Statistics 514: Block Designs

Fall 2020

Lecture 6: Block Designs

Montgomery: Chapter 4

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Nuisance Factor

- When present in experiment, nuisance factor has effect on response but its effect is not of interest
- ullet If unknown and uncontrollable o Protecting experiment through randomization
 - We do not know that the factor exists;
 - It may be changing levels as the experiment goes.
- If known (measurable) but uncontrollable → Analysis of Covariance (Chapter 15 Section 3)
- ullet If known and controllable o Blocking

Penicillin Experiment

Four penicillin manufacturing processes (A, B, C and D) were being investigated. Yield was the response. It was known that an important raw material, corn steep liquor, was quite variable. The experiment and its results were given below (subscripts indicate the experiment units):

	blend 1	blend 2	blend 3	blend 4	blend 5
\overline{A}	89_{1}	844	812	87_{1}	79_{3}
B	88_{3}	77_2	87_{1}	92_{3}	814
C	97_{2}	92_{3}	87_{4}	89_{2}	80_{1}
D	94_{4}	79_{1}	85_3	844	882

- Blend is a nuisance factor, treated as a block factor;
- (Complete) Blocking: all the treatments are applied within each block, and they are compared within blocks.
- Advantage: Eliminate blend-to-blend (between-block) variation from experimental error variance when comparing treatments.
- Cost: degree of freedom.

Randomized Complete Block Design

- ullet blocks each consisting of (partitioned into) a experimental units
- ullet a treatments are randomly assigned to the experimental units within each block
- Typically after the runs in one block have been conducted, then move to another block.
- Typical blocking factors: day, batch of raw material etc.
- Results in restriction on randomization because randomization is only within blocks.
- Data within a block are dependent on each other (sharing the same block effect).
- When a=2, randomized complete block design becomes paired two sample case (or matched pairs).

Statistical Model

- b blocks and a treatments
- Statistical model is

$$y_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij}$$

$$\begin{cases} i = 1, 2, \dots, a \\ j = 1, 2, \dots, b \end{cases}$$

 μ - grand mean

 au_i - ith treatment effect

 β_i - jth block effect

$$\epsilon_{ij} \sim N(0, \sigma^2)$$

- The model is additive because within a fixed block, the block effect is fixed; for a fixed treatment, the treatment effect is fixed across blocks. In other words, blocks and treatments do not interact.
- parameter constraints: $\sum_{i=1}^{a} \tau_i = 0;$ $\sum_{j=1}^{b} \beta_j = 0$

Estimates for Parameters

• Rewrite observation y_{ij} as:

$$y_{ij} = \overline{y}_{..} + (\overline{y}_{i.} - \overline{y}_{..}) + (\overline{y}_{.j} - \overline{y}_{..}) + (y_{ij} - \overline{y}_{i.} - \overline{y}_{.j} + \overline{y}_{..})$$

Compare with the model

$$y_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij}$$

We have

$$\hat{\mu} = \overline{y}_{..}$$

$$\hat{\tau}_{i} = \overline{y}_{i.} - \overline{y}_{..}$$

$$\hat{\beta}_{j} = \overline{y}_{.j} - \overline{y}_{..}$$

$$\hat{\epsilon}_{ij} = y_{ij} - \overline{y}_{i.} - \overline{y}_{.j} + \overline{y}_{..}$$

Sum of Squares (SS)

• Can partition $SS_T = \sum \sum (y_{ij} - \overline{y}_{..})^2$ into

$$b\sum_{i}(\overline{y}_{i.}-\overline{y}_{..})^{2}+a\sum_{i}(\overline{y}_{.j}-\overline{y}_{..})^{2}+\sum_{i}\sum_{j}(y_{ij}-\overline{y}_{i.}-\overline{y}_{.j}+\overline{y}_{..})^{2}$$

$$SS_{\text{Treatment}} = b \sum (\overline{y}_{i.} - \overline{y}_{..})^{2} = b \sum \hat{\tau}_{i}^{2} \quad \text{df} = a - 1$$

$$SS_{\text{Block}} = a \sum (\overline{y}_{.j} - \overline{y}_{..})^{2} = a \sum \hat{\beta}_{j}^{2} \quad \text{df} = b - 1$$

$$SS_{\text{E}} = \sum \sum (y_{ij} - \overline{y}_{i.} - \overline{y}_{.j} + \overline{y}_{..})^{2} = \sum \sum \hat{\epsilon}_{ij}^{2} \quad \text{df} = (a - 1)(b - 1)$$

