Linear Mixed Models

Appendix to An R and S-PLUS Companion to Applied Regression

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1 Introduction

The normal linear model (described, for example, in Chapter 4 of the text),

$$y_i = \beta_1 x_{1i} + \beta_2 x_{2i} + \dots + \beta_p x_{pi} + \varepsilon_i$$

 $\varepsilon_i \sim \text{NID}(0, \sigma^2)$

has one random effect, the error term ε_i . The parameters of the model are the regression coefficients, $\beta_1, \beta_2, ..., \beta_p$, and the error variance, σ^2 . Usually, $x_{1i} = 1$, and so β_1 is a constant or intercept.

For comparison with the linear mixed model of the next section, I rewrite the linear model in matrix form,

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$
 $\boldsymbol{\varepsilon} \sim \mathbf{N}_n(\mathbf{0}, \sigma^2 \mathbf{I}_n)$

where $\mathbf{y} = (y_1, y_2, ..., y_n)'$ is the response vector; \mathbf{X} is the model matrix, with typical row $\mathbf{x}_i' = (x_{1i}, x_{2i}, ..., x_{pi})$; $\boldsymbol{\beta} = (\beta_1, \beta_2, ..., \beta_p)'$ is the vector of regression coefficients; $\boldsymbol{\varepsilon} = (\varepsilon_1, \varepsilon_2, ..., \varepsilon_n)'$ is the vector of errors; \mathbf{N}_n represents the *n*-variable multivariate-normal distribution; $\mathbf{0}$ is an $n \times 1$ vector of zeroes; and \mathbf{I}_n is the order-n identity matrix.

So-called *mixed-effect models* (or just *mixed models*) include additional random-effect terms, and are often appropriate for representing clustered, and therefore dependent, data — arising, for example, when data are collected hierarchically, when observations are taken on related individuals (such as siblings), or when data are gathered over time on the same individuals.

There are several facilities in R and S-PLUS for fitting mixed models to data, the most ambitious of which is the nlme library (an acronym for non-linear mixed effects), described in detail by Pinheiro and Bates (2000). Despite its name, this library includes facilities for fitting linear mixed models (along with nonlinear mixed models), the subject of the present appendix. There are plans to incorporate generalized linear mixed models (for example, for logistic and Poisson regression) in the nlme library. In the interim, the reader may wish to consult the documentation for the glmmPQL function in Venables and Ripley's (1999) MASS library.¹

Mixed models are a large and complex subject, and I will only scrape the surface here. I recommend Raudenbush and Bryk (2002) as a general, relatively gentle, introduction to the subject for social scientists, and Pinheiro and Bates (2000), which I have already mentioned, as the definitive reference for the nlme library.

2 The Linear Mixed Model

Linear mixed models may be expressed in different but equivalent forms. In the social and behavioral sciences, it is common to express such models in hierarchical form, as explained in the next section. The

¹Version 6.3-2 of the MASS library (or, I assume, a newer version) is required.

lme (linear mixed effects) function in the nlme library, however, employs the *Laird-Ware form* of the linear mixed model (after a seminal paper on the topic published by Laird and Ware, 1982):

$$y_{ij} = \beta_1 x_{1ij} + \dots + \beta_p x_{pij}$$

$$+b_{i1} z_{1ij} + \dots + b_{iq} z_{qij} + \varepsilon_{ij}$$

$$b_{ik} \sim N(0, \psi_k^2), Cov(b_k, b_{k'}) = \psi_{kk'}$$

$$\varepsilon_{ij} \sim N(0, \sigma^2 \lambda_{ijj}), Cov(\varepsilon_{ij}, \varepsilon_{ij'}) = \sigma^2 \lambda_{ijj'}$$

$$(1)$$

where

- y_{ij} is the value of the response variable for the jth of n_i observations in the ith of M groups or clusters.
- β_1, \ldots, β_n are the fixed-effect coefficients, which are identical for all groups.
- x_{1ij}, \ldots, x_{pij} are the fixed-effect regressors for observation j in group i; the first regressor is usually for the constant, $x_{1ij} = 1$.
- b_{i1}, \ldots, b_{iq} are the random-effect coefficients for group i, assumed to be multivariately normally distributed. The random effects, therefore, vary by group. The b_{ik} are thought of as random variables, not as parameters, and are similar in this respect to the errors ε_{ij} .
- z_{1ij}, \ldots, z_{qij} are the random-effect regressors.
- ψ_k^2 are the variances and $\psi_{kk'}$ the covariances among the random effects, assumed to be constant across groups. In some applications, the ψ 's are parametrized in terms of a relatively small number of fundamental parameters.
- ε_{ij} is the error for observation j in group i. The errors for group i are assumed to be multivariately normally distributed.
- $\sigma^2 \lambda_{ijj'}$ are the covariances between errors in group *i*. Generally, the $\lambda_{ijj'}$ are parametrized in terms of a few basic parameters, and their specific form depends upon context. For example, when observations are sampled independently within groups and are assumed to have constant error variance (as in the application developed in the following section), $\lambda_{ijj} = \sigma^2$, $\lambda_{ijj'} = 0$ (for $j \neq j'$), and thus the only free parameter to estimate is the common error variance, σ^2 . Similarly, if the observations in a "group" represent longitudinal data on a single individual, then the structure of the λ 's may be specified to capture autocorrelation among the errors, as is common in observations collected over time.

Alternatively but equivalently, in matrix form,

$$egin{array}{lll} \mathbf{y}_i &=& \mathbf{X}_i oldsymbol{eta} + \mathbf{Z}_i \mathbf{b}_i + oldsymbol{arepsilon}_i \ &\sim & \mathbf{N}_q(\mathbf{0}, oldsymbol{\Psi}) \ arepsilon_i &\sim & \mathbf{N}_{n_i}(\mathbf{0}, oldsymbol{\sigma}^2 oldsymbol{\Lambda}_i) \end{array}$$

where

- \mathbf{y}_i is the $n_i \times 1$ response vector for observations in the *i*th group.
- \mathbf{X}_i is the $n_i \times p$ model matrix for the fixed effects for observations in group i.
- β is the $p \times 1$ vector of fixed-effect coefficients.
- \mathbf{Z}_i is the $n_i \times q$ model matrix for the random effects for observations in group i.
- \mathbf{b}_i is the $q \times 1$ vector of random-effect coefficients for group i.
- ε_i is the $n_i \times 1$ vector of errors for observations in group i.
- Ψ is the $q \times q$ covariance matrix for the random effects.
- $\sigma^2 \mathbf{\Lambda}_i$ is the $n_i \times n_i$ covariance matrix for the errors in group i.

