

# Linear Mixed Effects Models

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Duke STA 610

Introduction

Fixed and random effects

Model fitting

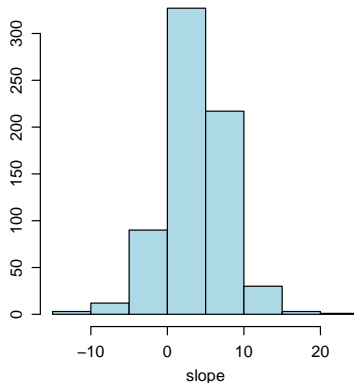
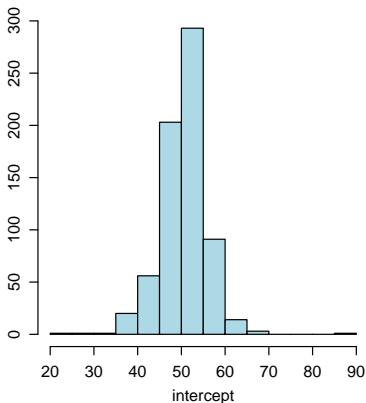
Group-level characteristics

General LME Model

## Heterogeneity of $\hat{\beta}_j$ 's for the NELS data

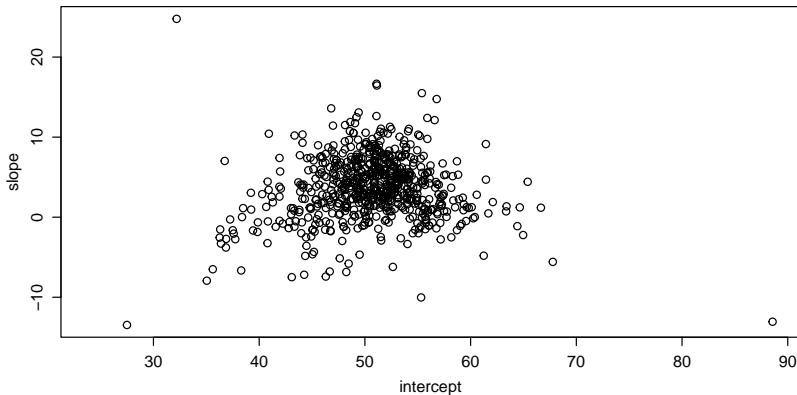
$$\hat{\beta}_j = (\mathbf{X}_j^T \mathbf{X}_j)^{-1} \mathbf{X}_j^T \mathbf{y}_j$$

```
hist(BETA.OLS[,1]) hist(BETA.OLS[,2])
```



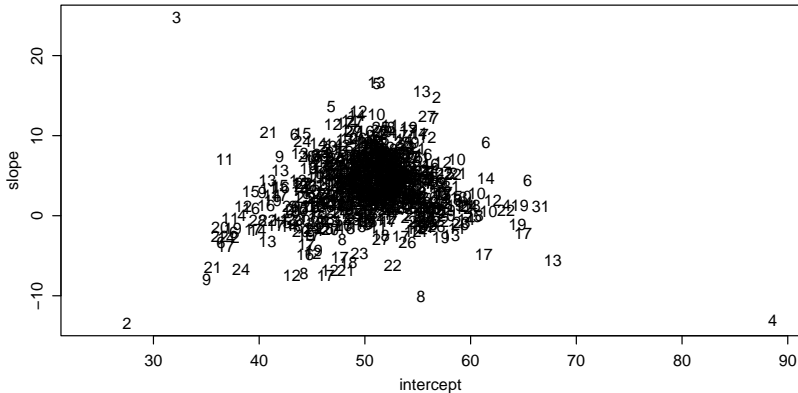
## Heterogeneity of $\hat{\beta}_j$ 's

```
plot(BETA.OLS)
```



$$\text{Var}[\hat{\beta}_j] = \sigma^2 (\mathbf{X}_j^T \mathbf{X}_j)^{-1}$$

## Heterogeneity as a function of sample size



$$\text{Var}[\hat{\beta}_j] = \sigma^2 (\mathbf{X}_j^T \mathbf{X}_j)^{-1}$$

## Modeling heterogeneity

In the hierarchical normal model:

$$\theta_j = \{\mu_j, \sigma^2\}$$

$$y_{i,j} = \mu_j + \sigma^2, \{e_{i,j}\} \sim \text{i.i.d. normal}(\mu_j, \sigma^2)$$

$$\mu_1, \dots, \mu_m \sim \text{i.i.d. normal}(\mu, \tau^2)$$

What should we do for a hierarchical regression model?

