.000	0.164	0.130
3	60.000	1.000	0.227	0.174
4	80.000	1.000	0.284	0.213
5	100.000	1.000	0.343	0.254
6	120.000	1.000	0.403	0.298
7	140.000	1.000	0.452	0.336
8	160.000	1.000	0.509	0.379
9	180.000	1.000	0.549	0.417
10	200.000	1.000	0.597	0.451
11	220.000	1.000	0.639	0.487
12	240.000	1.000	0.672	0.519
13	260.000	1.000	0.710	0.553
14	280.000	1.000	0.744	0.583
15	300.000	1.000	0.771	0.614

So here we see that when we truly use a multinomial distribution, the powers obtained are smaller. We next need to tie up the gender predictor with the school gender predictor.

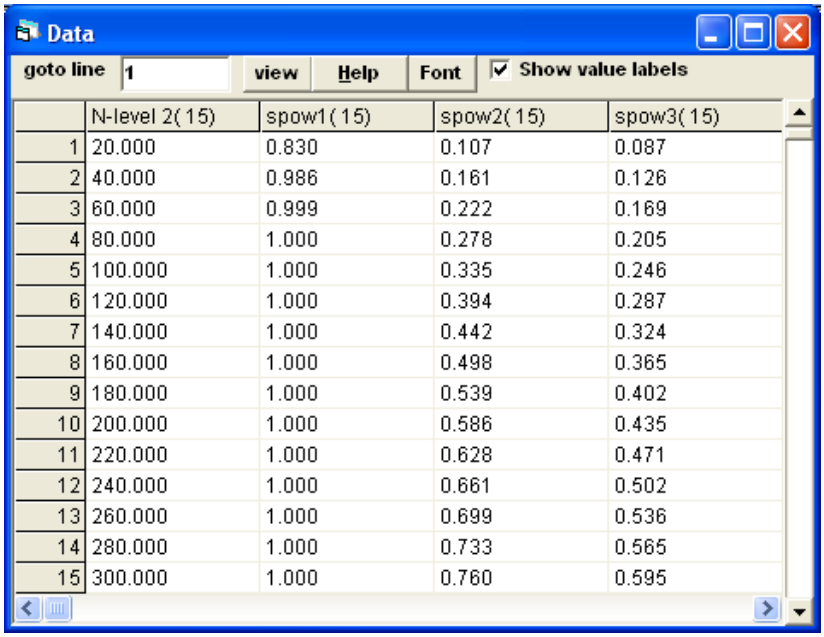
5.2.3 Linking gender to school gender

So far, the modelling has assumed independence between gender and school gender, which means that the code will generate simulated datasets where single sex schools have both boys and girls. We will now change the macro so that for girls' schools all pupils are girls and for boys' schools all pupils are boys. In the mixed schools, 48.8% of pupils are girls, and school identifier only explains about 10% of the variability in pupil gender. With regard to the gender predictor, we will assume that for mixed schools we have a probability of 0.5 for each pupil being a girl. Once more, we need to modify the file *setup.txt* to implement this change (the lines of code we have added are again in italics):

```
LOOP b40 1 b41
  NOTE BRAN b23 c11 0.600000 1
  BRAN b23 c11 0.5 1
  URAN b22 c589
  CALC c590 = c589< 0.15
  REPE b21 c590  c12
  CALC c590 = (c589 > 0.15)&(c589 < 0.45)
  REPE b21 c590 c13
  CALC c11 = c13 + c11*((c12==0)&(c13==0))
```

Here we have changed 2 lines. Firstly we have updated the probability of being a girl to 0.5, as this now corresponds to mixed schools only. Secondly, whilst the gender

response is created as before, in the last line its value is only taken if both c12 and c13 are 0: i.e. only for mixed schools. Otherwise, all pupils have gender 1 for girls' schools, and gender 0 for boys' schools. If we again run the macros with these changes, we will get the following results:



	N-level 2(15)	spow1(15)	spow2(15)	spow3(15)
1	20.000	0.830	0.107	0.087
2	40.000	0.986	0.161	0.126
3	60.000	0.999	0.222	0.169
4	80.000	1.000	0.278	0.205
5	100.000	1.000	0.335	0.246
6	120.000	1.000	0.394	0.287
7	140.000	1.000	0.442	0.324
8	160.000	1.000	0.498	0.365
9	180.000	1.000	0.539	0.402
10	200.000	1.000	0.586	0.435
11	220.000	1.000	0.628	0.471
12	240.000	1.000	0.661	0.502
13	260.000	1.000	0.699	0.536
14	280.000	1.000	0.733	0.565
15	300.000	1.000	0.760	0.595

Here we see that the power for the gender predictor reduces when we use this better simulation of the predictors. Again, this makes sense, since for the single sex schools you will not be able to separate both the gender effect and the school gender effect, and so for the gender predictor you are relying on the mixed effect schools. The school gender power is also slightly reduced for the same reasons.

5.2.4 Performing a deviance test

Generally one would test the inclusion of a group of predictors as a group using a single test. For example, we would often use a deviance test in which we record the difference in deviance (-2*loglike) between models fitted both with, and without, the terms to be tested. To do this here, we will use the LIKE command to store the deviance for each model. We will need to change both the *setup.txt* macro and the *analyse.txt* macro.

With regard to the *setup.txt* macro, we need to change one line at the top as follows:

ERASE c1011 c1012 c1013

(i.e. the addition of c1013 to the existing line), together with the following changes to the bottom of *setup.txt* macro:

```
SIMU c5
METH 1
EXPL 0 c12
EXPL 0 c13
START
```

```
  LIKE b52
  EXPL 1 c12
  EXPL 1 c13
  START
  LIKE b53
  CALC b53 = b52 - b53
  JOIN c1098 c1096 c1011 c1011
  JOIN c1099 c1097 c1012 c1012
  JOIN c1013 b53 c1013
ENDL
```

Here we have added several commands to change the model, fitting the model with, and without, the two school gender predictors. We will then store the difference in deviance in c1013. We need to add some code to the bottom of *analyse.txt* to deal with the deviance test results. Here we will hardwire things for our example, and assume we are interested in the 0.025 significance level again (i.e. a 2-sided test with a significance level of 0.05). The change in deviance follows a chi-squared distribution with 2 degrees of freedom; the 0.975 value is 7.38, and so we will use this in the macro. The following lines are added to the bottom of *analyse.txt*:

```
CALC c1014 = c1013 > 7.38
AVER c1014 b202 b203 b204 b205
JOIN c235 b203 c235
```