3 An Illustrative Application to Hierarchical Data

Applications of mixed models to hierarchical data have become common in the social sciences, and nowhere more so than in research on education. The following example is borrowed from Bryk and Raudenbush's influential (1992) text on hierarchical linear models, and also appears in a paper by Singer (1998), which shows how such models can be fit by the MIXED procedure in SAS.²

The data for the example, from the 1982 "High School and Beyond" survey, and pertain to 7185 high-school students from 160 schools, are present in the data frames MathAchieve and MathAchSchool, distributed with the nlme library:³

```
> library(nlme)
Loading required package: nls
> library(lattice) # for Trellis graphics
Loading required package: grid
> data(MathAchieve)
> MathAchieve[1:10,]
                       # first 10 students
Grouped Data: MathAch ~
                         SES | School
   School Minority
                       Sex
                               SES MathAch MEANSES
     1224
                 No Female -1.528
                                     5.876
                                            -0.428
1
2
     1224
                 No Female -0.588
                                    19.708
                                            -0.428
3
     1224
                 No
                      Male -0.528
                                    20.349
                                            -0.428
4
     1224
                 No
                      Male -0.668
                                     8.781
                                            -0.428
5
     1224
                      Male -0.158
                 No
                                    17.898
                                             -0.428
6
     1224
                 No
                      Male
                           0.022
                                     4.583
                                             -0.428
7
     1224
                 No Female -0.618
                                    -2.832
                                            -0.428
8
     1224
                      Male -0.998
                                     0.523
                                            -0.428
                 No Female -0.888
                                     1.527
9
     1224
                                            -0.428
10
     1224
                      Male -0.458
                                    21.521
> data(MathAchSchool)
> MathAchSchool[1:10,] # first 10 schools
                    Sector PRACAD DISCLIM HIMINTY MEANSES
     School Size
1224
       1224 842
                    Public
                              0.35
                                     1.597
                                                  0
                                                     -0.428
1288
       1288 1855
                    Public
                              0.27
                                     0.174
                                                  0
                                                      0.128
                             0.32
                                    -0.137
                                                     -0.420
1296
       1296 1719
                    Public
                                                  1
1308
       1308
             716 Catholic
                             0.96
                                    -0.622
                                                  0
                                                      0.534
                             0.95
                                   -1.694
1317
       1317
             455 Catholic
                                                  1
                                                      0.351
1358
       1358 1430
                    Public
                              0.25
                                     1.535
                                                  0
                                                     -0.014
1374
       1374 2400
                    Public
                             0.50
                                     2.016
                                                  0
                                                     -0.007
1433
       1433
             899 Catholic
                              0.96
                                    -0.321
                                                  0
                                                      0.718
1436
       1436
             185 Catholic
                              1.00
                                    -1.141
                                                  0
                                                      0.569
```

1461

1461 1672

Public

The first data frame pertains to students, and there is therefore one row in the data frame for each of the 7185 students; the second data frame pertains to schools, and there is one row for each of the 160 schools. We shall require the following variables:

2.096

0.78

• School: an identification number for the student's school. Although it is not required by lme, students in a specific school are in consecutive rows of the data frame, a convenient form of data organiza-

0

0.683

²The data were obtained from Singer. There is now a second edition of Bryk and Raudenbush's text, Raudenbush and Bryk (2002)

³These are actually grouped-data objects, which include some additional information along with the data. See the discussion below.

tion. The schools define groups — it is unreasonable to suppose that students in the same school are independent of one-another.

- SES: the socioeconomic status of the student's family, centered to an overall mean of 0 (within rounding error).
- MathAch: the student's score on a math-achievement test.
- Sector: a factor coded 'Catholic' or 'Public'. Note that this is a school-level variable and hence is identical for all students in the same school. A variable of this kind is sometimes called an *outer variable*, to distinguish it from an *inner variable* (such as SES), which varies within groups. Because the variable resides in the school data set, we need to copy it over to the appropriate rows of the student data set. Such data-management tasks are common in preparing data for mixed-modeling.
- MEANSES: another outer variable, giving the mean SES for students in each school. Notice that this variable already appears in both data sets. The variable, however, seems to have been calculated incorrectly that is, its values are slightly different from the school means and I will therefore recompute it (using tapply see Section 8.4 of the text) and replace it in the student data set:

```
> attach(MathAchieve)
> mses <- tapply(SES, School, mean) # school means
> mses[as.character(MathAchSchool$School[1:10])]
                                                   # for first 10 schools
     1224
               1288
                         1296
                                    1308
                                              1317
                                                        1358
-0.434383
           0.121600 -0.425500
                               0.528000
                                         0.345333 -0.019667
     1374
               1433
                         1436
                                    1461
-0.012643 0.712000 0.562909
                              0.677455
> detach(MathAchieve)
```

The nlme and trellis Libraries in S-PLUS

In S-PLUS, the nlme library (called nlme3) and the trellis library are in the search path at the beginning of the session and need not be attached via the library function.

I begin by creating a new data frame, called Bryk, containing the inner variables that we require:

```
> Bryk <- as.data.frame(MathAchieve[, c("School", "SES", "MathAch")])
> names(Bryk) <- c("school", "ses", "mathach")</pre>
> sample20 <- sort(sample(7185, 20)) # 20 randomly sampled students
> Bryk[sample20, ]
     school
               ses mathach
20
       1224 -0.078 16.405
280
       1433 0.952
                    19.033
       2526 -0.708
1153
                     7.359
1248
       2629 -0.598
                    17.705
1378
       2655 -0.548
                    17.205
1939
       3152 -0.628
                    15.751
2182
       3499 0.592
                    10.491
2307
       3610 -0.678
                     8.565
2771
       4042 1.082
                    15.297
2779
       4042 0.292
                    20.672
2885
       4223 -0.188
                    17.984
3016
       4292 0.292 23.619
```

```
4308
       6144 -0.848
                      2.799
4909
       6816 -0.148
                     16.446
5404
       7345 -1.528
                      8.788
5704
       7890 0.802
                      3.744
5964
       8193 -0.828
                     10.748
6088
       8477 -0.398
                     16.305
6637
       9021 1.512
                      9.930
7154
       9586
            1.082
                    14.266
```

By using as.data.frame, I make Bryk an ordinary data frame rather than a grouped-data object. I rename the variables to lower-case in conformity with my usual practice — data frames start with upper-case letters, variables with lower-case letters.

