

# Lecture 11

## Random and Mixed Effects Models, Computer Experiments

Reading: Oehlert Chapter 11; Dean-Voss-Draguljić Chapters  
17 & 20

*DSA 8020 Statistical Methods II*

March 28 - April 1, 2022

Whitney Huang  
Clemson University

# Agenda

Random and Mixed  
Effects Models,  
Computer  
Experiments



Random and Mixed  
Effects Models

Computer Experiments

## 1 Random and Mixed Effects Models

## 2 Computer Experiments

Everything we have done so far has dealt with **fixed effects**

**CRD:**  $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$

**RCBD:**  $y_{ij} = \mu + \alpha_i + \beta_j + \epsilon_{ij}$

**Factorial:**  $y_{ij} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \epsilon_{ij}$

- The treatment effects are unknown but constants  $\Rightarrow$  if we ran the experiment over again, would expect the same treatment effects
- We can increase the power of all of our tests by increasing the sample size  $n$
- We perform inference on the treatment effects via t-tests and F-tests

Random effects models look very similar to fixed effects models. For example, we could have

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij}.$$

The difference is in the **assumptions** we make for the treatment effects

### Fixed Effects

Treatment effects  $\alpha_i$ s are unknown **constants** that add to zero (or some other constraint)

### Random Effects

- $\alpha_i$ s  $\sim N(0, \sigma_\alpha^2)$
- $\alpha_i$ s are independent of  $\epsilon_{ij}$

# How and Why Are Things So Different?

## Fixed effects:

- The treatments are the treatments and they are unchanging
- If we rerun the experiment, we are still studying the same treatments

## Random effects:

- The treatments are a random sample from a population of potential treatments
- If we rerun the experiment, we are looking at an entirely new sample of treatments
- Inference is on the population of potential treatments

## Fixed effects:

- $\text{Var}(y_{ij}) = \sigma^2$
- All  $y_{ij}$ s are independent of each other
- Interest is about  $\alpha_i$ s

## Random effects:

- $\text{Var}(y_{ij}) = \sigma_\alpha^2 + \sigma^2$
- $$\text{Cor}(y_{ij}, y_{kl}) = \begin{cases} 0 & \text{if } i \neq k \\ \frac{\sigma_\alpha^2}{\sigma_\alpha^2 + \sigma^2} & \text{if } i = k; j \neq l \\ 1 & \text{if } i = k; j = l \end{cases}$$
- Interest is (mostly) about  $\sigma_\alpha^2$

# An Example of Fixed Effects vs Random Effects

- 1 Compare reading ability of 10 2nd grade classes in NY:

Select  $g = 10$  specific classes of interest. Randomly choose  $n$  students from each classroom. Want to compare  $\alpha_i$ s (class-specific effects)  $\Rightarrow$  **Fixed effects**

- 2 Compare variability among all 2nd grade classes in NY:

Randomly choose  $g = 10$  classes from large number of classes. Randomly choose  $n$  students from each classroom. Want to assess  $\sigma_\alpha^2$  (class to class variability)  $\Rightarrow$  **Random effects**

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij},$$

where

- $\mu$  is the overall mean
- $\alpha_i$ :  $i$ th treatment effect and  $\alpha_i \sim N(0, \sigma_\alpha^2)$
- $\{\alpha_i\}$  and  $\{\epsilon_{ij}\}$  independent
- The hypotheses are:

$$H_0 : \sigma_\alpha^2 = 0$$

$$H_a : \sigma_\alpha^2 > 0$$

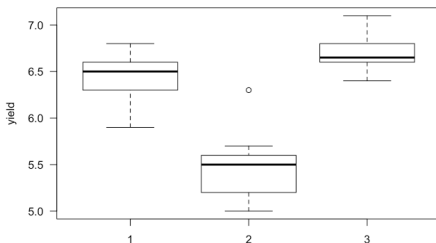
One can use either “old school” method (ANOVA) or “**new school**” method (REML) to make inference about  $\sigma_\alpha^2$



## Random Effects Example

Suppose that an agronomist is studying a large number of varieties of soybeans for yield. The agronomist randomly selects three varieties, and then randomly assigns each of those varieties to 10 of 30 available plots.