Here we have a 0/1 approach which we store in column c235. These macros will take longer to run as they fit two models for each simulated dataset. The results of running the macros after these changes can be seen below:

Data

goto line 1 | view | Help | Font | Show value labels

	N-level 2(15)	zpow2(15)	zpow3(15)	spow2(15)	spow3(15)	c235(15)
1	20.000	0.126	0.106	0.107	0.087	0.072
2	40.000	0.187	0.157	0.161	0.126	0.122
3	60.000	0.229	0.181	0.222	0.169	0.161
4	80.000	0.292	0.211	0.278	0.205	0.191
5	100.000	0.327	0.256	0.335	0.246	0.245
6	120.000	0.411	0.279	0.394	0.287	0.306
7	140.000	0.489	0.346	0.442	0.324	0.378
8	160.000	0.480	0.348	0.498	0.365	0.395
9	180.000	0.512	0.426	0.539	0.402	0.439
10	200.000	0.584	0.450	0.586	0.435	0.507
11	220.000	0.664	0.475	0.628	0.471	0.578
12	240.000	0.661	0.519	0.661	0.502	0.590
13	260.000	0.717	0.530	0.699	0.536	0.658
14	280.000	0.731	0.571	0.733	0.565	0.693
15	300.000	0.747	0.582	0.760	0.595	0.702

Here we see that the power values from the deviance test (c235) start lower than the two independent Z test powers, as might be expected. Then, as the sample size increases, the power sits somewhere between the power when testing the 2 individual school gender terms.

5.3 An example using R

As discussed elsewhere in this document, MLPowSim can create either MLwiN macros, or R code, as specified by the user. Above, we discussed editing the outputted MLwiN macros to accommodate models which cannot be specified in the MLPowSim interface; here, we will do the same for the R code produced

5.3.1 The R code produced by MLPowSim: *powersimu.r*

We will again consider the example studied in Section 5.1. In MLPowSim, if we request output for R rather than MLwiN, and then enter the same inputs as in Section 5.1 (requesting ML estimation, and asking for the confidence intervals to be included in the output), the code (saved in a file called *powersimu.r*) produced will be as follows:

```
###     A programme to obtain the power of parameters in 2 level
#       balanced model  with  Normal response
#                    generated on 17/12/08
###~~~~~~~~~~~~~~~~~    Required packages  ~~~~~~~~~~~~~~~~~~~~~###
    library(MASS)
    library(lme4)
###~~~~~~~~~~~~~~~~~~     Initial inputs    ~~~~~~~~~~~~~~~~~~~###

set.seed(1)
siglevel<-0.025
z1score<-abs(qnorm(siglevel))
simus<-1000
n1low<-40
n1high<-40
n1step<-10
n2low<-20
n2high<-300
n2step<-20
npred<-2
randsize<-1
beta<-c(-0.226000,0.257000,0.146000)
betasize<-length(beta)
effectbeta<-abs(beta)
sgnbeta<-sign(beta)
randcolumn<-0
meanpred<-c(0,0.600000,0.462000)
varpred<-matrix(c(0.120000,0.000000,0.000000,0.000000),npred,npred)
varpred2<-matrix(c(0.125000,0.045000,0.045000,0.249000),npred,npred)
sigma2u<-matrix(c(0.156000),randsize,randsize)
sigmae<-sqrt(0.839000)
n1range<-seq(n1low,n1high,n1step)
n2range<-seq(n2low,n2high,n2step)
n1size<-length(n1range)
n2size<-length(n2range)
totalsize<-n1size*n2size
finaloutput<-matrix(0,totalsize,6*betasize)
rowcount<-1
##-----------------        Inputs for model fitting       -----------------##

fixname<-c("x0","x1","x2")
fixform<-"1+x1+x2"
randform<-"(1|l2id)"
expression<-paste(c(fixform,randform),collapse="+")
modelformula<-formula(paste("y ~",expression))
data<-vector("list",2+length(fixname))
names(data)<-c("l2id","y",fixname)

#####--------- Initial input for power in two approaches ----------------#####

   powaprox<-vector("list",betasize)
```

```
    names(powaprox)<-c("b0","b1","b2")
     powsde<-powaprox

cat("               The programme was executed at", date(),"\n")
cat("   ------------------------------------------------------------------------\n")

 for(n2 in seq(n2low,n2high,n2step)){
  for(n1 in seq(n1low,n1high,n1step)){

                                          length=n1*n2
                                         x<-matrix(1,length,betasize)
                                        z<-matrix(1,length,randsize)
                                       l2id<-rep(c(1:n2),each=n1)
                                      sdepower<-matrix(0,betasize,simus)
                                     powaprox[1:betasize]<-rep(0,betasize)
                                    powsde<-powaprox

cat(" Start of simulation for sample sizes of ",n1," micro and ",n2,"macro units\n")
  for(iter in 1:simus){

                      if(iter/10==floor(iter/10)){
                                             cat(" Iteration remain=",simus-
iter,"\n")
                                            }
#######------------       To set up X matrix           --------------########

            micpred<-mvrnorm(length,meanpred[-1],varpred)
             macpred<-mvrnorm(n2,rep(0,npred),varpred2)
              x[,(2:dim(x)[2])]<-micpred+macpred[l2id,]
#####-------------------------------------------------------------------------#####
                  e<-rnorm(length,0,sigmae)
                   u<-mvrnorm(n2,rep(0,randsize),sigma2u)
                    fixpart<-x%*%beta
                     randpart<-rowSums(z*u[l2id,])
                      y<-fixpart+randpart+e
##-------------------        Inputs for model fitting       ---------------##

  data$l2id<-as.factor(l2id)
  data$y<-y
    data$x0<-x[,1]
    data$x1<-x[,2]
    data$x2<-x[,3]
###~~~~~~~~~~      Fitting the model using lmer funtion    ~~~~~~~~~~###

(fitmodel <- lmer(modelformula,data,method="ML"))

######~~~~~~~~~~   To obtain the power of parameter(s) ~~~~~~~~~~######

estbeta<-fixef(fitmodel)
 sdebeta<-sqrt(diag(vcov(fitmodel)))
  for(l in 1:betasize)
  {
   cibeta<-estbeta[l]-sgnbeta[l]*z1score*sdebeta[l]
    if(beta[l]*cibeta>0)              powaprox[[l]]<-powaprox[[l]]+1
      sdepower[l,iter]<-as.numeric(sdebeta[l])
  }
##-------------------------------------------------------------------------##
        } ##  iteration end here

 ###---------                  Powers and their CIs             ---------###

                       for(l in 1:betasize){

meanaprox<-powaprox[[l]]<-unlist(powaprox[[l]]/simus)
Laprox<-meanaprox-z1score*sqrt(meanaprox*(1-meanaprox)/simus)
Uaprox<-meanaprox+z1score*sqrt(meanaprox*(1-meanaprox)/simus)
meansde<-mean(sdepower[l,])
varsde<-var(sdepower[l,])
USDE<-meansde-z1score*sqrt(varsde/simus)
LSDE<-meansde+z1score*sqrt(varsde/simus)
powLSDE<- pnorm(effectbeta[l]/LSDE-z1score)
powUSDE<- pnorm(effectbeta[l]/USDE-z1score)
powsde[[l]]<-pnorm(effectbeta[l]/meansde-z1score)


               ###---------   Restrict the CIs within 0 and 1       ---------##
                             if(Laprox<0) Laprox<-0
```

```
                                if(Uaprox>1) Uaprox<-1
                                if(powLSDE<0) powLSDE<-0
                                if(powUSDE>1) powUSDE<-1

finaloutput[rowcount,(6*l-5):(6*l-3)]<-c(Laprox,meanaprox,Uaprox)
finaloutput[rowcount,(6*l-2):(6*l)]<-c(powLSDE,powsde[[l]],powUSDE)

                                            }

###~~~~~~~~~~            Set out the results in a data frame    ~~~~~~~~~~###

rowcount<-rowcount+1
cat("------------------------------------------------------------------------\n")
                                 } ## end of the loop  over the first level
                              } ## end of the loop  over the second level

 ###---------         Export output in a file                       ---------###

finaloutput<-as.data.frame(round(finaloutput,3))
 output<-data.frame(cbind(rep(n2range,each=n1size),rep(n1range,n2size),finaloutput))
  names(output)<-
c("N","n","zLb0","zpb0","zUb0","sLb0","spb0","sUb0","zLb1","zpb1","zUb1","sLb1","spb1"
,"sUb1","zLb2","zpb2","zUb2","sLb2","spb2","sUb2")
write.table(output,"powerout.txt",sep="\t
",quote=F,eol="\n",dec=".",col.names=T,row.names=F,qmethod="double")
```