Next, I add the outer variables to the data frame, in the process computing a version of SES, called cses, that is centered at the school mean:

```
> Bryk$meanses <- mses[as.character(Bryk$school)]
> Bryk$cses <- Bryk$ses - Bryk$meanses

> sector <- MathAchSchool$Sector
> names(sector) <- row.names(MathAchSchool)
> Bryk$sector <- sector[as.character(Bryk$school)]</pre>
```

> Bryk[sample20,]

```
school
               ses mathach
                             meanses
                                          cses
                                                 sector
20
       1224 -0.078
                    16.405 -0.434383
                                      0.35638
280
       1433 0.952
                    19.033
                            0.712000
                                      0.24000 Catholic
1153
       2526 -0.708
                     7.359
                            0.326912 -1.03491 Catholic
1248
       2629 -0.598
                    17.705 -0.137649 -0.46035 Catholic
1378
       2655 -0.548
                    17.205 -0.701654
                                      0.15365
                                                 Public
       3152 -0.628
                            0.031038 -0.65904
1939
                    15.751
                                                 Public
2182
       3499 0.592
                    10.491
                            0.449895
                                     0.14211 Catholic
2307
       3610 -0.678
                     8.565
                            0.120125 -0.79813 Catholic
2771
       4042 1.082
                    15.297
                            0.402000 0.68000 Catholic
2779
       4042 0.292
                    20.672
                            0.402000 -0.11000 Catholic
2885
       4223 -0.188
                    17.984 -0.094000 -0.09400 Catholic
3016
       4292 0.292
                    23.619 -0.486154 0.77815 Catholic
4308
       6144 -0.848
                     2.799 -0.437535 -0.41047
                                                 Public
       6816 -0.148
4909
                    16.446
                            0.528909 -0.67691 Catholic
5404
       7345 -1.528
                     8.788
                            0.033250 -1.56125
                                                 Public
5704
       7890 0.802
                     3.744 -0.522706
                                     1.32471
                                                 Public
5964
       8193 -0.828
                    10.748 -0.176605 -0.65140 Catholic
6088
       8477 -0.398
                    16.305 -0.196108 -0.20189
6637
       9021 1.512
                     9.930 0.626643 0.88536 Catholic
       9586 1.082 14.266 0.621153 0.46085 Catholic
```

The following steps are a bit tricky:

- The students' school numbers (in Bryk\$school) are converted to character values, used to index the outer variables in the school dataset. This procedure assigns the appropriate values of meanses and sector to each student.
- To make this indexing work for the Sector variable in the school data set, the variable is assigned to the global vector sector, whose names are then set to the row names of the school data frame.

Following Bryk and Raudenbush, we will ask whether math achievement is related to socioeconomic status; whether this relationship varies systematically by sector; and whether the relationship varies randomly across schools within the same sector.

3.1 Examining the Data

As in all data analysis, it is advisable to examine the data before embarking upon statistical modeling. There are too many schools to look at each individually, so I start by selecting samples of 20 public and 20 Catholic schools, storing each sample as a grouped-data object:

Grouped-data objects are enhanced data frames, provided by the nlme library, incorporating a model formula that gives information about the structure of the data. In this instance, the formula mathach "ses | school, read as "mathach is modeled as ses given school," indicates that mathach is the response variable, ses is the principal within-group (i.e., inner) covariate, and school is the grouping variable.

Although nlme provides a plot method for grouped-data objects, which makes use of Trellis graphics, the graphs are geared more towards longitudinal data than hierarchical data. In the present context, therefore, I prefer to use Trellis graphics directly, as follows:

- The call to trellis.device creates a graphics-device window appropriately set up for Trellis graphics; in this case, I have specified monochrome graphics (color = F) so that this appendix will print well in black-and-white; the default is to use color.
- The xyplot function draws a Trellis display of scatterplots of math achievement against socioeconomic status, one scatterplot for each school, as specified by the formula mathach ~ ses | school. The school number appears in the strip label above each plot. I created one display for Catholic schools (Figure 1) and another for public schools (Figure 2). The argument main to xyplot supplies the title of each graph.
- The content of each cell (or *panel*) of the Trellis display is determined by the **panel** argument to xyplot, here an anonymous function defined "on the fly." This function takes two arguments, x and y, giving respectively the horizontal and vertical coordinates of the points in a panel, and successively calls three standard panel functions:

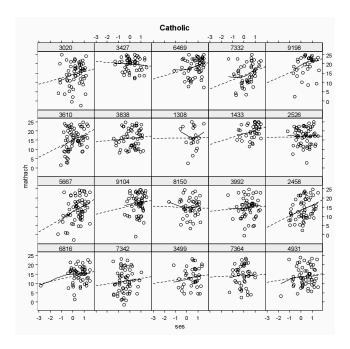


Figure 1: Trellis display of math achievement by socio-economic status for 20 randomly selected Catholic schools. The broken lines give linear least-squares fits, the solid lines local-regression fits.

- panel.xyplot (which is the default panel function for xyplot) creates a basic scatterplot.
- panel.loess draws a local regression line on the plot. Because there is a relatively small number
 of observations for each school, I set the span of the local-regression smoother to 1. (See the
 Appendix on nonparametric regression for details.)
- panel.lmline similarly draws a least-squares line; the argument 1ty=2 produces a broken line.

Examining the scatterplots in Figures 1 and 2, there is a weak positive relationship between math achievement and SES in most Catholic schools, although there is variation among schools: In some schools the slope of the regression line is near zero or even negative. There is also a positive relationship between the two variables for most of the public schools, and here the average slope is larger. Considering the small number of students in each school, linear regressions appear to do a reasonable job of capturing the within-school relationships between math achievement and SES.

The nlme library includes the function lmList for fitting a linear model to the observations in each group, returning a list of linear-model objects, which is itself an object of class "lmList". Here, I fit the regression of math-achievement scores on socioeconomic status for each school, creating separate lmList objects for Catholic and public schools:

```
> cat.list <- lmList(mathach ~ ses | school, subset = sector=='Catholic',
+ data=Bryk)
> pub.list <- lmList(mathach ~ ses | school, subset = sector=='Public',
+ data=Bryk)
>
```

Several methods exist for manipulating lmList objects. For example, the generic intervals function has a method for objects of this class that returns (by default) 95-percent confidence intervals for the regression coefficients; the confidence intervals can be plotted, as follows:

```
> plot(intervals(cat.list), main='Catholic')
> plot(intervals(pub.list), main='Public')
>
```

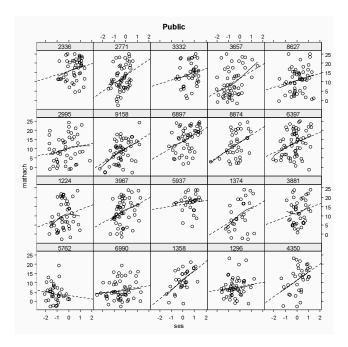


Figure 2: Trellis display of math achievement by socio-economic status for 20 randomly selected public schools.

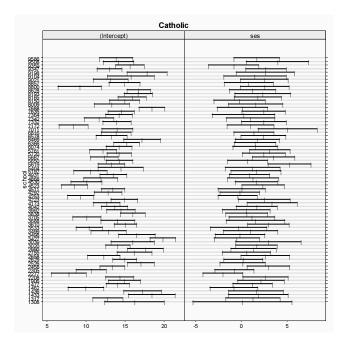


Figure 3: 95-percent confidence intervals for the intercepts and slopes of the within-schools regressions of math achievement on SES, for Catholic schools.