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## HLM

### MVN model for across-group heterogeneity:

$$\beta_1, \dots, \beta_m \sim \text{i.i.d. multivariate normal}(\beta, \Sigma_\beta)$$

The parameters in this model include

$\beta$ , an across-group mean regression vector

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## Ad-hoc estimates

```
## rough estimate of beta
apply(BETA.OLS, 2, mean, na.rm=TRUE)

## (Intercept)          xj
## 50.618228      3.672483
```

This estimator of  $\beta$  equally weights all schools.

Generally, we want to assign a lower weight to schools with less data.

```
## rough estimate of Sigma_beta
cov(BETA.OLS, use="complete.obs")

##              (Intercept)          xj
## (Intercept) 26.795851  1.001585
## xj          1.001585 15.818939
```

This is a *very rough* estimate of  $\Sigma_\beta$ :

- It ignores sample size differences;
- It ignores the variability of  $\hat{\beta}_j$  around  $\beta_j$ .

$$\text{Var}[\hat{\beta}_j\text{'s around } \hat{\beta}] \approx \text{Var}[\beta_j\text{'s around } \beta] + \text{Var}[\hat{\beta}_j\text{'s around } \beta_j\text{'s}]$$

$$\text{Sample covariance of } \hat{\beta}_j\text{'s} \approx \Sigma_\beta + \text{Estimation error}$$

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## Fixed and random effects

Recall the following:

$$\mu_j \sim N(\mu, \tau^2) \Leftrightarrow \mu_j = \mu + a_j, \quad a_j \sim N(0, \tau^2)$$

Analogously,

$$\beta_j \sim N(\beta, \Sigma_\beta) \Leftrightarrow \beta_j = \beta + b_j, \quad b_j \sim N(0, \Sigma_\beta)$$

Therefore, our hierarchical model says that

$$\begin{aligned} \mathbf{y}_j &= \mathbf{X}_j \beta_j + \epsilon_j \\ &= \mathbf{X}_j (\beta + \mathbf{b}_j) + \epsilon_j \\ &= \mathbf{X}_j \beta + \mathbf{X}_j \mathbf{b}_j + \epsilon_j \end{aligned}$$

- $\beta$  is sometimes called a *fixed effect*, as it is fixed across all groups.
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“random” as it varies across groups, or

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→ *fixed effect* and *random effect* are not to be confused with the terms *fixed* and *random* in the context of the group-level parameters being sampled.

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### Recall the HNM:

$$y_{i,j} = \mu + a_j + \epsilon_{i,j}$$

What was the within-group covariance?

$$\begin{aligned}\text{Cov}[y_{i_1,j}, y_{i_2,j}] &= E[(y_{i_1,j} - \mu)(y_{i_2,j} - \mu)] \\ &= E[(a_j + \epsilon_{i_1,j})(a_j + \epsilon_{i_2,j})] \\ &= E[a_j^2] + 0 + 0 + 0 \\ &= \tau^2\end{aligned}$$

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More generally, we might want the *within-group covariance matrix*:

$$\mathbf{y}_j = \begin{pmatrix} y_{1,j} \\ \vdots \\ y_{n,j} \end{pmatrix} \quad \text{Cov}[\mathbf{y}_j] = \begin{pmatrix} \text{Var}[y_{1,j}] & \text{Cov}[y_{1,j}, y_{2,j}] & \cdots & \text{Cov}[y_{1,j}, y_{n,j}] \\ \text{Cov}[y_{1,j}, y_{2,j}] & \text{Var}[y_{2,j}] & \cdots & \text{Cov}[y_{2,j}, y_{n,j}] \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}[y_{1,j}, y_{n,j}] & \text{Cov}[y_{2,j}, y_{n,j}] & \cdots & \text{Var}[y_{n,j}] \end{pmatrix}$$

Our calculations have shown that for the HNM

$$\text{Cov}[\mathbf{y}_j] = \begin{pmatrix} \sigma^2 + \tau^2 & \tau^2 & \cdots & \tau^2 \\ \vdots & & & \vdots \\ \tau^2 & \tau^2 & \cdots & \sigma^2 + \tau^2 \end{pmatrix}$$



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**Marginal dependence:** If I don't know  $\beta_j$  (or  $\mathbf{b}_j$ ), then knowing  $y_{i_1,j}$  gives me a bit of information about  $\beta_j$ , which in turn gives me information about  $y_{i_2,j}$ , and so the observations are dependent: My information about  $y_{i_2,j}$  depends on the value of  $y_{i_1,j}$  if I don't know  $\beta_j$ .