As can be seen, the code is organised into various sections, and we will now look at each of these in turn.

5.3.1.1 "Required packages"

The first line(s) of code in *powersimu.r* (not including comments, which in the R language are denoted by a # sign) specify the packages that are required for the subsequent code to execute correctly: in this case *MASS* and *lme4* (note that it is not necessary to load the package *lme4* to fit one-level models, since the command *glm* is used for model fitting, and this is already available in the package *MASS*).

5.3.1.2 "Initial Inputs"

The next section of code includes some of the variables and objects which will be used as inputs in later commands and functions. The first line (*set.seed*) declares the random seed, i.e. the value for the random number generator. The significance level is specified in the second line (*siglevel*); in this example, it is set to 0.025 (for a 2-sided test with a significance level of 0.05). The third line (*z1score*) represents the absolute value of the quantile of the standard Normal distribution evaluated at the specified significance level. Next the number of simulations to be conducted, for each sample size combination, is declared (*simus*).

Lines 5 to 10 specify the minimum sample size (*low*), maximum sample size (*high*), and intervening step size (*step*) for each level (*n1* and *n2*). Line 11 (*npred*) specifies the number of fixed predictors (not including the intercept), whilst the following line (*randsize*) specifies the number of unique elements in the variance matrix at level 2.

Next, the fixed coefficients are stored in the vector variable *beta*, with the next three lines indicating the length (*betasize*), effect size (*effectbeta*) and sign (*sgnbeta*) of this vector. The last of these variables is required in order to obtain the confidence

intervals for the power estimates calculated using the zero/one method (e.g. see Section 1.4.1).

The variable *randcolumn* is only important for random slopes models, and so here is set to zero. The next three lines (*meanpred, varpred* & *varpred2*) store the mean and variances of the predictors (at the first and second levels). The following two lines (*sigma2u* & *sigmae*) define the variances of the residuals at the second and first levels, respectively.

The range of sample units at each level, along with their length (i.e. how many different sizes of sample units there are at each level), are then specified in the next few lines (*n1range, n2range, n1size* & *n2size*). From these sample ranges, the total number of sample size combinations is determined, and this is saved as the variable *totalsize.*

Next, the variable *finaloutput* defines a matrix structure, with the columns representing the power estimates, together with corresponding confidence intervals, generated from each of the two different methods (i.e. zero/one and standard error), with a separate row for each sample unit combination. The final line in this section of code, *rowcount*, acts as a counter.

5.3.1.3 "Inputs for model fitting"

The next section of code creates a structure for the grouped data which will be used as an argument when fitting the model using the function *lmer*; the grouped data structure consists of a formula and a data set (a data frame object). The predictors are specified by the variable *fixname*, and the model formula is then created by combining the form of the fixed and random parts (*fixform, randform, expression*). If further explanation is required, we recommend that the reader consults the relevant available documentation discussing model formulae in mixed effect models in R (e.g. Pinheiro and Bates (2000)).

Finally, we build a data structure (*modelformula* & *data*) and assign relevant names (*names*), so that at the end of this section we have a grouped data structure consisting of the formula for the hierarchical structure, together with the names of the variables in the data. Note that in each simulation, the dataset changes, whilst the formula and names of the variables remains fixed.

5.3.1.4 "Initial inputs for power in two approaches"

The next section of code creates two vector lists corresponding to the zero/one and standard error method, and gives their corresponding column names the same names as the fixed parameters in the model. In our current example, the parameters are b0, b1 and b2.

The command *cat*, which can be combined with other arguments (e.g. *date*), prints the material between the subsequent quotation marks; therefore, the next two commands print the time and date the code is run in R, above a long dashed line.

We then start to loop (*for*) over the sample size units in the second and first levels, respectively. Note that the inner loop is over the lowest level. The total number of observations depends on the sample size combination, and this is calculated in the following lines (*length*).

The design matrices for the fixed (*x*) and random (*z*) effects, respectively, are then initialised. In order to identify the structure of the grouped data, we create a vector for the second level (*l2id*), and use this as a grouping factor when fitting the model. Next, matrices are initialised to store the power estimates (*sdepower, powaprox* & *powsde*). Then, just before the simulation starts, a message is printed (*cat*) declaring the current sample size combination being simulated. Using the *if* command, together with *cat*, the number of remaining iterations is then printed after every tenth iteration.