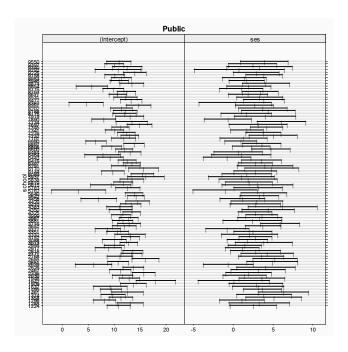


Figure 4: 95-percent confidence intervals for the intercepts and slopes of the within-schools regressions of math achievement on SES, for public schools.

The resulting graphs are shown in Figures 3 and 4. In interpreting these graphs, we need to be careful to remember that I have not constrained the scales for the plots to be the same, and indeed the scales for the intercepts and slopes in the public schools are wider than in the Catholic schools. Because the SES variable is centered to zero, the intercepts are interpretable as the predicted levels of math achievement in each school at an overall average level of SES. It is clear that there is substantial variation in the intercepts among both Catholic and public schools; the confidence intervals for the slopes, in contrast, overlap to a much greater extent, but there is still apparent school-to-school variation.

To facilitate comparisons between the distributions of intercepts and slopes across the two sectors, I draw parallel boxplots for the coefficients:

```
> cat.coef <- coef(cat.list)
> cat.coef[1:10,]
     (Intercept)
                       ses
1308
         16.1890
                   0.12602
1317
         12.7378
                   1.27391
1433
         18.3989
                   1.85429
1436
         17.2106
                   1.60056
          9.9408 -0.82881
1462
1477
         14.0321
                   1.23061
1906
         14.8855
                   2.14551
2208
         14.2889
                   2.63664
2277
          7.7623 -2.01503
2305
         10.6466 -0.78211
> pub.coef <- coef(pub.list)</pre>
> pub.coef[1:10,]
     (Intercept)
1224
         10.8051 2.508582
1288
         13.1149 3.255449
```

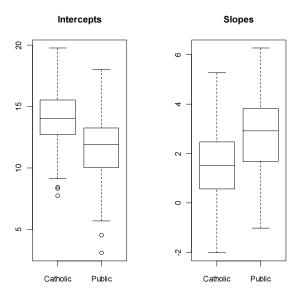


Figure 5: Boxplots of intercepts and slopes for the regressions of math achievement on SES in Catholic and public schools.

```
1296
          8.0938 1.075959
1358
         11.3059 5.068009
1374
          9.7772 3.854323
         12.5974 6.266497
1461
1499
          9.3539 3.634734
1637
          9.2227 3.116806
1909
         13.7151 2.854790
1942
         18.0499 0.089383
> old <- par(mfrow=c(1,2))</pre>
 boxplot(cat.coef[,1], pub.coef[,1], main='Intercepts',
      names=c('Catholic', 'Public'))
  boxplot(cat.coef[,2], pub.coef[,2], main='Slopes',
      names=c('Catholic', 'Public'))
 par(old)
```

The calls to coef extract matrices of regression coefficients from the lmList objects, with rows representing schools. Setting mfrow to 1 row and 2 columns produces the side-by-side pairs of boxplots in Figure 5; mfrow is then returned to its previous value. At an average level of SES, the Catholic schools have a higher average level of math achievement than the public schools, while the average slope relating math achievement to SES is larger in the public schools than in the Catholic schools.

3.2 Fitting a Hierarchical Linear Model with 1me

Following Bryk and Raudenbush (1992) and Singer (1998), I will fit a hierarchical linear model to the mathachievement data. This model consists of two equations: First, within schools, we have the regression of math achievement on the individual-level covariate SES; it aids interpretability of the regression coefficients to center SES at the school average; then the intercept for each school estimates the average level of math achievement in the school.

Using centered SES, the individual-level equation for individual j in school i is

$$\operatorname{mathach}_{ij} = \alpha_{0i} + \alpha_{1i} \operatorname{cses}_{ij} + \varepsilon_{ij} \tag{2}$$

At the school level, also following Bryk and Raudenbush, I will entertain the possibility that the school intercepts and slopes depend upon sector and upon the average level of SES in the schools:

$$\alpha_{0i} = \gamma_{00} + \gamma_{01} \text{meanses}_i + \gamma_{02} \text{sector}_i + u_{0i}$$

$$\alpha_{1i} = \gamma_{10} + \gamma_{11} \text{meanses}_i + \gamma_{12} \text{sector}_i + u_{1i}$$
(3)

This kind of formulation is sometimes called a coefficients-as-outcomes model.

Substituting the school-level equation 3 into the individual-level equation 2 produces

$$\text{mathach}_{ij} = \gamma_{00} + \gamma_{01} \text{meanses}_i + \gamma_{02} \text{sector}_i + u_{0i} \\
 + (\gamma_{10} + \gamma_{11} \text{meanses}_i + \gamma_{12} \text{sector}_i + u_{1i}) \text{cses}_{ij} + \varepsilon_{ij}$$

Rearranging terms,

$$\begin{split} \text{mathach}_{ij} &= \gamma_{00} + \gamma_{01} \text{meanses}_i + \gamma_{02} \text{sector}_i + \gamma_{10} \text{cses}_{ij} \\ &+ \gamma_{11} \text{meanses}_i \text{cses}_{ij} + \gamma_{12} \text{sector}_i \text{cses}_{ij} \\ &+ u_{0i} + u_{1i} \text{cses}_{ij} + \varepsilon_{ij} \end{split}$$

Here, the γ 's are fixed effects, while the u's (and the individual-level errors ε_{ij}) are random effects. Finally, rewriting the model in the notation of the linear mixed model (equation 1),

$$\text{mathach}_{ij} = \beta_1 + \beta_2 \text{meanses}_i + \beta_3 \text{sector}_i + \beta_4 \text{cses}_{ij}$$

$$+ \beta_5 \text{meanses}_i \text{cses}_{ij} + \beta_6 \text{sector}_i \text{cses}_{ij}$$

$$+ b_{i1} + b_{i2} \text{cses}_{ij} + \varepsilon_{ij}$$

$$(4)$$

The change is purely notational, using β 's for fixed effects and b's for random effects. (In the data set, however, the school-level variables — that is, meanses and sector — are attached to the observations for the individual students, as previously described.) I place no constraints on the covariance matrix of the random effects, so

$$\mathbf{\Psi} = V \begin{bmatrix} b_{i1} \\ b_{i2} \end{bmatrix} = \begin{bmatrix} \psi_1^2 & \psi_{12} \\ \psi_{12} & \psi_2^2 \end{bmatrix}$$

but assume that the individual-level errors are independent within schools, with constant variance:

$$V(\boldsymbol{\varepsilon}_i) = \sigma^2 \mathbf{I}_{n_i}$$

As mentioned in Section 2, linear mixed models are fit with the lme function in the nlme library. Specifying the fixed effects in the call to lme is identical to specifying a linear model in a call to lm (see Chapter 4 of the text). Random effects are specified via the random argument to lme, which takes a one-sided model formula.