Hence:

- $SS_T = SS_{Treatment} + SS_{Block} + SS_E$
- The Mean Squares are

$$\mathrm{MS_{Treatment}} = \mathrm{SS_{Treatment}}/(a-1), \ \mathrm{MS_{Block}} = \mathrm{SS_{Block}}/(b-1),$$
 and $\mathrm{MS_E} = \mathrm{SS_E}/(a-1)(b-1).$

Testing Basic Hypotheses

- $H_0: \tau_1 = \tau_2 = \ldots = \tau_a = 0$ vs $H_1:$ at least one is not
- Can show:

$$\begin{split} &\mathsf{E}(\mathsf{MS_E}) \texttt{=} \sigma^2 \\ &\mathsf{E}(\mathsf{MS_{Treatment}}) \texttt{=} \sigma^2 + b \sum_{i=1}^a \tau_i^2/(a-1) \\ &\mathsf{E}(\mathsf{MS_{Block}}) \texttt{=} \sigma^2 + a \sum_{j=1}^b \beta_j^2/(b-1) \end{split}$$

• Use F-test to test H_0 :

$$F_0 = \frac{\text{MS}_{\text{Treatment}}}{\text{MS}_{\text{E}}} = \frac{\text{SS}_{\text{Treatment}}/(a-1)}{\text{SS}_{\text{E}}/((a-1)(b-1))}$$

- Caution testing block effects
 - Usually not of interest.
 - Randomization is restricted: Differing opinions on F-test for testing blocking effects.
 - Can use ratio MS_{Block}/MSE to check if blocking successful.
 - Block effects can be random effects.

Analysis of Variance Table

Source of	Sum of	Degrees of	Mean	F_0
Variation	Squares	Freedom	Square	
Blocks	SS_{Block}	b-1	MS_{Block}	
Treatment	$SS_{\mathrm{Treatment}}$	a-1	$MS_{\mathrm{Treatment}}$	F_0
Error	SS_E	(b-1)(a-1)	MS_{E}	
Total	SS_{T}	ab-1		

$$\mathrm{SS}_{\mathrm{T}} = \sum \sum y_{ij}^2 - y_{\cdot \cdot}^2/N$$

$$SS_{Treatment} = \frac{1}{b} \sum y_{i.}^2 - y_{..}^2 / N$$

$$SS_{Block} = \frac{1}{a} \sum y_{.j}^2 - y_{..j}^2 / N$$

$$\mathsf{SS}_E \texttt{=} \mathsf{SS}_T \texttt{-} \mathsf{SS}_{Treatment} \texttt{-} \mathsf{SS}_{Block}$$

Decision Rule: If $F_0 > F_{\alpha,a-1,(b-1)(a-1)}$ then reject H_0

Example: Detergents

An experiment was designed to study the performance of four different detergents in cleaning clothes. The following "cleanness" readings (higher=cleaner) were obtained with specially designed equipment for three different types of common stains. Is there a difference between the detergents?

	Stain 1	Stain 2	Stain 3
Detergent 1	45	43	51
Detergent 2	47	46	52
Detergent 3	48	50	55
Detergent 4	42	37	49

$$\sum \sum y_{ij} = 565$$
 and $\sum \sum y_{ij}^2 = 26867$

$$y_{1.}=139, y_{2.}=145, y_{3.}=153$$
 and $y_{4.}=128; y_{.1}=182, y_{.2}=176,$ and $y_{.3}=207$

$$SS_T = 26867 - 565^2/12 = 265$$

$$SS_{Trt} = (139^2 + 145^2 + 153^2 + 128^2)/3 - 565^2/12 = 111$$

$$\mathrm{SS}_{\mathrm{Block}} = (182^2 + 176^2 + 207^2)/4 - 565^2/12 = 135$$

$$SS_E = 265 - 111 - 135 = 19$$
; $F_0 = (111/3)/(19/6) = 11.6$; P-value < 0.01

Checking Assumptions (Diagnostics)