5.3.1.5 "To set up X matrix"

The components of the design matrix are a mixture of random variables at different levels, and so in the next section of code we combine the random vectors generated for the first and second levels to create the predictors (*micpred, macpred* & *x*). If appropriate, we would derive the design matrix of the random effects in the next few sections; however, since we have only a random intercept in this example, with a design matrix consisting of a vector of ones, no such commands are included.

We are now at the stage of creating the residuals at both levels, and deriving the response vector; therefore, we generate the random vector corresponding to the level one residual in the next line (*e*), and then simulate the level two residuals (*u*). Matrix manipulations are then used to build the fixed part (*fixpart*) and random part (*randpart*), which correspond to $X\beta$ and ZU in mathematical formulae; these are then added to the level one residual to create the response vector, *y*.

5.3.1.6 "Inputs for model fitting"

We now save the generated objects (*l2id, y* & *x*) in the data frame before fitting the model, allocating each element of the data frame to a corresponding object.

5.3.1.7 "Fitting the model using lmer function"

Immediately after storing all the required objects in our data frame, we can fit the model (*fitmodel*) for the *i*-th iteration of the current simulation run. The model is fitted using the *lmer* function, along with any required arguments. In this example, maximum likelihood estimation, *ML*, is used to fit the model. However, by changing the *method* argument, other estimation methods, such as *REML* (the default method when calling the *lmer* function), can be implemented instead.

5.3.1.8 "To obtain the power of parameter(s)"

In the next section of code we obtain our estimated powers by extracting the estimated fixed effects (*estbeta*) and their standard errors (*sdebeta*), before closing the loop. For the zero/one method of calculating power, we construct an upper/lower bound for the fixed effects (*cibeta*), whilst for the standard error method of calculating power, we just accumulate the standard errors of the estimated fixed effects (*sdepower*). The entire procedure is then set in a loop over the fixed effects in the model, and once this loop finishes, we are ready to go ahead to the next stage.

5.3.1.9 "Powers and their CIs"

The section of code which follows derives the power estimates and their confidence intervals. Here, for the zero/one method, the estimated power (*meanaprox*) is taken as the average of the 0s and 1s (*powaprox*) obtained for each simulation. Then, as this is a binary variable, the confidence interval (*Laprox* (lower) & *Uaprox* (upper)) is derived using a Normal approximation. For the standard error method, the mean (*meansde*) and variance (*varsde*) of the vector of the standard errors for the fixed parameters is first derived, and then the confidence interval about the mean is obtained (*USDE*, *LSDE*). Finally, the mean (*powsde*) and its confidence interval (*powLSDE*, *powUSDE*) are plugged into the approximated formula

$$\frac{\gamma}{SE(\gamma)} \approx z_{1-\alpha} + z_{1-\beta}$$

to obtain the approximated power and confidence intervals.

Since the confidence intervals are approximate, the lower and upper bounds may be less than zero or greater than one, respectively, and therefore the next section of code (the four lines beginning with *if*) constrains such values to zero and one.

The relevant information is then saved in the correct row and correct columns of the matrix object *finaloutput*. The row counter (*rowcount*) then increases by one, and the two loops over the sample units in the first and second level, respectively, end.

5.3.1.10 "Export output in a file"

In this final section of code the matrix object *finaloutput* is first converted to a data frame. Then, after adding two extra columns detailing the sample size units at each level (in the line beginning *output*), each column is identified with an appropriate name (*names*). Finally, the data frame *output* is saved into the text file *powerout.txt* via the *write.table* command.

5.3.2 The output file produced by R: *powerout.txt*

As mentioned earlier, MLPowSim produces R code output which it saves in a file called *powersimu.r*, an example of which we reviewed above. Once this code has run to completion in R (see Section 1.5.1 for details on how to execute the code), an output text file called *powerout.txt* is saved; this presents the estimated power and confidence intervals (if requested) for both the zero/one and standard error method. If

we run the R code we have been discussing in this section, we get the following results (for details of how to view the estimates outputted by R, see Section 1.5.1; please note that here we only show a selected portion of the output):

N	zpb1	spb1	zpb2	spb2
20	0.818	0.827	0.142	0.117
40	0.981	0.983	0.2	0.192
60	0.999	0.999	0.288	0.267
80	1	1	0.333	0.341
100	1	1	0.431	0.406
120	1	1	0.475	0.475
140	1	1	0.531	0.529
160	1	1	0.606	0.589
180	1	1	0.625	0.64
200	1	1	0.692	0.687
220	1	1	0.717	0.726
240	1	1	0.735	0.764
260	1	1	0.771	0.794
280	1	1	0.822	0.824
300	1	1	0.852	0.848

A quick look at the estimated powers indicates that they are similar to those we obtained earlier in MLwiN (see Section 5.1), especially those derived from the standard error method.

As mentioned earlier, the R code produced by MLPowSim does not automatically produce plots of the power curves, and this task is left to the user. However, below we give an example of how one can go about plotting power curves in R.

5.3.3 Plotting the output

Unlike the output for MLwiN, MLPowSim does not generate R code to generate graphs (i.e. this task is left to the user). Whilst it's possible to plot the outputs using some simple graphics tools available in the *MASS* library, we provide an example here of how to do so using the *lattice* package:

```
library(lattice)
output<-read.table("powerout.txt",header =T,sep = " ", dec = ".")
method<-rep(c("Zero/one method","Standard error method"),each=length(n2range),times=betasize)
sample<-rep(n2range,times=2*betasize)
parameter<-rep(c("b0","b1","b2"),each=2*length(n2range))
power<-c(output$zpb0,output$spb0,output$zpb1,output$spb1,output$zpb2,output$spb2)
Lpower<-c(output$zLb0,output$sLb0,output$zLb1,output$sLb1,output$zLb2,output$sLb2)
Upower<-c(output$zUb0,output$sUb0,output$zUb1,output$sUb1,output$zUb2,output$sUb2)
dataset<-data.frame(method,sample,parameter,Lpower,power,Upower)
xyplot(power~sample | method*parameter ,data=dataset,xlab="Sample size of second level",
        scales=list(x=list(tick.number=12,at=sample),y=list(tick.number=12,at=seq(0,1,.1))),
        as.table=T,subscripts=T,
        panel=function(x,y,subscripts)
       {
         panel.grid(h=15,v=15)
         panel.xyplot(x,y,type="l")
```