Soybean	Yield
V1	6.6, 6.4, 5.9, 6.6, 6.2, 6.7, 6.3, 6.5, 6.5, 6.8
V2	5.6, 5.2, 5.3, 5.1, 5.7, 5.6, 5.6, 6.3, 5.0, 5.4
V3	6.9, 7.1, 6.4, 6.7, 6.5, 6.6, 6.6, 6.6, 6.8, 6.8



```
> fixef <- lm(yield ~ var)
```

```
> anova(fixef)
```

Analysis of Variance Table

Response: yield

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
var	2	8.306	4.1530	49.593	9.114e-10 ***
Residuals	27	2.261	0.0837		

---

Signif. codes:

0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

```
> coefficients(fixef)
```

(Intercept)	var2	var3
6.45	-0.97	0.25

## Random Effects Analysis

```
> library(lme4)
> randef <- lmer(yield ~ 1 + (1|var), REML = TRUE)
> summary(mod1)
```

Linear mixed model fit by maximum likelihood . t-tests  
use Satterthwaite's method [lmerModLmerTest]  
Formula: yield ~ 1 + (1 | var)

AIC	BIC	logLik	deviance	df.resid
27.2	31.4	-10.6	21.2	27

Scaled residuals:

Min	1Q	Median	3Q	Max
-1.8755	-0.6033	0.1245	0.5068	2.7574

Random effects:

Groups	Name	Variance	Std.Dev.
var	(Intercept)	0.26849	0.5182
Residual		0.08374	0.2894

Number of obs: 30, groups: var, 3

Fixed effects:

	Estimate	Std. Error	df	t value	Pr(> t )
(Intercept)	6.2100	0.3038	3.0000	20.44	0.000256

## Concrete Cylinder Example Revisited

Suppose you are manufacturing concrete cylinders for bridge supports. There are three ways of drying concrete (say A, B, and C), and you want to find the one that gives you the best compressive strength. The concrete is mixed in batches that are large enough to produce exactly three cylinders, and your production engineer believes that there is substantial variation in the quality of the concrete from batch to batch.

Treatment	Batch					Trt Sum
	1	2	3	4	5	
A	52	47	44	51	42	236
B	60	55	49	52	43	259
C	56	48	45	44	38	231
Batch Mean	168	150	138	147	123	726

If we were treat the batch effects as random effects, then we have a **Mixed Effects Model**

## Concrete Cylinder Example: Mixed Effects Analysis

```
> randef <- lmer(x ~ trt + (1|blk), REML = TRUE, data = dat)
> summary(randef)
```

Linear mixed model fit by REML. t-tests use

Satterthwaite's method [lmerModLmerTest]

Formula: x ~ trt + (1 | blk)

Data: dat

REML criterion at convergence: 71.1

Scaled residuals:

Min	1Q	Median	3Q	Max
-1.1417	-0.6147	-0.1494	0.5772	1.3390

Random effects:

Groups	Name	Variance	Std.Dev.
blk	(Intercept)	28.35	5.324
Residual		5.85	2.419

Number of obs: 15, groups: blk, 5

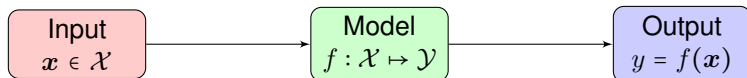
Fixed effects:

	Estimate	Std. Error	df	t value	Pr(> t )
(Intercept)	47.200	2.615	5.054	18.047	8.76e-06
trtB	4.600	1.530	8.000	3.007	0.0169
trtC	-1.000	1.530	8.000	-0.654	0.5316

## What is a Computer Experiment

In some situations it is economically, ethically, or simply not possible to run a **physical experiment**. Instead, the following scenario might be feasible:

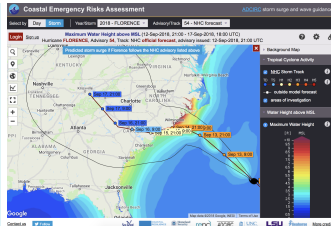
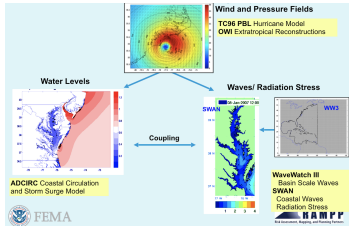
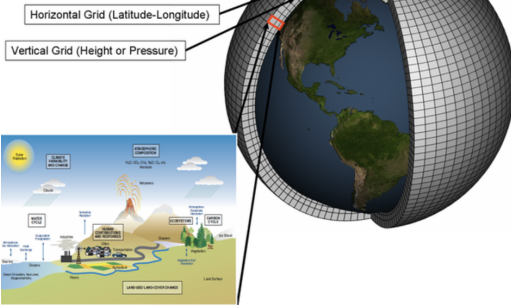
- the physical process can be described by a mathematical model (e.g., a system of differential equations)
- computer code (simulator) can be written to compute the response from the mathematical model



In this case, a researcher can conduct a **computer experiment** by running the computer code, which serves as a proxy for the physical process, to compute a “response” at any combination of values of the inputs