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- $\mathbf{X}_j \boldsymbol{\Sigma} \mathbf{X}_j^T$  is  $n_j \times n_j$ , the covariances between observations within a group.

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 &= \Sigma_{1,1} + \Sigma_{1,2}(x_{1,j} + x_{2,j}) + \Sigma_{2,2}x_{1,j}x_{2,j} \\
 &= \text{Var}[\beta_{0,j}] + \text{Var}[\beta_{1,j}]x_{1,j}x_{2,j} + \text{Cov}[\beta_{0,j}, \beta_{1,j}](x_{1,j} + x_{2,j})
 \end{aligned}$$

- Intercept variance positively correlates the observations within a group.
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## Within-group covariance

Consider the case that  $\mathbf{x}_{i,j} = \{1, x_{i,j}\}$  and  $\boldsymbol{\beta}_j = \{\beta_{0,j}, \beta_{1,j}\}$ .

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## Within-group covariance

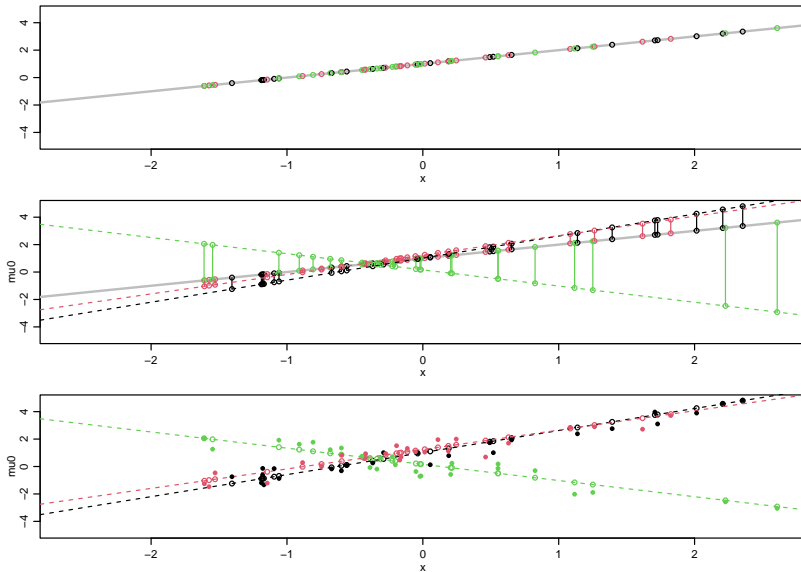
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## Sources of variation and correlation



## Fitting a HLM

Assuming data are independent *across* groups, the likelihood at a value  $(\beta, \Sigma_\beta, \sigma^2)$  can be computed as follows:

0. Set  $ll = 0$ .
1. Set  $ll = ll + \text{ldmvnorm}(\mathbf{y}_1, \mathbf{X}_1\beta, \mathbf{X}_1\Sigma_\beta\mathbf{X}_1 + \sigma^2\mathbf{I})$ .
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- ...
- m. Set  $ll = ll + \text{ldmvnorm}(\mathbf{y}_m, \mathbf{X}_m\beta, \mathbf{X}_m\Sigma_\beta\mathbf{X}_m + \sigma^2\mathbf{I})$ .

We can then numerically optimize the likelihood to find the MLEs.