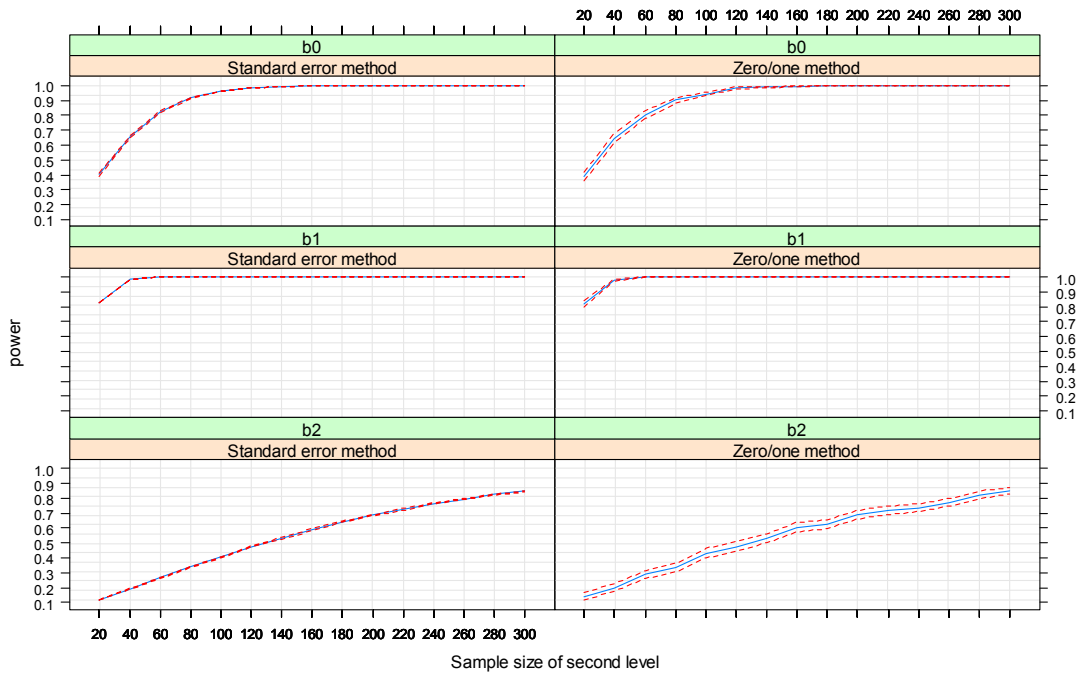
```
  panel.lines(dataset$sample[subscripts],dataset$Lpower[subscripts],lty=2,col=2)
  panel.lines(dataset$sample[subscripts],dataset$Upower[subscripts],lty=2,col=2)
})
```

We'll go through these commands line by line, and then look at the resulting power curves. The first line loads the *lattice* package, which we will use for plotting the data. Then we load the file *powerout.txt*, and store this as a table (*output*), keeping the column headings and the space between the columns and rows.

Next, we create a data frame indicating the method used to obtain the power estimates (*method*; i.e. zero/one or standard error), the sample size combinations (*sample*), the parameters in the model (*parameter*), and the power estimates (*power*) with their corresponding lower and upper confidence intervals (*Lpower*, *Upower*). These objects are then combined to form the data frame *dataset*.

The command *xyplot* is then used to plot the output stored in the data frame. This command involves a number of arguments, including a formula which describes the form of the plot, together with arguments specifying the axis labels and tick markers. The *panel* function is then used to specify how each panel will be plotted; for example, the *panel.lines* command draws the confidence intervals as dashed lines around the estimated powers.

After copying and pasting these lines into the R console, the following graph should appear.



5.4 Modifying the example in R to include a multiple category predictor

5.4.1 Initial changes

In this section we will look at how we might change the R code generated by MLPowSim. We will consider the same example we studied in Section 5.2, when we were adjusting macros in MLwiN. The input data is the same as that which appeared in Section 5.2.1, except that R, instead of MLwiN, is chosen, together with ML estimation, and also we start the sample size for the second level at 60, instead of 20. Running the generated R code in the R console will lead to the following output (which, again, we have abridged):

N	spb1	spb2	spb3
60	1	0.243	0.178
80	1	0.312	0.224
100	1	0.378	0.271
120	1	0.434	0.312
140	1	0.49	0.354
160	1	0.546	0.395
180	1	0.596	0.436
200	1	0.64	0.474
220	1	0.681	0.512
240	1	0.722	0.549
260	1	0.753	0.58
280	1	0.786	0.612
300	1	0.809	0.641

5.4.2 Creating a multiple category predictor

As mentioned in Section 5.2.2, there is currently no option in MLPowSim to specify a multinomial density when one is asked to choose a distribution for the predictor(s). In our example dataset it would be useful to assume a multinomial distribution for the school gender predictor. Here, we will look at how the R code produced by MLPowSim can be altered to accommodate such a model, by changing the independent continuous predictors to multinomial variables. Here, we change the design matrix as follows; in the section of code entitled *To set up X matrix,* we replace the following eight lines:

```
micpred<-rnorm(length,meanpred[3],sqrt(varpred[3]))
 macpred<-rnorm(n2,0,sqrt(varpred2[3]))
  macpred<-rep(macpred,each=n1)
   x[,3]<-micpred+macpred
micpred<-rnorm(length,meanpred[4],sqrt(varpred[4]))
 macpred<-rnorm(n2,0,sqrt(varpred2[4]))
  macpred<-rep(macpred,each=n1)
   x[,4]<-micpred+macpred
```

with these three lines:

```
macpred<-rmultinom(n2,1,c(0.15,0.30,0.55))
x[,3]<-macpred[1,][l2id]
x[,4]<-macpred[2,][l2id]
```

There is no change in the first predictor, but the second (school gender) is constructed differently. First, we generate *n2* multinomial variables of size one, with probabilities which corresponding to boys' schools, girls' schools and mixed schools, respectively. As can be seen, the first two probabilities correspond to the means of the two predictors, treating them as continuous variables. The first and second rows of the generated variable indicate the presence or absence of a boys' school or girls' school.

Since the probability of choosing a boys' school is low, we may have all zeroes in the first row of the generated multinomial variable: i.e. no boys' schools in *n2* schools generated. Consequently, the whole of the third column of the design matrix for the fixed parameters, *X*, would then be zero. In such instances it would not be possible to estimate the parameters, and attempting to fit this model would lead to an error message in R. Therefore we start the sample size for the second level from 60 rather than 20 to avoid this. Note that in MLwiN this would also occur however MLwiN identifies the problem and in such cases sets the associated fixed effect to zero.