# Examples of Computer Models

## Schematic for Global Atmospheric Model



Random and Mixed  
Effects Models,  
Computer  
Experiments

CLEMSON  
UNIVERSITY

Random and Mixed  
Effects Models

Computer Experiments

# Computer Experiments vs. Physical Experiments

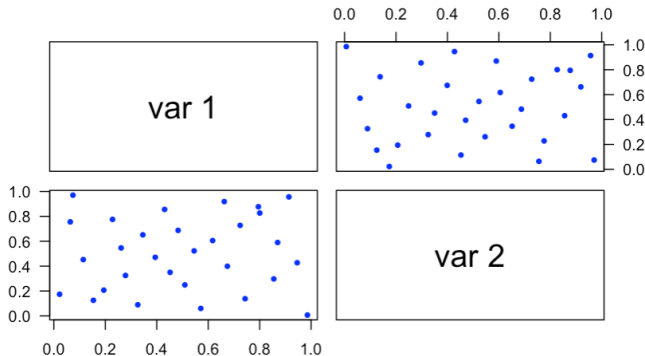
- *“Experimental results are believed by everyone, except for the person who ran the experiment”*
- *“Computational results are believed by no one, except the person who wrote the code”*

Replication, randomization and blocking are irrelevant for a computer experiment because many **computer codes are deterministic** and **all the inputs to the code are known and can be controlled**



**Design:** where to make the runs, i.e., the selection of inputs  $\{x_i\}_{i=1}^n$  for a given computational budget  $n$ .

**Example:**  $x_i = (x_{i1}, x_{i2})^T$  and  $n = 30$



This is an example of [space-filling design](#)

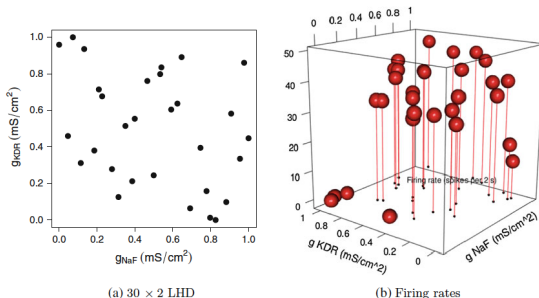
**Analysis:** fit a statistical model to the computer model inputs-output  $\{y_i, \mathbf{x}_i\}_{i=1}^n$  to “emulate” the simulator and to quantify the prediction uncertainty for  $y(\mathbf{x}_{\text{new}})$  via a **Gaussian Process Model** GP ( $m(\cdot), K(\cdot, \cdot)$ ), where

- $m(\mathbf{x}) = \mathbb{E}[y(\mathbf{x})]$  is the **mean function**, usually takes a simple form, e.g.,  $m(\mathbf{x}) = \mu$
- $K(\mathbf{x}, \mathbf{x}') = \text{Cov}(y(\mathbf{x}), y(\mathbf{x}'))$  is the **covariance function**, usually parametrized by “distance”. e.g.,  
$$K(\mathbf{x}, \mathbf{x}') = C(\mathbf{x}, \mathbf{x}'; \boldsymbol{\theta}) = \sigma^2 \prod_{j=1}^p C_j(d(\mathbf{x}_j, \mathbf{x}'_j); \theta_j).$$

Fit a GP model to  $\{y_i, \mathbf{x}_{i=1}^n\}$  to obtain the maximum likelihood estimates  $\hat{\mu}$ ,  $\hat{\sigma}^2$  and  $\{\theta_j\}_{j=1}^p$  in order to predict  $y(\mathbf{x}_{\text{new}})$  and to quantify its prediction uncertainty

## Neuron Experiment [pp.776-778, Dean-Voss-Draguljić, 2017]

The firing rate of a neuron at +380 pA current injection of a young monkey is modeled as a deterministic function of two input variables;  $x_1$  was the maximal conductance of the transient sodium, denoted  $g_{NaF}$ , and  $x_2$  was the maximal conductance of the delayed-rectifier potassium, denoted  $g_{KDR}$



**Source:** Fig. 20.6, Dean-Voss-Draguljić, 2017

The goal here is to reconstruct the 2D firing rate surface within the input space

## Neuron Experiment Result

After fitting a GP with squared exponential covariance function (i.e.,  $C(\mathbf{x}, \mathbf{x}') = \sigma^2 e^{-[\theta_1(x_1 - x'_1)^2 + \theta_2(x_2 - x'_2)^2]}$ ), we obtain  $\hat{\mu} = 27.61$ ,  $\hat{\sigma}^2 = 251.86$ ,  $\hat{\theta}_1 = \hat{\theta}_{\text{NaF}} = 5.03$ ,  $\hat{\theta}_2 = \hat{\theta}_{\text{KDR}} = 50.22$ . With these estimated parameters we can calculate the predictions and their prediction uncertainties