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## Fitting the HLM with lmer

```
library(lme4)
fit.lme<-lmer( y.nels ~ ses.nels + (ses.nels | g.nels),REML=FALSE)
```

```
summary(fit.lme)

## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: y.nels ~ ses.nels + (ses.nels | g.nels)
##
##          AIC          BIC    logLik deviance df.resid
##  92553.1    92597.9 -46270.5   92541.1     12968
##
## Scaled residuals:
##      Min       1Q   Median       3Q      Max
## -3.8910 -0.6382  0.0179  0.6669  4.4613
##
## Random effects:
##   Groups      Name            Variance Std.Dev. Corr
##   g.nels      (Intercept)  12.223     3.496
##             ses.nels       1.515     1.231    0.11
##   Residual                    67.345     8.206
## Number of obs: 12974, groups: g.nels, 684
##
## Fixed effects:
##              Estimate Std. Error t value
## (Intercept)  50.6767    0.1551   326.70
## ses.nels      4.3594    0.1231    35.41
##
## Correlation of Fixed Effects:
##              (Intr)
## ses.nels  0.007
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## Extracting results - fixed effects

```
### fixed effects
beta.hat<-fixef(fit.lme)
beta.hat

## (Intercept)      ses.nels
##    50.676702      4.359396

### variance-covariance of fixed effects estimates
VBETA<-vcov(fit.lme)
VBETA

## 2 x 2 Matrix of class "dpoMatrix"
##              (Intercept)      ses.nels
## (Intercept) 0.0240607576 0.0001310263
## ses.nels    0.0001310263 0.0151611175

### standard errors
sqrt(diag(VBETA))

## (Intercept)      ses.nels
##    0.1551153    0.1231305

### t-values
beta.hat/sqrt(diag(VBETA))

## (Intercept)      ses.nels
##    326.70343     35.40469
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## Extracting results - variance components

```
### within-group variance
s2.hat<-sigma(fit.lme)^2
```

```
### across-group variance
VarCorr(fit.lme)$g.nels
```

```
##                (Intercept)  ses.nels
## (Intercept)   12.2232568  0.4888068
## ses.nels       0.4888068  1.5148390
## attr(,"stddev")
## (Intercept)    ses.nels
##      3.496177    1.230788
## attr(,"correlation")
##                (Intercept)  ses.nels
## (Intercept)    1.0000000  0.1135954
## ses.nels       0.1135954  1.0000000
```

```
### remove the S4 ugliness
VB<-matrix(VarCorr(fit.lme)$g.nels,2,2)
```

```
VB
```

```
##                [,1]      [,2]
## [1,] 12.2232568  0.4888068
## [2,]  0.4888068  1.5148390
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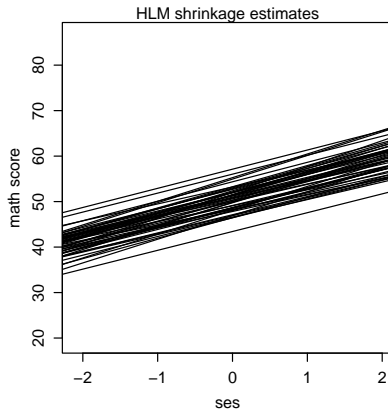
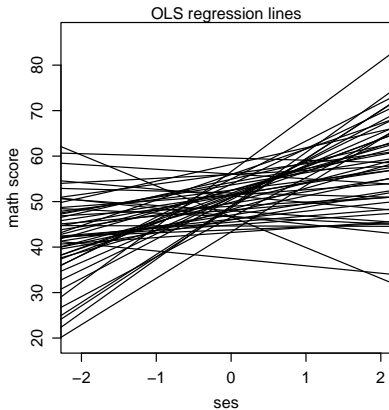
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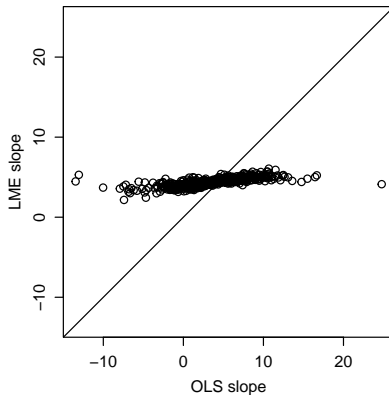
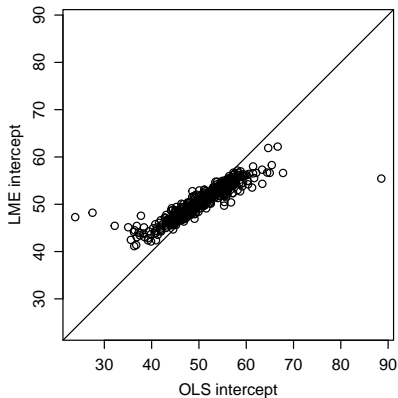
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```

## Random effects estimates