After storing the above changes and running the entire code once more in R, we get the following output (which again, we have abridged):

N	spb1	spb2	spb3
60	1	0.226	0.174
80	1	0.284	0.214
100	1	0.344	0.256
120	1	0.398	0.297
140	1	0.454	0.339
160	1	0.507	0.377
180	1	0.552	0.413
200	1	0.594	0.448
220	1	0.642	0.488
240	1	0.676	0.52
260	1	0.71	0.553
280	1	0.742	0.583
300	1	0.772	0.612

As can be seen, the powers associated with each of the parameters, particularly the last two, have decreased, because the multinomial variable provides less information about them.

5.4.3 Linking gender to school gender

Following our discussion in Section 5.2.3, we need to further alter the changes made in the previous section to link gender to school gender. In fact, two changes need to be made. First, we need to adjust the probability of being a girl to 0.5; this represents what is expected in the mixed schools, since boys and girls have an equal chance of being chosen. Then, we need to specify the correct number for the gender predictor:

i.e. fix it to 1 if the chosen school is a girls' school, fix it to 0 if it is boys' school, and keep its initial generated value if it is a mixed school. To do this, we make the following changes to the section of R code entitled *To set up X matrix*:

we alter:

```
x[,2]<-rbinom(length,1,xprob[2])
```

so that it now reads:

```
x[,2]<-rbinom(length,1,0.5)
```

In addition, under the line:

```
x[,4]<-macpred[2,][l2id]
```

we add the following:

```
x[,2]<-x[,4]+x[,2]*(x[,3]==0&x[,4]==0)
```

If we store these changes, then run the R code again, this results in the following output:

N	spb1	spb2	spb3
60	0.999	0.221	0.169
80	1	0.278	0.207
100	1	0.336	0.247
120	1	0.389	0.286
140	1	0.445	0.327
160	1	0.497	0.363
180	1	0.541	0.399
200	1	0.583	0.433
220	1	0.63	0.471
240	1	0.665	0.503
260	1	0.699	0.535
280	1	0.731	0.565
300	1	0.761	0.593

Here we see very similar estimates to those derived from MLwiN in Section 5.2.3, again with a slight decrease in power compared to the preceding model.

5.4.4 Performing the deviance test

As discussed in Section 5.2.4, comparisons between whole groups of predictors can be conducted using deviance tests, comparing likelihood statistics from models with, and without, certain predictors. We can achieve this in R using the command *deviance*.

In this section we will describe several changes to the code that allow us to perform the deviance test, and also to display the result in our final output.

We first need to add an extra column to the output to contain the deviance information and can do this by changing the following line:

```
finaloutput<-matrix(0,totalsize,6*betasize)
```

to:

```
finaloutput<-matrix(0,totalsize,6*betasize+1)
```

To the section of code entitled *Inputs for model fitting* we add a formula that specifies a model without the two school gender predictors; we will subsequently fit this model, and then find the difference in deviance between it and the fitted model with the gender predictors. Under the line:

```
names(data)<-c("l2id","y",fixname)
```

we add the following:

```
modelformula1<-formula(y~1+x1+(1|l2id))
devtestsim <- rep(0,simus)
```

Note the second line simply initialises a vector which will store the difference in deviance for each dataset. We next need to change the code in the inner loop that fits the model, so that it now fits the model with, and without, the school gender terms, and we then need to compare the deviance. So, after the line:

```
(fitmodel <- lmer(modelformula,data,method="ML"))
```

we add the following:

```
(fitmodel1 <- lmer(modelformula1,data,method="ML"))
devtestsim[iter] <- deviance(fitmodel1) - deviance(fitmodel)
```

The first line fits the model we specified above, whilst the second line calculates the difference in deviance between the two fitted models.

The next step is to summarise the variable *devtestsim* in terms of how often it is greater than the critical value of 7.38 (see Section 5.2.4), and we do this when piecing together the *finaloutput* object. After the lines:

```
finaloutput[rowcount,(6*l-5):(6*l-3)]<-c(Laprox,meanaprox,Uaprox)
finaloutput[rowcount,(6*l-2):(6*l)]<-c(powLSDE,powsde[[l]],powUSDE)
```

we add:

```
finaloutput[rowcount,6*l+1] <- mean(devtestsim > 7.38)
```

The final change we need to make is simply to include a column heading for the deviance test output, and we can do this by adding the relevant name at the end of the names line, as follows:

```
names(output)<-
c("N","n","zLb0","zpb0","zUb0","sLb0","spb0","sUb0","zLb1","zpb1","zU
b1","sLb1","spb1","sUb1","zLb2","zpb2","zUb2","sLb2","spb2","sUb2","z
Lb3","zpb3","zUb3","sLb3","spb3","sUb3","devtest")
```

If we save these changes, and run this code anew, we get the following results (again we present only selected portions of the output here):

N	zpb2	spb2	zpb3	spb3	devtest
60	0.229	0.221	0.191	0.169	0.158
80	0.296	0.278	0.211	0.207	0.197
100	0.332	0.336	0.265	0.247	0.237
120	0.394	0.389	0.264	0.286	0.283
140	0.477	0.445	0.35	0.327	0.38
160	0.496	0.497	0.359	0.363	0.394
180	0.524	0.541	0.38	0.399	0.453
200	0.602	0.583	0.416	0.433	0.505
220	0.649	0.63	0.476	0.471	0.557
240	0.65	0.665	0.495	0.503	0.571
260	0.713	0.699	0.539	0.535	0.648
280	0.713	0.731	0.561	0.565	0.669
300	0.756	0.761	0.602	0.593	0.707

The results are similar to those we found in Section 5.2.4 (with MLwiN): i.e. the power estimates for the deviance test are initially lower than those for each predictor, but as sample size increases they reach values somewhere between the power for testing the two individual gender terms.

5.5 The Wang and Gelfand (2002) method

When using MLPowSim we are required to give point estimates for all parameters of interest in our model, for both effect sizes and variances. Our power calculations are then based on assuming these estimates are correct and simulating data conditional on these estimates. This approach therefore does not take account of uncertainty in the estimates themselves. Wang and Gelfand (2002) discuss using simulation-based techniques for power calculations in a Bayesian framework. Their paper contains many interesting ideas but we will here focus only on one: namely allowing uncertainty in the estimated effect sizes and variances.

Wang and Gelfand (2002) use MCMC methods to fit their models in a Bayesian framework, and consequently all their parameters have prior distributions which, for clarity, they describe as ‘fitting priors’. They then argue for a second set of ‘sampling priors’ which are used to cope with the uncertainty in the estimated effect sizes and variances. Basically the ‘sampling priors’ are used during the creation of the simulated datasets, while the ‘fitting priors’ are used in the fitting of models to the simulated data created. Typically the ‘fitting priors’ will be more ‘diffuse’ as they are meant to represent the priors we would anticipate using once the data is obtained.