- Assumptions
 - Model is additive (no interaction between treatment effects and block effects, i.e., additivity assumption)
 - Errors are independent and normally distributed
 - Constant variance
- Checking normality:
 - Histogram, QQ plot of residuals, Shapiro-Wilk Test.
- Checking constant variance
 - Residual Plot: Residuals vs \hat{y}_{ij}
 - Residuals vs blocks
 - Residuals vs treatments

Checking Assumptions (Continued)

- Additivity
 - Interaction Plot: \hat{y}_{ij} vs. treatment levels for each block
 - Parallel lines: block effects are same for different treatments, so NO interaction
 - * Lines are not parallel: block effects can be different for different treatments, so possible interaction between block and treatment
 - Formal test: Tukey's One-degree Freedom Test of Non-additivity
- If interaction exists, usually try transformation to eliminate interaction

Treatments Comparison

- Multiple Comparisons/Contrasts
 - procedures (methods) are similar to those for Completely Randomized
 Design (CRD)

n is replaced by b in all formulas

Degrees of freedom error is (b-1)(a-1)

- Example : Comparison of Detergents
 - Tukey's Method ($\alpha=.05$)

$$q_{\alpha}(a, df) = q_{\alpha}(4, 6) = 4.896.$$

$$CD = \frac{q_{\alpha}(4,6)}{\sqrt{2}} \sqrt{\text{MSE}(\frac{1}{b} + \frac{1}{b})} = 4.896 \sqrt{\frac{19}{6*3}} = 5.001$$

Estimated treatment means

Using SAS

```
data wash; input stain soap y 00; cards;
1 1 45 1 2 47 1 3 48 1 4 42 2 1 43 2 2 46
2 3 50 2 4 37 3 1 51 3 2 52 3 3 55 3 4 49
;
proc glm data=wash;
  class stain soap;
  model y = soap stain;
  means soap/alpha=0.05 tukey lines;
  output out=diag r=res p=pred;
proc univariate noprint normal;
  gqplot res/normal (L=1 mu=est sigma=est);
  histogram res/normal (L=1 mu=est sigma=est) kernel(L=2 K=quadratic);
proc gplot; plot res*pred;
symbol1 v=circle i=joint;
proc gplot data=diag; plot y*soap=stain; run;
                                                   quit;
```

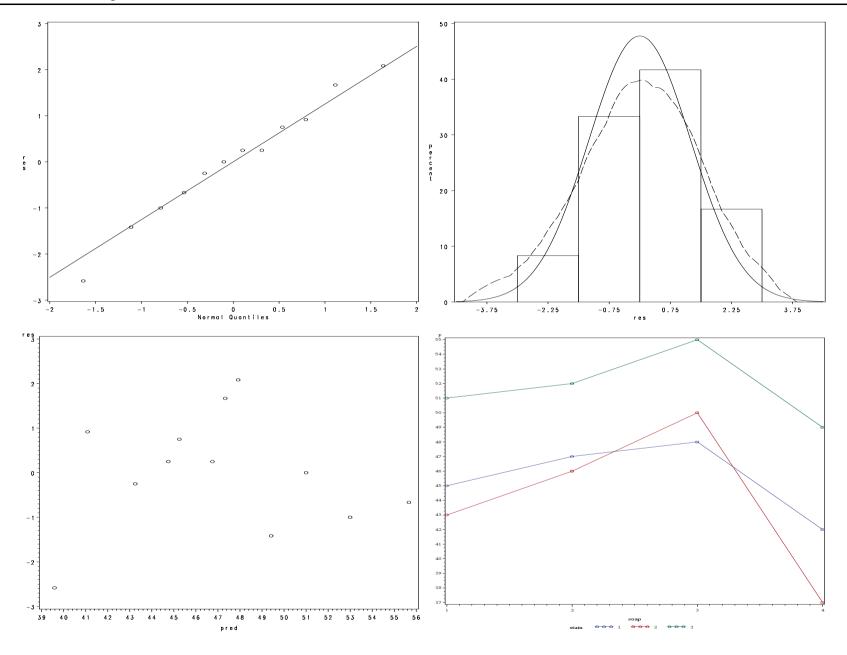
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SAS Output