```
B.LME<-as.matrix(ranef(fit.lme)$g.nels)  
BETA.LME<-sweep( B.LME , 2 , beta.hat, "+" )
```



## Range of shrinkage estimates





## Formula for shrinkage estimates

### Intuitively:

$$\tilde{\beta}_j = w_j \hat{\beta}_j + (1 - w_j) \hat{\beta}$$

where  $w_j$  depends on  $\Sigma_b$  and  $\sigma^2(\mathbf{X}_j^T \mathbf{X}_j)^{-1}$ :

- $w_j$  is big if  $\sigma^2(\mathbf{X}_j^T \mathbf{X}_j)^{-1}$  small compared to  $\Sigma_b$ ;
- $w_j$  is small if  $\sigma^2(\mathbf{X}_j^T \mathbf{X}_j)^{-1}$  large compared to  $\Sigma_b$ .

This is almost right. Averaging has to be done using matrices. The BLUP is:

$$\tilde{\beta}_j = \left( \mathbf{X}_j^T \mathbf{X}_j / \sigma^2 + \Sigma_\beta^{-1} \right)^{-1} \left( \mathbf{X}_j \mathbf{y}_j / \sigma^2 + \Sigma_\beta^{-1} \hat{\beta} \right)$$

In practice,  $\sigma^2, \Sigma_\beta, \hat{\beta}$  are usually replaced with  $\hat{\sigma}^2, \hat{\Sigma}_\beta, \hat{\beta}$ .

**Quiz:** How does  $\tilde{\beta}_j$  vary with  $\mathbf{X}_j$ ,  $\sigma^2$  and  $\Sigma_\beta$ ?

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This is almost right. Averaging has to be done using matrices. The BLUP is:

$$\tilde{\beta}_j = \left( \mathbf{X}_j^T \mathbf{X}_j / \sigma^2 + \Sigma_\beta^{-1} \right)^{-1} \left( \mathbf{X}_j \mathbf{y}_j / \sigma^2 + \Sigma_\beta^{-1} \hat{\beta} \right)$$

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**Quiz:** How does  $\tilde{\beta}_j$  vary with  $\mathbf{X}_j$ ,  $\sigma^2$  and  $\Sigma_\beta$ ?

## Formula for shrinkage estimates

### Intuitively:

$$\tilde{\beta}_j = w_j \hat{\beta}_j + (1 - w_j) \hat{\beta}$$

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## Derivation of shrinkage formula

- $\hat{\beta}_j | \beta_j \sim N(\beta_j, \sigma^2(\mathbf{X}_j^\top \mathbf{X}_j)^{-1})$
- $\beta_j \sim N(\boldsymbol{\beta}, \boldsymbol{\Sigma}_\beta)$

Then Bayes rule says  $\beta_j \sim N(\mathbf{m}, \mathbf{V})$  where

$$\mathbf{V} = (\mathbf{X}_j^\top \mathbf{X}_j / \sigma^2 + \boldsymbol{\Sigma}_\beta^{-1})^{-1}$$

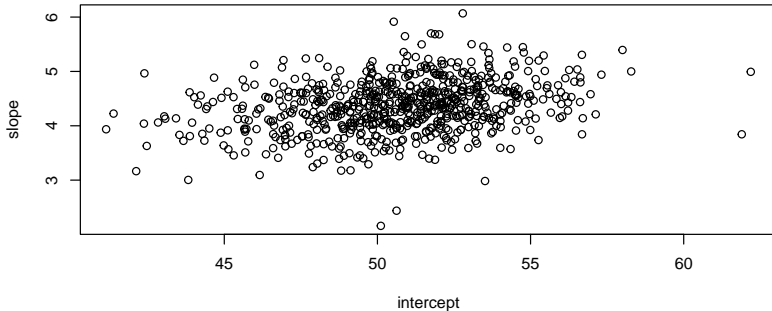
$$\mathbf{m} = V(\mathbf{X}_j^\top \mathbf{y}_j / \sigma^2 + \boldsymbol{\Sigma}_\beta^{-1} \boldsymbol{\beta})$$

The BLUP/Bayes estimator is the conditional expectation:

$$\tilde{\beta}_j = \left( \mathbf{X}_j^\top \mathbf{X}_j / \sigma^2 + \boldsymbol{\Sigma}_\beta^{-1} \right)^{-1} \left( \mathbf{X}_j \mathbf{y}_j / \sigma^2 + \boldsymbol{\Sigma}_\beta^{-1} \boldsymbol{\beta} \right)$$

## Macro-level effects

### LME regression estimates:



### Questions:

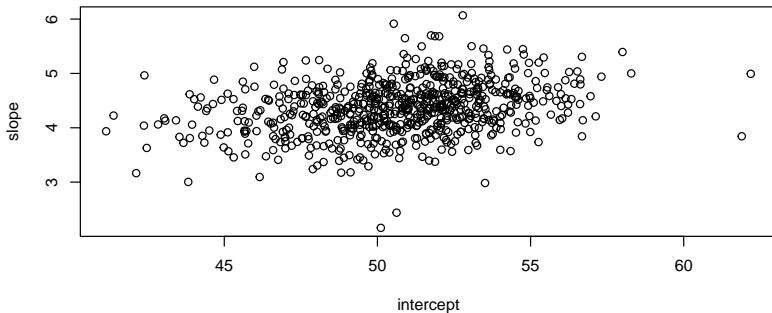
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Can we relate *macro-level parameters* to *macro-level effects* ?



## Macro-level effects

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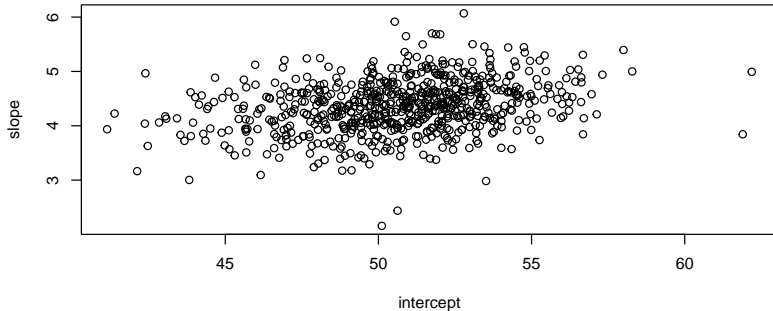
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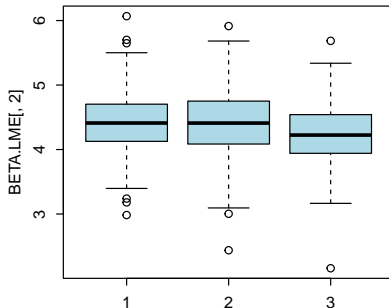
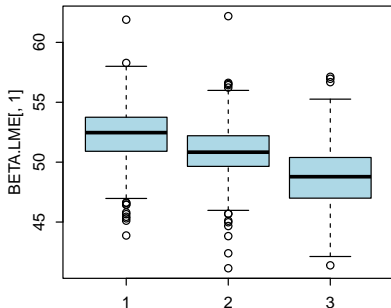
Can we relate *macro-level parameters* to *macro-level effects* ?

## Macro-level effects