Before fitting a mixed model to the math-achievement data, I reorder the levels of the factor sector so that the contrast coding the sector effect will use the value 0 for the public sector and 1 for the Catholic sector, in conformity with the coding employed by Bryk and Raudenbush (1992) and by Singer (1998):

- > Bryk\$sector <- factor(Bryk\$sector, levels=c('Public', 'Catholic'))
- > contrasts(Bryk\$sector)

Catholic

Public 0 Catholic 1

Reminder: Default Contrast Coding in S-PLUS

Recall that in S-PLUS, the default contrast function for unordered factors is contr.helmert rather than contr.treatment. As described in Section 4.2 of the text, there are several ways to change the contrast coding, including resetting the global default: options(contrasts=c('contr.treatment', 'contr.poly')).

Having established the contrast-coding for sector, the linear mixed model in equation 4 is fit as follows:

```
> bryk.lme.1 <- lme(mathach ~ meanses*cses + sector*cses,
     random = ~ cses | school,
     data=Bryk)
> summary(bryk.lme.1)
Linear mixed-effects model fit by REML
 Data: Bryk
    AIC
          BIC logLik
  46525 46594 -23252
Random effects:
Formula: ~cses | school
Structure: General positive-definite, Log-Cholesky parametrization
            StdDev
                    Corr
(Intercept) 1.541177 (Intr)
cses
            0.018174 0.006
Residual
            6.063492
Fixed effects: mathach ~ meanses * cses + sector * cses
                      Value Std.Error
                                        DF t-value p-value
                                            60.886 <.0001
(Intercept)
                    12.1282
                              0.19920 7022
meanses
                     5.3367
                              0.36898 157
                                            14.463
                                                    <.0001
                     2.9421
                              0.15122 7022
                                            19.456
                                                    <.0001
cses
sectorCatholic
                     1.2245
                              0.30611 157
                                             4.000
                                                     1e-04
                     1.0444
                              0.29107 7022
                                             3.588
                                                     3e-04
meanses:cses
cses:sectorCatholic -1.6421
                              0.23312 7022
                                            -7.044
                                                    <.0001
Correlation:
                    (Intr) meanss cses
                                         sctrCt mnss:c
                     0.256
meanses
cses
                     0.000 0.000
                    -0.699 -0.356 0.000
sectorCatholic
meanses:cses
                     0.000 0.000 0.295
                                          0.000
cses:sectorCatholic 0.000 0.000 -0.696
                                          0.000 - 0.351
Standardized Within-Group Residuals:
     Min
                 Q1
                                     QЗ
                          Med
                                              Max
-3.170106 -0.724877 0.014892 0.754263 2.965498
Number of Observations: 7185
Number of Groups: 160
```

Notice that the formula for the random effects includes only the term for centered SES; as in a linear-model formula, a random intercept is implied unless it is explicitly excluded (by specifying -1 in the random formula). By default, 1me fits the model by restricted maximum likelihood (REML), which in effect corrects the maximum-likelihood estimator for degrees of freedom. See Pinheiro and Bates (2000) for details on this

and other points.

The output from the summary method for lme objects consists of several panels:

- The first panel gives the AIC (Akaike information criterion) and BIC (Bayesian information criterion), which can be used for model selection (see Section 6.5.2 of the text), along with the log of the maximized restricted likelihood.
- The next panel displays estimates of the variance and covariance parameters for the random effects, in the form of standard deviations and correlations. The term labelled Residual is the estimate of σ . Thus, $\hat{\psi}_1 = 1.541$, $\hat{\psi}_2 = 0.018$, $\hat{\sigma} = 6.063$, and $\hat{\psi}_{12} = 0.006 \times 1.541 \times 0.018 = 0.0002$.
- The table of fixed effects is similar to output from 1m; to interpret the coefficients in this table, refer to the hierarchical form of the model given in equations 2 and 3, and to the Laird-Ware form of the linear mixed model in equation 4 (which orders the coefficients differently from the 1me output). In particular:
 - The fixed-effect intercept coefficient $\hat{\beta}_1 = 12.128$ represents an estimate of the average level of math achievement in public schools, which are the baseline category for the dummy regressor for sector.
 - Likewise, the coefficient labelled sectorCatholic, $\widehat{\beta}_3=1.225$, represents the difference between the average level of math achievement in Catholic schools and public schools.
 - The coefficient for cses, $\hat{\beta}_4=2.942$, is the estimated average slope for SES in public schools, while the coefficient labelled cses:sectorCatholic, $\hat{\beta}_6=-1.642$, gives the difference in average slopes between Catholic and public schools. As we noted in our exploration of the data, the average level of math achievement is higher in Catholic than in public schools, and the average slope relating math achievement to students' SES is larger in public than in Catholic schools.
 - Given the parametrization of the model, the coefficient for meanses, $\hat{\beta}_2 = 5.337$, represents the relationship of schools' average level of math achievement to their average level of SES
 - The coefficient for the interaction meanses:cses, $\hat{\beta}_5 = 1.044$, gives the average change in the within-school SES slope associated with a one-unit increment in the school's mean SES. Notice that all of the coefficients are highly statistically significant.
- The panel labelled Correlation gives the estimated sampling correlations among the fixed-effect coefficient estimates, which are not usually of direct interest. Very large correlations, however, are indicative of an ill-conditioned model.
- Some information about the standardized within-group residuals $(\hat{\epsilon}_{ij}/\hat{\sigma})$, the number of observations, and the number of groups, appears at the end of the output.

Different Solutions from 1me in R and S-PLUS

The results for $\hat{\psi}_2$ (the standard deviation of the random effects of cses) and $\hat{\psi}_{12}$ (the covariance between the random intercepts and slopes) are different in S-PLUS, where lme uses a different (and more robust) optimizer than in R.

Comparing the maximized log-likelihoods for the two programs suggests that the R version of 1me has not converged fully to the REML solution. Checking confidence intervals for the variance components in the R solution [by the command intervals(bryk.lme.1)] shows that the confidence interval for ψ_2 in particular is extremely wide, raising the possibility that the problem is ill-conditioned. (These normal-theory confidence intervals for variance components should not be trusted, but they do help to reveal estimates that are not well determined by the data.)

In the S-PLUS solution, in contrast, the confidence interval for ψ_2 is much narrower, but the confidence interval for the correlation between the two sets of random effects is very wide. Not coincidentally, it turns out that ψ_2 and ψ_{12} can be dropped from the model.