Here we will adapt the MLwiN macro output from MLPowSim so that we use a method similar to that of Wang and Gelfand (2002); in fact, the only difference is that

we revert to classical frequentist inference for model fitting (if we were to instead use MCMC, then our method would essentially replicate that of Wang and Gelfand, apart from the choice of model performance criteria).

For simplicity, here we will consider the first single level model that we studied back in Section 1.3.2. You may recall that in that section we were interested in whether boys fared worse than average in exams, and we had an effect size of -0.140 and a population variance estimate of 1.051. As is standard with power calculations, our approach assumed that these values are fixed and known, but what if instead we thought there was some uncertainty in these measures? Wang and Gelfand (2002) often use Uniform priors in their examples, and so let us instead assume that the effect size (β_0) has a Uniform[-0.18,-0.1] sampling prior and σ^2_e has a Uniform[0.8051,1.2051] prior.

We will firstly repeat our earlier inputs in MLPowSim by working through Section 1.3.2 to create the macros. We will then need to modify the macro *setup.txt* to allow for the sampling priors. We will create 1000 draws from the sampling priors for β_0 and σ^2_e in columns c501 and c502, respectively. We can generate from a Uniform[0,1] distribution via the URAN command, and then manipulate the values so that they are from the correct uniform prior. We then pick these values when we fit each model. The modified *setup.txt* macro looks as follows (with added/modified lines in italics):

```
NOTE MLwiN macro code generated by MLPowSim
NOTE b23 - number of units
ERASE c1011 c1012
GENErate 1 b23 c1
PUT b23 1 c4
PUT b23 1 c5
NAME c1 'l1id' c4 'cons' c5 'resp'
RESP c5
IDEN 1 c1
EXPL 1 c4
SETV 1 c4
ERROR 0
BATCH 1
PREF 0
POST 0
URAN b41 c501
CALC c501 = (c501-0.5)*0.08
PICK 1 c598 b51
CALC c501 = c501+b51
URAN b41 c502
CALC c502 = (c502-0.5)*0.4
PICK 1 c596 b51
CALC c502 = c502+b51
LOOP b40 1 b41
  PICK b40 c501 b51
  EDIT 1 c1098 b51
  PICK b40 c502 b51
  EDIT 1 c1096 b51
```

```
  SIMU c5
  METH 1
  START
  JOIN c1098 c1096 c1011 c1011
  JOIN c1099 c1097 c1012 c1012
ENDL
OBEY analyse.txt
PAUSE 1
```

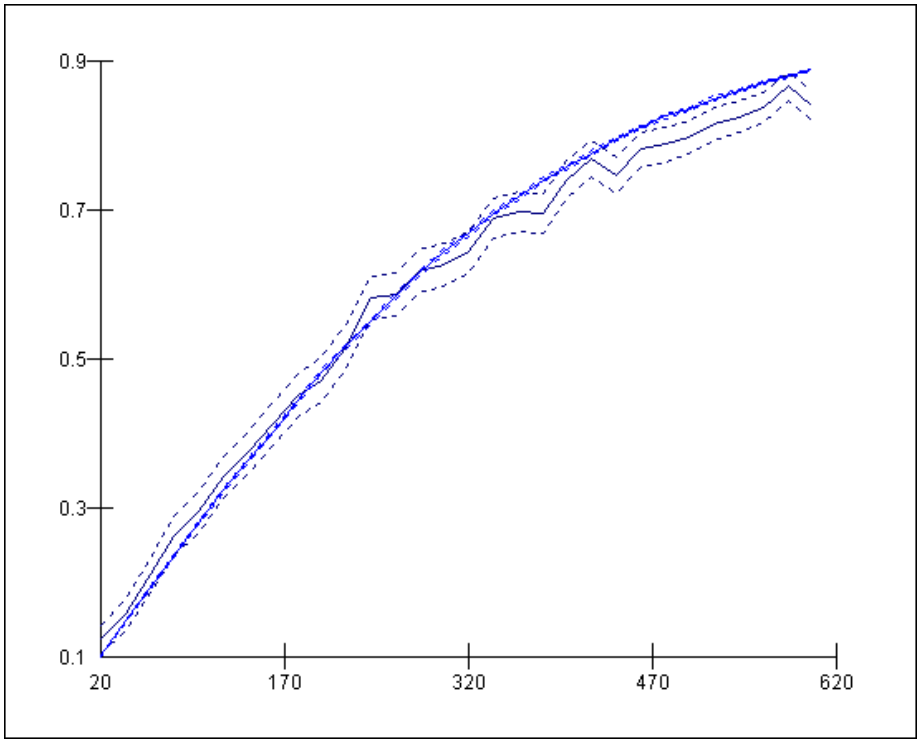
If we save this macro and then run the macro *simu.txt* in the usual way (as detailed in Section 1.4), then by viewing columns C210, C211 and C231 we see the following:

Data

goto line 1 | view | Help | Font | Show value l

	Samplesize(30)	zpow0(30)	spow0(30)
1	20.000	0.115	0.092
2	40.000	0.150	0.141
3	60.000	0.206	0.188
4	80.000	0.261	0.234
5	100.000	0.295	0.280
6	120.000	0.344	0.325
7	140.000	0.379	0.368
8	160.000	0.419	0.409
9	180.000	0.459	0.452
10	200.000	0.481	0.493
11	220.000	0.528	0.529
12	240.000	0.598	0.563
13	260.000	0.602	0.599
14	280.000	0.634	0.632
15	300.000	0.644	0.663
16	320.000	0.662	0.688
17	340.000	0.709	0.716
18	360.000	0.719	0.739
19	380.000	0.717	0.764
20	400.000	0.764	0.780
21	420.000	0.793	0.801
22	440.000	0.770	0.821
23	460.000	0.807	0.838
24	480.000	0.813	0.853
25	500.000	0.824	0.864
26	520.000	0.842	0.878
27	540.000	0.852	0.889
28	560.000	0.865	0.901
29	580.000	0.895	0.910
30	600.000	0.868	0.918

We can also run the macro *graphs.txt* (as detailed in Section 1.4.3) to get the following:



In fact, allowing for the sampling priors here hasn't made much difference to the SE method (the smoother line) when comparing this graph to the equivalent one in Section 1.4.3, but it has resulted in a slight reduction in power for the 0/1 method (the more erratic line) for larger sample sizes, and an increase for smaller sample sizes. Strictly speaking, the SE method is still using the point estimate of -0.140 in its power calculations after the 1000 simulations have run, and so it isn't truly using the sampling prior correctly. In fact, it's very close to the standard method without the sampling prior (i.e. as in Section 1.4.3), and so it is useful for comparison.