```
### FLP variable
flp.school<-tapply( flp.nels , g.nels, mean)
table(flps.school)

## flps.school
##    1    2    3
## 226 257 201

### RE and FLP association
mpar()
par(mfrow=c(1,2))
boxplot(BETA.LME[,1]~flps.school,col="lightblue")
boxplot(BETA.LME[,2]~flps.school,col="lightblue")
```



## Macro-level effects

It seems that  $\beta_{0,j}$  and possibly  $\beta_{1,j}$  are associated with  $flp_j$ .

- Testing: Is there evidence for the association?
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These questions can be addressed by expanding the model:

**Old model:**

$$\begin{aligned}
 y_{i,j} &= \beta_{0,j} + \beta_{1,j} \times ses_{i,j} + \epsilon_{i,j} \\
 &= (\beta_0 + b_{0,j}) + (\beta_1 + b_{1,j}) \times ses_{i,j} + \epsilon_{i,j}
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**New model:**

$$\begin{aligned}
 y_{i,j} &= \beta_{0,j} + \beta_{1,j} \times ses_{i,j} + \epsilon_{i,j} \\
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Note that under this model,

- The intercept for school  $j$  is  $\beta_{0,j} = (\beta_0 + \alpha_0 \times flp_j + b_{0,j})$
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## Macro-level fixed effects

$$\begin{aligned}y_{i,j} &= \beta_{0,j} + \beta_{1,j} \times \text{ses}_{i,j} + \epsilon_{i,j} \\ &= (\beta_0 + \alpha_0 \times \text{flp}_j + b_{0,j}) + (\beta_1 + \alpha_1 \times \text{flp}_j + b_{1,j}) \times \text{ses}_{i,j} + \epsilon_{i,j}\end{aligned}$$

- $\alpha_0$  represents the macro effect of  $\text{flp}_j$  on the intercept/mean in group  $j$
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Rearranging, we get

$$y_{i,j} = \beta_0 + \alpha_0 \times flp_j + \beta_1 \times ses_{i,j} + \alpha_1 \times flp_j \times ses_{i,j} + \\ b_{0,j} + b_{1,j} \times ses_{i,j} + \\ \epsilon_{i,j}$$

**Fixed effects regression:**  $\beta_0 + \alpha_0 \times flp_j + \beta_1 \times ses_{i,j} + \alpha_1 \times flp_j \times ses_{i,j}$

**Random effects regression:**  $b_{0,j} + b_{1,j} \times ses_{i,j}$

### Note:

- The predictors for the two regressions are different.
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## Macro-level fixed effects

$$y_{i,j} = (\beta_0 + \alpha_0 \times flp_j + b_{0,j}) + (\beta_1 + \alpha_1 \times flp_j + b_{1,j}) \times ses_{i,j} + \epsilon_{i,j}$$

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## Group-level representation

### Micro-level representation:

$$y_{i,j} = \boldsymbol{\beta}^T \mathbf{x}_{i,j} + \mathbf{b}_j^T \mathbf{z}_{i,j} + \epsilon_{i,j}$$

### Combining observations within a group:

$$\begin{pmatrix} y_{1,j} \\ \vdots \\ y_{n,j} \end{pmatrix} = \begin{pmatrix} \mathbf{x}_{1,j} \rightarrow \\ \vdots \\ \mathbf{x}_{n,j} \rightarrow \end{pmatrix} \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_p \end{pmatrix} + \begin{pmatrix} \mathbf{z}_{1,j} \rightarrow \\ \vdots \\ \mathbf{z}_{n,j} \rightarrow \end{pmatrix} \begin{pmatrix} b_{1,j} \\ \vdots \\ b_{p,j} \end{pmatrix} + \begin{pmatrix} \epsilon_{1,j} \\ \vdots \\ \epsilon_{n,j} \end{pmatrix}$$