Dependent	Variable: y					
		Sum of				
Source	DF	Squares	Mean Square	F	Value	Pr > F
Model	5	246.0833333	49.2166667		15.68	0.0022
Error	6	18.8333333	3.1388889			
Corrected	Total 11	264.9166667				
R-Square	Coeff Va:	r Root MSE	y Mean			
0.928908	3.762883	3 1.771691	47.08333			
Source	DF	Type I SS	Mean Square	F	Value	Pr > F
soap	3	110.9166667	36.9722222		11.78	0.0063
stain	2	135.1666667	67.5833333		21.53	0.0018
Source	DF	Type III SS	Mean Square	F	Value	Pr > F
soap	3	110.9166667	36.9722222		11.78	0.0063
stain	2	135.1666667	67.5833333		21.53	0.0018

Tukey's Studentized Range (HSD) Test for res
Alpha 0.05
Error Degrees of Freedom 6
Error Mean Square 3.138889
Critical Value of Studentized Range 4.89559
Minimum Significant Difference 5.007
Means with the same letter are not significantly different.

Tukey	Group	ing	Mean	N	soap
		A	51.000	3	3
		A			
		A	48.333	3	2
		A			
	В	A	46.333	3	1
	В				
	В		42.667	3	4



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Tukey's Test for Non-Additivity

- Additivity assumption (or no interaction assumption) is crucial for block designs or experiments.
- ullet To check the interaction between block and treatment **fully** needs (a-1)(b-1) degree of freedom. It is not affordable when without replicates.
- Instead consider a special type of interaction. Assume following model (pages 182-185)

$$y_{ij} = \mu + \tau_i + \beta_j + \gamma \tau_i \beta_j + \epsilon_{ij}$$

• $H_0: \gamma = 0 \text{ vs } H_1: \gamma \neq 0$

Sum of Squares caused by possible interaction:

$$\mathrm{SS}_N = \frac{\left[\sum_i \sum_j y_{ij} y_{i.} y_{.j} - y_{..} (\mathrm{SS}_{\mathrm{Trt}} + \mathrm{SS}_{\mathrm{Blk}} + y_{..}^2/ab)\right]^2}{ab\mathrm{SS}_{\mathrm{Trt}} \mathrm{SS}_{\mathrm{Blk}}} \quad df = 1.$$

Remaining error SS: $SS'_{E} = SS_{E} - SS_{N}$, df = (a-1)(b-1) - 1

Test Statistic:

$$F_0 = \frac{\mathrm{SS}_N/1}{\mathrm{SS}_F'/[(a-1)(b-1)-1]} \sim F_{1,(a-1)(b-1)-1}$$

• Decision rule: Reject H_0 if $F_0 > F_{\alpha,1,(a-1)(b-1)-1}$.

A Convenient Procedure to Calculate SS_N, SS/_E and F_0

- 1. Fit additive model $y_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij}$
- 2. Obtain \hat{y}_{ij} and $q_{ij} = \hat{y}_{ij}^2$
- 3. Fit the model $y_{ij} = \mu + \tau_i + \beta_j + \theta q_{ij} + \epsilon_{ij}$

Use the test for $H_0: \theta = 0$ in the ANOVA table with type III SS and ignore the tests for the treatment and block factors.

- Brief review on different types of SS (model y=trt blk q)
 - Type I SS: difference in SSM when variables are added sequentially in the model,
 i.e., SS(trt), SS(blk|trt), SS(q|blk,trt). Each observation is weighted equally.
 - Type II SS: difference in SSM when a variable is included last in the model or not, i.e., SS(trt|blk,q), SS(blk|trt,q), SS(q|blk,trt). Each observation is weighted equally.
 - Type III SS: similar to Type II SS, but adjust for the cells having different numbers of observations. Calculated using regression.

Example 5.2 from Montgomery

 Impurity in chemical product is affected by temperature and pressure. We will assume temperature is a blocking factor. The data is shown below. We will test for non-additivity.

	i iessuie				
Temp	25	30	35	40	45
100	5	4	6	3	5
125	3	1	4	2	3
150	1	1	3	1	2

Praccura

$$SS_N = 0.0985, SS'_F = 1.9015, F_0 = .36, P - value = 0.566$$

Do Not Reject, there appears to be no interaction between block and treatment.