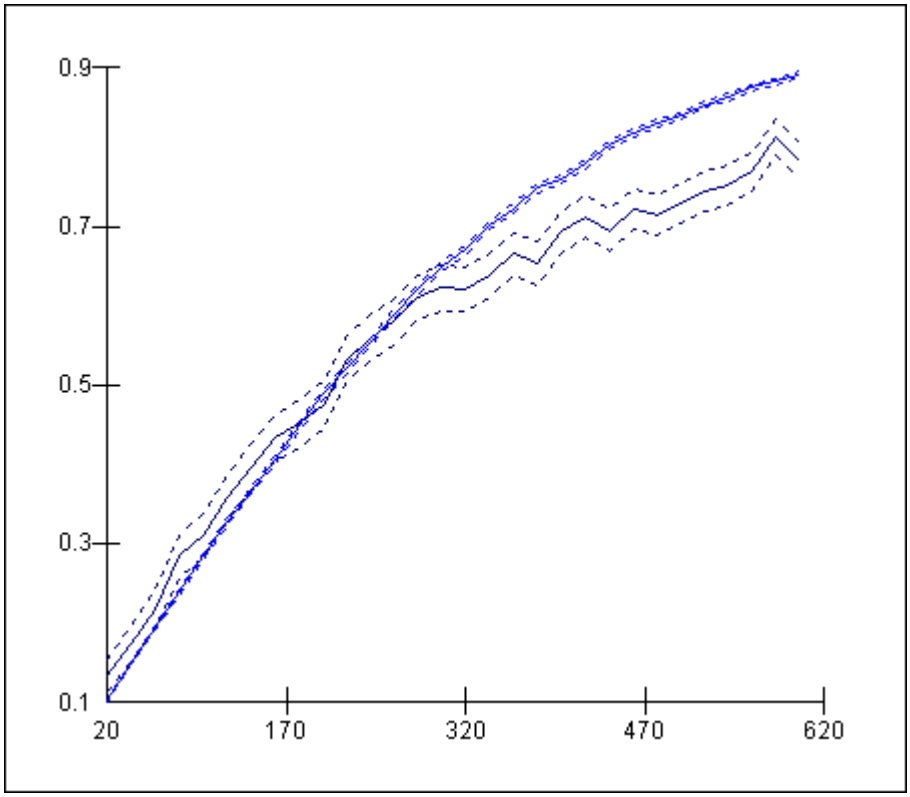
We could increase our uncertainty in our effect sizes by doubling the widths of the Uniform priors, i.e. change the following lines in the *setup.txt* macro:

*CALC c501 = (c501-0.5)*0.08*
and
*CALC c502 = (c502-0.5)*0.4*

to

*CALC c501 = (c501-0.5)*0.16*
and
*CALC c502 = (c502-0.5)*0.8*

If we were to restart MLwiN and rerun the macros then we would now get the following graphs:



Here we see a larger drop in power for higher sample sizes and a slightly larger increase in power for smaller sample sizes. To understand what is going on we need to think what adding uncertainty to our effect size is actually doing. If our effect size is fixed then we know that increasing our sample size will increase power. Allowing the effect size to vary means that for some simulations the effect size will need a smaller sample size to give a prescribed power, and for some simulations the effect size will need a larger sample size to give the same prescribed power. When the sample size is such that power to detect is normally high, the occasional small effect sizes will pull the power down; in contrast, when we have small sample sizes and the power to detect is low, then the occasional large effect sizes will increase the power. If we continue to increase the width of our priors we begin to include effect sizes of differing signs and, assuming a one-sided hypothesis, these are more likely not to be rejected as we increase sample size; this means that as the prior intervals get arbitrarily big we should end up with a power of 0.5 for all sample sizes. Note that if we make the prior interval arbitrarily big and consider a 2-sided alternative, then the probability of generating an effect size (for use in simulations) that is close to 0 becomes arbitrarily small, and so a power of 1 for all sample sizes will be the result.

Clearly this motivates the practice of an assumed (known) effect size and also highlights the fact that if one uses the Wang and Gelfand approach, one should not use a ‘sampling’ prior that is too diffuse.

REFERENCES

Afshartous, D. (1995). Determination of sample size for multilevel model design. In: V.S. Williams, L.V. Jones and I. Olkin (Eds.), *Perspectives on statistics for educational research: Proceedings of the National Institute of Statistical Sciences (NISS) (Tech. Rep. No. 35).*

Bosker R.J., Snijders T.A.B, and Guldemond, H. (2003). PINT (Power IN Two-level designs) User Manual.

Browne, W.J. (2003). *MCMC Estimation in MLwiN*. London: Institute of Education.

Browne, W.J. and Draper, D. (2006). A comparison of Bayesian and likelihood-based methods for fitting multilevel models. *Bayesian Analysis* **1**: 473-550

Gelman, A. and Hill, J. (2007) *Data Analysis Using Regression and Multilevel / Hierarchical Models.* Cambridge University Press: Cambridge.

Goldstein, H. and J. Rasbash. (1996). Improved approximations for multilevel models with binary responses. *Journal of the Royal Statistical Society (Series A)* **159**: 505-513.

Langford, I.H., Bentham, G. and McDonald, A. (1998). Multilevel modelling of geographically aggregated health data: a case study on malignant melanoma mortality and UV exposure in the European community. *Statistics in Medicine* **17**: 41-58.

Mok, M. (1995) Sample Size Requirements for 2-Level Designs in Educational Research *Multilevel Modelling Newsletter* **7** (2): 11-15

Nuttall DL, Goldstein H, Prosser R & Rasbash J. (1989). Differential School Effectiveness. *International Journal of Educational Research*, **13:** 769-776.

Pinheiro, J.C. and Bates, D.M. (2000). *Mixed-Effects Models in S and S-PLUS.* New York, NY: Springer-Verlag.

Rasbash, J., Steele, F., Browne, W.J. and Prosser, B. (2004). *A User's Guide to MLwiN.* London: Institute of Education.

Snijders T.A.B, and Bosker R.J. (1993) Standard Errors And Sample Sizes For 2-Level Research. *Journal Of Educational Statistics* **18** (3): 237-259.

Wang, F. and Gelfand, A.E. (2002). A simulation-based approach to Bayesian sample size determination for performance under a given model and for separating models. *Statistical Science,* **17**(2), 193-208.