I am grateful to Douglas Bates and José Pinheiro for clarifying the source of the differences in the results from the R and S-PLUS versions of nlme.

In addition to estimating and testing the fixed effects, it is of interest to determine whether there is evidence that the variances of the random effects in the model are different from 0. We can test hypotheses about the variances and covariances of random effects by deleting random-effects terms from the model and noting the change in the log of the maximized restricted likelihood, calculating log likelihood-ratio statistics. We must be careful, however, to compare models that are identical in their fixed effects.

For the current illustration, we may proceed as follows:

```
> bryk.lme.2 <- update(bryk.lme.1,
      random = ~ 1 | school) # omitting random effect of cses
> anova(bryk.lme.1, bryk.lme.2)
           Model df
                      AIC
                            BIC logLik
                                         Test
                                                 L.Ratio p-value
bryk.lme.1
               1 10 46525 46594 -23252
                  8 46521 46576 -23252 1 vs 2 0.0032069 0.9984
bryk.lme.2
> bryk.lme.3 <- update(bryk.lme.1,
      random = ~ cses - 1 | school)
                                     # omitting random intercept
> anova(bryk.lme.1,
                   bryk.lme.3)
           Model df
                      AIC
                            BIC logLik
                                         Test L.Ratio p-value
               1 10 46525 46594 -23252
bryk.lme.1
bryk.lme.3
               2 8 46740 46795 -23362 1 vs 2 219.44 <.0001
```

Each of these likelihood-ratio tests is on 2 degrees of freedom, because excluding one of the random effects removes not only its variance from the model but also its covariance with the other random effect. There is strong evidence, then, that the average level of math achievement (as represented by the intercept) varies from school to school, but not that the coefficient of SES varies, once differences between Catholic and public schools are taken into account, and the average level of SES in the schools is held constant.

Model bryk.lme.2, fit above, omits the non-significant random effects for cses; the fixed-effects estimates are nearly identical to those for the initial model bryk.lme.1, which includes these random effects:

```
> summary(bryk.lme.2)
> summary(bryk.lme.2)
Linear mixed-effects model fit by REML
Data: Bryk
    AIC    BIC logLik
    46521 46576 -23252
```

```
Random effects:
Formula: ~1 | school
        (Intercept) Residual
StdDev:
             1.5412
                      6.0635
Fixed effects: mathach ~ meanses * cses + sector * cses
                      Value Std.Error
                                        DF t-value p-value
(Intercept)
                    12.1282
                              0.19920 7022
                                           60.885
                                                    <.0001
meanses
                     5.3367
                              0.36898
                                      157
                                            14.463
                     2.9421
                              0.15121 7022
                                            19.457
                                                     <.0001
cses
sectorCatholic
                     1.2245
                              0.30612
                                      157
                                              4.000
                                                      1e-04
                     1.0444
                              0.29105 7022
                                             3.589
                                                      3e-04
meanses:cses
cses:sectorCatholic -1.6422
                              0.23309 7022
                                            -7.045
Correlation:
                    (Intr) meanss cses
                                         sctrCt mnss:c
                     0.256
meanses
                     0.000 0.000
cses
sectorCatholic
                    -0.699 -0.356
                                   0.000
meanses:cses
                     0.000 0.000 0.295
                                          0.000
cses:sectorCatholic 0.000 0.000 -0.696 0.000 -0.351
Standardized Within-Group Residuals:
                          Med
      Min
                 01
                                     QЗ
-3.170115 -0.724877 0.014845 0.754242 2.965513
Number of Observations: 7185
Number of Groups: 160
```

4 An Illustrative Application to Longitudinal Data

To illustrate the use of linear mixed models for longitudinal research, I draw on as-yet unpublished data collected by Blackmoor and Davis on the exercise histories of 138 teenaged girls hospitalized for eating disorders, and on a group of 93 'control' subjects.⁴ The data are in the data frame Blackmoor in the car library:

```
> library(car) # for data only
> data(Blackmoor) # from car
> Blackmoor[1:20,] # first 20 observations
   subject
             age exercise
                             group
       100 8.00
                     2.71 patient
1
2
       100 10.00
                     1.94 patient
3
       100 12.00
                     2.36 patient
4
       100 14.00
                     1.54 patient
5
       100 15.92
                     8.63 patient
6
       101 8.00
                     0.14 patient
7
       101 10.00
                     0.14 patient
8
       101 12.00
                     0.00 patient
9
       101 14.00
                     0.00 patient
10
       101 16.67
                     5.08 patient
```

⁴These data were generously made available to me by Elizabeth Blackmoor and Caroline Davis of York University.

```
11
       102 8.00
                     0.92 patient
12
       102 10.00
                     1.82 patient
13
       102 12.00
                     4.75 patient
                    24.72 patient
15
       102 15.08
16
       103 8.00
                     1.04 patient
                     2.90 patient
17
       103 10.00
18
       103 12.00
                     2.65 patient
20
       103 14.08
                     6.86 patient
21
       104 8.00
                     2.75 patient
22
       104 10.00
                     6.62 patient
```

The variables are:

- subject: an identification code; there are several observations for each subject, but because the girls were hospitalized at different ages, the number of observations, and the age at the last observation, vary.
- age: the subject's age in years at the time of observation; all but the last observation for each subject were collected retrospectively at intervals of two years, starting at age eight.
- exercise: the amount of exercise in which the subject engaged, expressed as estimated hours per week.
- group: a factor indicating whether the subject is a 'patient' or a 'control'.⁵

4.1 Examining the Data

Initial examination of the data suggested that it is advantageous to take the log of exercise: Doing so makes the exercise distribution for both groups of subjects more symmetric and linearizes the relationship of exercise to age. Because there are some 0 values of exercise, I use "started" logs in the analysis reported below (see Section 3.4 of the text on transforming data), adding five minutes (5/60 of an hour) to each value of exercise prior to taking logs (and using logs to the base 2 for interpretability):

```
> Blackmoor$log.exercise <- log(Blackmoor$exercise + 5/60, 2)
> attach(Blackmoor)
```

As in the analysis of the math-achievement data in the preceding section, I begin by sampling 20 subjects from each of the patient and control groups, plotting log.exercise against age for each subject:

⁵To avoid the possibility of confusion, I point out that the variable group represents groups of independent patients and control subjects, and is *not* a factor defining clusters. Clusters in this longitudinal data set are defined by the variable subject.

The graphs appear in Figure 6.