Using SAS

```
options nocenter ls=75;
data impurity;
  input trt blk y 00; cards;
1 1 5 1 2 3 1 3 1 2 1 4 2 2 1 2 3 1 3 1 6 3 2 4 3 3 3
4 1 3 4 2 2 4 3 1 5 1 5 5 2 3 5 3 2
proc glm data=impurity;
  class blk trt;
  model y=blk trt;
  output out=one r=res p=pred;
data two;
  set one;
  q=pred*pred;
proc glm data=two;
  class blk trt;
  model y=blk trt q/ss3;
                            run;
```

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SAS Output

		Sum of			
Source	DF	Squares	Mean Square	F Value	Pr > F
Model	6	34.93333333	5.8222222	23.29	0.0001
Error	8	2.00000000	0.2500000		
Corrected Total	14	36.93333333			
Source	DF	Type I SS	Mean Square	F Value	Pr > F
blk	2	23.33333333	11.66666667	46.67	<.0001
trt	4	11.60000000	2.9000000	11.60	0.0021

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		Sum of			
Source	DF	Squares	Mean Square	F Value	Pr > F
Model	7	35.03185550	5.00455079	18.42	0.0005
Error	7	1.90147783	0.27163969		
Corrected Total	14	36.93333333			
Source	DF	Type III SS	Mean Square	F Value	Pr > F
blk	2	1.25864083	0.62932041	2.32	0.1690 XXX
trt	4	1.09624963	0.27406241	1.01	0.4634 XXX
q	1	0.09852217	0.09852217	0.36	0.5660

XXX: not meaningful for testing blocks and treatments

Choice of Sample Size

- Same as determining the number of blocks (b)
- Similar idea in designing completely randomized experiment (Lecture 5).
- ullet Test $H_0: au_1 = \dots = au_a = 0$ vs. $H_1:$ at least one of $\{ au_1, \dots, au_a\}$ is NOT zero
 - Test statistic: $F_0 = \mathsf{MS}_{\mathrm{Treatment}}/\mathsf{MS}_{\mathrm{E}} \overset{H_0}{\sim} F_{a-1,(a-1)(b-1)}$

$$F_0 \stackrel{H_1}{\sim} F_{a-1,(a-1)(b-1)}(\delta), \quad \delta = b \sum_{i=1}^a \tau_i^2 / \sigma^2$$

- When using the OC curve in Chart V, $\Phi^2 = \delta/a$.
- Test $H_0: \tau_i = \tau_k$ vs. $H_1: \tau_i \neq \tau_k$
 - Test statistic: $t_0=(\bar{Y}_{i.}-\bar{Y}_{k.})/\sqrt{2\mathrm{MS_E}/b}\stackrel{H_0}{\sim}t_{(a-1)(b-1)}$

$$t_0 \stackrel{H_1}{\sim} t_{(a-1)(b-1)}(\delta), \quad \delta = (\tau_i - \tau_k) / \sqrt{2\sigma^2/b}$$

Detergent Example: Overall F-Test

```
data new; a=4; alpha=.05; d=5; var=3.1389;
   do b=2 to 6;
       df = (a-1)*(b-1); /* compared to a*(n-1) in CRD */
       nc = b*d*d/(2*var);
       fcut = finv(1-alpha, a-1, df);
       beta = probf(fcut,a-1,df,nc);
       power = 1-beta; output;
   end;
proc print;
   var b df nc beta power; run;
Obs
            df
                              beta
       b
                                        power
                     nc
  1
             3 7.9646
                           0.76134
                                      0.23866
  2.
       3
             6 11.9469 0.45857 0.54143
       4
             9 15.9291
                       0.22741 0.77259
       5
            12 19.9114 0.09858 0.90142
  4
       6
            15 23.8937 0.03870
                                      0.96130
```

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Detergent Example: Multiple Comparisons