### Two-level HLM: General form

$$\mathbf{y}_j = \mathbf{X}_j \boldsymbol{\beta} + \mathbf{Z}_j \mathbf{b}_j + \boldsymbol{\epsilon}_j$$

**Note:** This formulation allows the *fixed effects predictors* to be different from the *random effects predictors*.

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$$\mathbf{y}_j = \mathbf{X}_j \boldsymbol{\beta} + \mathbf{Z}_j \mathbf{b}_j + \boldsymbol{\epsilon}_j$$

**Note:** This formulation allows the *fixed effects predictors* to be different from the *random effects predictors*.

## Group-level representation

### Micro-level representation:

$$y_{i,j} = \boldsymbol{\beta}^T \mathbf{x}_{i,j} + \mathbf{b}_j^T \mathbf{z}_{i,j} + \epsilon_{i,j}$$

### Combining observations within a group:

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This is the general form of a *two-level* hierarchical linear model

$$\mathbf{y}_j = \mathbf{X}_j\boldsymbol{\beta} + \mathbf{Z}_j\mathbf{b}_j + \boldsymbol{\epsilon}_j$$

where  $\mathbf{b}_j$  and  $\boldsymbol{\epsilon}_j$  are multivariate normal.

- $\boldsymbol{\beta}$  are the *fixed effects coefficients*;
- $\mathbf{X}_j$  is the *design matrix for the fixed effects*.
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**Across-group heterogeneity:**  $\boldsymbol{\Psi}$  is the variance-covariance in  $\mathbf{b}_1, \dots, \mathbf{b}_m$ .

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$$\boldsymbol{\Sigma}_j = \sigma^2 \mathbf{I}_{n_j}.$$

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$$\begin{aligned}y_{i,j} &= \mu + a_j + \epsilon_{i,j} \\ \{a_j\} &\sim iid N(0, \tau^2) \\ \{\epsilon_{i,j}\} &\sim iid N(0, \sigma^2)\end{aligned}$$

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## Formula: y.nels ~ 1 + (1 | g.nels)
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##
## Scaled residuals:
##      Min       1Q   Median       3Q      Max
## -3.8112 -0.6534  0.0093  0.6732  4.6999
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## Random effects:
##   Groups      Name            Variance Std.Dev.
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$$\begin{aligned}y_{i,j} &= \beta^T \mathbf{x}_{i,j} + \mathbf{b}_j^T \mathbf{x}_{i,j} + \epsilon_{i,j} \\ \{\mathbf{b}_j\} &\sim iid N(0, \Psi) \\ \{\epsilon_{i,j}\} &\sim iid N(0, \sigma^2)\end{aligned}$$

**Exercise:** Express this model as  $\mathbf{y}_j = \mathbf{X}_j\beta + \mathbf{Z}_j\mathbf{b}_j + \epsilon_j$

- Design matrices:

$$\mathbf{X}_j = \mathbf{Z}_j = \begin{bmatrix} \mathbf{x}_{1,j} \rightarrow \\ \vdots \\ \mathbf{x}_{n_j,j} \rightarrow \end{bmatrix} \quad \text{for each } j \in \{1, \dots, m\}$$

- Regression parameters:

$$\beta = \beta, \quad \mathbf{b}_j = \mathbf{b}_j$$

- Covariance terms:

$$\Psi = \text{Cov}[\mathbf{b}_j], \quad \Sigma = \sigma^2 \mathbf{I}$$

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## Group-specific linear regression