- Each Trellis plot is constructed by using the default plot method for grouped-data objects.
- To make the two plots comparable, I have exercised direct control over the scale of the vertical axis (set to slightly larger than the range of the combined log-exercise values), the layout of the plot (5 columns, 4 rows)⁶, and the aspect ratio of the plot (the ratio of the vertical to the horizontal size of the plotting region in each panel, set here to 1.0).
- The print method for Trellis objects, normally automatically invoked when the returned object is not assigned to a variable, simply plots the object on the active graphics device. So as to print both plots on the same "page," I have instead called print explicitly, using the position argument to place each graph on the page. The form of this argument is c(xmin, ymin, xmax, ymax), with horizontal (x) and vertical (y) coordinates running from 0, 0 (the lower-left corner of the page) to 1, 1 (the upper-right corner). The argument more=T in the first call to print indicates that the graphics page is not yet complete.

There are few observations for each subject, and in many instances, no strong within-subject pattern. Nevertheless, it appears as if the general level of exercise is higher among the patients than among the controls. As well, the trend for exercise to increase with age appears stronger and more consistent for the patients than for the controls.

I pursue these impressions by fitting regressions of log.exercise on age for each subject. Because of the small number of observations per subject, we should not expect very good estimates of the within-subject regression coefficients. Indeed, one of the advantages of mixed models is that they can provide improved estimates of the within-subject coefficients (the random effects) by pooling information across subjects.⁷

The boxplots of regression coefficients are shown in Figure 7. I changed the origin of age to 8 years, which is the initial observation for each subject, so the intercept represents level of exercise at the start of the study. As expected, there is a great deal of variation in both the intercepts and the slopes. The median intercepts are similar for patients and controls, but there is somewhat more variation among patients. The slopes are higher on average for patients than for controls, for whom the median slope is close to 0.

⁶Notice the unusual ordering in specifying the layout — columns first, then rows.

⁷Pooled estimates of the random effects provide so-called best-linear-unbiased predictors (or BLUPs). See help(predict.lme) and Pinheiro and Bates (2000).

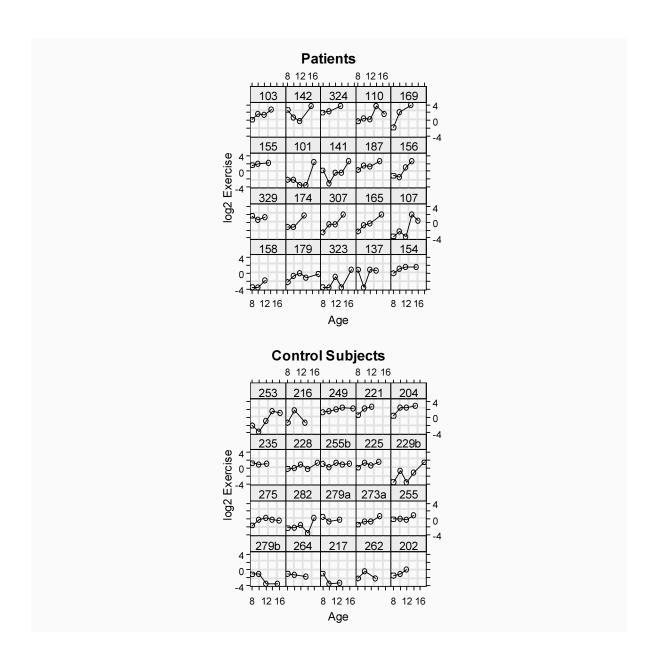


Figure 6: log₂ exercise by age for 20 randomly selected patients and 20 randomly selected control subjects.

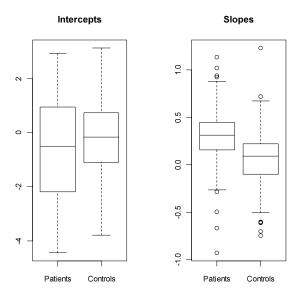


Figure 7: Coefficients for the within-subject regressions of log₂ exercise on age, for patients and control subjects

4.2 Fitting the Mixed Model

I proceed to fit a linear mixed model to the data, including fixed effects for age (again, with an origin of 8), group, and their interaction, and random intercepts and slopes:

```
> bm.lme.1 <- lme(log.exercise ~ I(age - 8)*group,
                     random = ~ I(age - 8) | subject,
+
                     data=Blackmoor)
> summary(bm.lme.1)
Linear mixed-effects model fit by REML
 Data: Blackmoor
     AIC
           BIC logLik
  3630.1 3668.9 -1807.1
Random effects:
Formula: ~I(age - 8) | subject
Structure: General positive-definite, Log-Cholesky parametrization
           StdDev Corr
(Intercept) 1.44356 (Intr)
I(age - 8) 0.16480 -0.281
Residual
            1.24409
Fixed effects: log.exercise ~ I(age - 8) * group
                          Value Std.Error DF t-value p-value
(Intercept)
                       -0.27602 0.182368 712 -1.5135 0.1306
I(age - 8)
                        0.06402 0.031361 712 2.0415 0.0416
grouppatient
                       -0.35400 0.235291 229 -1.5045 0.1338
I(age - 8):grouppatient 0.23986 0.039408 712 6.0866 <.0001
Correlation:
```

```
(Intr) I(g-8) grpptn
I(age - 8) -0.489
grouppatient -0.775 0.379
I(age - 8):grouppatient 0.389 -0.796 -0.489

Standardized Within-Group Residuals:
Min Q1 Med Q3 Max
-2.73486 -0.42451 0.12277 0.52801 2.63619

Number of Observations: 945
Number of Groups: 231
```

There is a small, and marginally statistically significant, average age trend in the control group (represented by the fixed-effect coefficient for age - 8), and a highly significant interaction of age with group, reflecting a much steeper average trend in the patient group. The small and nonsignificant coefficient for group indicates similar age-eight intercepts for the two groups.

I test whether the random intercepts and slopes are necessary, omitting each in turn from the model and calculating a likelihood-ratio statistic, contrasting the refit model with the original model:

```
> bm.lme.2 <- update(bm.lme.1, random = ~ 1 | subject)
> anova(bm.lme.1, bm.lme.2)
         Model df
                    AIC
                            BIC logLik
                                         Test L.Ratio p-value
            1 8 3630.1 3668.9 -1807.1
bm.lme.1
bm.lme.2
            2 6 3644.3 3673.3 -1816.1 1 vs 2 18.122
> bm.lme.3 <- update(bm.lme.1, random = ~ I(age - 8) - 1 | subject)
> anova(bm.lme.1, bm.lme.3)
        Model df
                    AIC
                           BIC logLik
                                         Test L.Ratio p-value
            1 8 3630.1 3668.9 -1807.1
bm.lme.1
            2 6 3834.1 3863.2 -1911.0 1 vs 2 207.95 <.0001
```

The tests are highly statistically significant, suggesting that both random intercepts and random slopes are required.