• Compare all pairs and detect any difference more than 12 with 80% power

```
data new1; a=4; alpha=.05; var=3.1389; d=5;
    do b=2 to 6;
        df = (a-1)*(b-1); nc = d/sqrt(var*2/b);
        crit = probmc("range",.,1-alpha,df,a)/sqrt(2); /*Tukey*/
        /*crit = probmc("dunnett2",.,1-alpha,df,a-1);/*Two-Sided Dunnett*/
        power=1-probt(crit, df, nc) + probt(-crit, df, nc); output;
    end;
proc print;
    var b df power; run;
Obs
             df
        b
                    power
  1
              3
                  0.23185
  2
                  0.54574
              6
        4
              9 0.78118
        5
             12 0.90817
  4
        6
  5
             15 0.96513
```

Random Block Effects

- ullet Could randomly select blocks, and result in modeling $eta_j \stackrel{iid}{\sim} N(0,\sigma_{eta}^2)$
 - Observations in the same blocks are dependent
- Expected Mean Squares (EMS)

$$E[MS_{Treatments}] = \sigma^2 + b \sum_{i=1}^{a} \tau_i^2 / (a-1)$$

$$E[MS_{Blocks}] = \sigma^2 + a\sigma_{\beta}^2$$

$$E[MS_E] = \sigma^2$$

ullet Test $H_0: au_1 = \dots = au_a = 0$ vs. $H_1:$ at least one au_i is not zero

$$F_0 = \frac{MS_{Treatment}}{MS_E}$$

- When there is an interaction between treatments and blocks
 - Interaction effects are considered random
 - Interaction variance appears in all EMS
 - Perform usual F-test (ratio of MS)
 - Use PROC MIXED instead of PROC GLM
- \bullet Could randomly select treatments, and result in modeling $\tau_i \stackrel{iid}{\sim} N(0,\sigma_\tau^2)$
- More about mixed effects models will be covered in later lectures.

RCBD with Replicates

- a treatments ($i = 1, 2, \ldots, a$)
- b blocks (j = 1, 2, ..., b)
- ullet n observations for each treatment in each block ($l=1,2,\ldots,n$)

Assume no interaction between Treatment and Block

$$y_{ijl} = \mu + \tau_i + \beta_j + \epsilon_{ijl}$$

$$\begin{cases} i = 1, 2, \dots, a \\ j = 1, 2, \dots, b \\ l = 1, 2, \dots, n \end{cases}$$

Similar assumptions/constraints as before:

$$\epsilon_{ijl} \stackrel{iid}{\sim} N(0, \sigma^2),$$

$$\sum_{i=1}^{a} \tau_i = 0, \qquad \sum_{j=1}^{b} \beta_j = 0$$

Source of	Sum of	Degrees of	Mean	\overline{F}
Variation	Squares	Freedom	Square	
Blocks	SS_{Block}	b-1	MS_{Block}	
Treatment	$SS_{\mathrm{Treatment}}$	a-1	$MS_{\mathrm{Treatment}}$	F_0
Error	SS_{E}	abn - b - a + 1	MS_{E}	
Total	SS_{T}	abn-1		

For multiple comparison, df_E becomes abn-a-b+1 and the number of replicates for a fixed treatment now is bn instead of n. Hence, the formulas need to be modified accordingly.

Do not assume no interaction between Treatment and Block

$$y_{ijl} = \mu + \tau_i + \beta_j + (\tau \beta)_{ij} + \epsilon_{ijl}$$

Similar assumptions but more constraints:

$$\sum_{i=1}^{a} \tau_i = 0, \quad \sum_{j=1}^{b} \beta_j = 0,$$
$$\sum_{i=1}^{a} (\tau \beta)_{ij} = 0, \quad \sum_{j=1}^{b} (\tau \beta)_{ij} = 0$$

Source of	Sum of	Degrees of	Mean	\overline{F}
Variation	Squares	Freedom	Square	
Blocks	SS_{Block}	b-1	MS_{Block}	
Treatment	$SS_{\mathrm{Treatment}}$	a-1	$MS_{\mathrm{Treatment}}$	F_0
Blk*Trt	${\sf SS}_{{ m Blk*Trt}}$	(b-1)(a-1)	$MS_{\mathrm{Blk*Trt}}$	
Error	SS_E	ab(n-1)	$MS_{\mathbf{E}}$	
Total	SS_{T}	abn-1		

• Assess additivity (no interaction) by SS_{Trt^*Blk} : $F_0 = ?$