```
fit.1<-lmer(y.nels~ ses.nels + (ses.nels|g.nels), REML=FALSE)
```

```
summary(fit.1)

## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: y.nels ~ ses.nels + (ses.nels | g.nels)
##
##          AIC          BIC    logLik deviance df.resid
##  92553.1   92597.9 -46270.5  92541.1     12968
##
## Scaled residuals:
##      Min       1Q   Median       3Q      Max
## -3.8910 -0.6382  0.0179  0.6669  4.4613
##
## Random effects:
##   Groups      Name      Variance Std.Dev. Corr
##   g.nels      (Intercept) 12.223   3.496
##             ses.nels    1.515   1.231   0.11
## Residual                67.345   8.206
## Number of obs: 12974, groups: g.nels, 684
##
## Fixed effects:
##              Estimate Std. Error t value
## (Intercept)  50.6767    0.1551  326.70
## ses.nels      4.3594    0.1231   35.41
##
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\* modulo different sample sizes.

### Review of benefits of model extension:

- Group-specific regressors should appear in  $\mathbf{X}_j$  but not  $\mathbf{Z}_j$ ;
- If  $\{b_{k,1}, \dots, b_{k,m}\}$  shows little variability ( $\psi_{k,k}$  small), we may want to remove  $x_{i,j,k}$  from the random effects model, and include it as a fixed effect only.
- Within-group covariances other than  $\Sigma = \sigma^2 \mathbf{I}$  might be useful:
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# General LME

```
fit.2<-lmer(y.nels~ flp.nels + ses.nels + flp.nels*ses.nels + (ses.nels | g.nels), REML=FALSE)
summary(fit.2)

## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: y.nels ~ flp.nels + ses.nels + flp.nels * ses.nels + (ses.nels |
##      g.nels)
##
##           AIC          BIC    logLik deviance df.resid
##  92396.3   92456.0 -46190.1  92380.3      12966
##
## Scaled residuals:
##      Min       1Q   Median       3Q      Max
## -3.9773 -0.6417  0.0201  0.6659  4.5202
##
## Random effects:
##   Groups      Name      Variance Std.Dev. Corr
##   g.nels  (Intercept)  9.012    3.002
##           ses.nels    1.571    1.254    0.06
##   Residual              67.260    8.201
## Number of obs: 12974, groups:  g.nels, 684
##
## Fixed effects:
##              Estimate Std. Error t value
## (Intercept)    55.3975    0.3860 143.524
## flp.nels        -2.4062    0.1819 -13.230
## ses.nels         4.4909    0.3326  13.500
## flp.nels:ses.nels -0.1931    0.1587  -1.216
##
## Correlation of Fixed Effects:
##              (Intr) flp.nl ss.nls
## flp.nels      -0.930
## ses.nels      -0.158  0.088
## flp.nls:ss.   0.086 -0.007 -0.926
```