Let us next consider the possibility that the within-subject errors (the ε_{ij} 's in the mixed model) are auto-correlated — as may well be the case, since the observations are taken longitudinally on the same subjects. The lme function incorporates a flexible mechanism for specifying correlation structures, and supplies constructor functions for several such structures.⁸ Most of these correlation structures, however, are appropriate only for equally spaced observations. An exception is the corCAR1 function, which permits us to fit a continuous first-order autoregressive process in the errors. Suppose that ε_{it} and $\varepsilon_{i,t+s}$ are errors for subject i separated by s units of time, where s need not be an integer; then, according to the continuous first-order autoregressive model, the correlation between these two errors is $\rho(s) = \phi^{|s|}$ where $0 \le \phi < 1$. This appears a reasonable specification in the current context, where there are at most $n_i = 5$ observations per subject.

Fitting the model with CAR1 errors to the data produces the following results:

```
> bm.lme.4 <- update(bm.lme.1, correlation = corCAR1(form = ~ age |subject))
> summary(bm.lme.4)
Linear mixed-effects model fit by REML
Data: Blackmoor
    AIC    BIC logLik
    3607.1 3650.8 -1794.6
```

Random effects:

⁸ A similar mechanism is provided for modeling non-constant variance, via the weights argument to lme. See the documentation for lme for details.

```
Formula: ~I(age - 8) | subject
Structure: General positive-definite, Log-Cholesky parametrization
            StdDev
                   Corr
(Intercept) 1.053381 (Intr)
I(age - 8) 0.047939 0.573
Residual
            1.514138
Correlation Structure: Continuous AR(1)
Formula: ~age | subject
Parameter estimate(s):
   Phi
0.6236
Fixed effects: log.exercise ~ I(age - 8) * group
                            Value Std.Error DF t-value p-value
                        -0.306202   0.182027 712 -1.6822   0.0930
(Intercept)
I(age - 8)
                        0.072302 0.032020 712 2.2580
                                                         0.0242
grouppatient
                        -0.289267 0.234968 229 -1.2311 0.2196
I(age - 8):grouppatient 0.230054 0.040157 712 5.7289 <.0001
Correlation:
                        (Intr) I(g-8) grpptn
I(age - 8)
                        -0.509
grouppatient
                        -0.775 0.395
I(age - 8):grouppatient 0.406 -0.797 -0.511
Standardized Within-Group Residuals:
    Min
               Q1
                       Med
                                 QЗ
                                         Max
-2.67829 -0.46383 0.16530 0.58823 2.11817
Number of Observations: 945
```

The correlation structure is given in the correlation argument to lme (here as a call to corCAR1); the form argument to corCAR1 is a one-sided formula defining the time dimension (here, age) and the group structure (subject). The estimated autocorrelation, $\hat{\phi} = 0.62$, is quite large, but the fixed-effects estimates and their standard errors have not changed much. A likelihood-ratio test establishes the statistical significance of the error autocorrelation:

Number of Groups: 231

Because the specification of the model has changed, we can re-test whether random intercepts and slopes are required; as it turns out, the random age term may now be removed from the model, but not the random intercepts:

⁹The large correlation between the random effects for the intercept and slope, however, suggests that the problem may be ill-conditioned.

Differences in the Results in R and S-PLUS

As in the analysis of the Bryk and Raudenbush data, the lme function in S-PLUS produces different estimates of the standard deviation of the slopes [here, the random effects for I(age - 8)] and of the correlation between the slopes and intercepts. This time, however, the R version of the software does a slightly better job of maximizing the restricted likelihood.

As before, this difference is evidence of an ill-conditioned problem, as may be verified by examining confidence intervals for the estimates: In R, the confidence interval for the correlation runs from nearly -1 to almost +1, while lme in S-PLUS is unable to calculate the confidence intervals because the estimated covariance matrix for the random effects is not positive-definite. Also as before, the random slopes can be removed from the model (see below).

To get a more concrete sense of the fixed effects, using model bm.lme.5 (which includes autocorrelated errors, random intercepts, but not random slopes), I employ the predict method for lme objects to calculate fitted values for patients and controls across the range of ages (8 to 18) represented in the data:

```
> pdata <- expand.grid(age=seq(8, 18, by=2), group=c('patient', 'control'))</pre>
> pdata$log.exercise <- predict(bm.lme.5, pdata, level=0)</pre>
> pdata$exercise <- (2^pdata$log.exercise) - 5/60</pre>
> pdata
   age
         group log.exercise exercise
                  -0.590722 0.58068
    8 patient
    10 patient
2
                   0.009735 0.92344
3
    12 patient
                   0.610192 1.44313
4
    14 patient
                   1.210650 2.23109
5
    16 patient
                   1.811107 3.42578
6
    18 patient
                   2.411565 5.23718
7
     8 control
                  -0.307022 0.72498
8
    10 control
                  -0.161444 0.81080
9
    12 control
                  -0.015866 0.90573
10
   14 control
                   0.129712
                              1.01074
                   0.275291 1.12690
11
    16 control
   18 control
                   0.420869 1.25540
```

Specifying level=0 in the call to predict produces estimates of the fixed effects. The expression

```
(2^pdataslog.exercise) - 5/60
```

translates the fitted values of exercise from the log₂ scale back to hours/week.

Finally, I plot the fitted values (Figure 8):

```
> plot(pdata$age, pdata$exercise, type='n',
+     xlab='Age (years)', ylab='Exercise (hours/week)')
> points(pdata$age[1:6], pdata$exercise[1:6], type='b', pch=19, lwd=2)
> points(pdata$age[7:12], pdata$exercise[7:12], type='b', pch=22, lty=2, lwd=2)
> legend(locator(1), c('Patients', 'Controls'), pch=c(19, 22), lty=c(1,2), lwd=2)
```

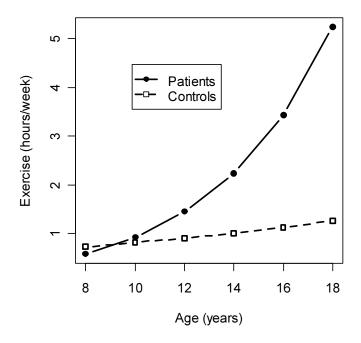


Figure 8: Fitted values representing estimated fixed effects of group, age, and their interaction.

Notice that the legend is placed interactively with the mouse. It is apparent that the two groups of subjects have similar average levels of exercise at age 8, but that thereafter the level of exercise increases much more rapidly for the patient group than for the controls.

Reminder: Use of legend in S-PLUS

The plotting characters for the legend function in S-PLUS are specified via the marks argument, rather than via pch as in R. As well, in S-PLUS, you may wish to use plotting characters 16 and 0 in place of 19 and 22.

References

Bryk, A. S. & S. W. Raudenbush. 1992. Hierarchical Linear Models: Applications and Data Analysis Methods. Newbury Park CA: Sage.

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