Factorial Designs

Design of Experiments - Montgomery
Sections 5-1 - 5-3
Overview of Design of Experiments

• Two primary categories of structure in an experiment
  – Treatment structure - factors of interest in study
  – Design structure - grouping of EUs into homogeneous group or blocks

• To date, focus has been on a one-way treatment structure under different design structures
  – CRD - no design structure
  – RCBD - one blocking factor, all trts randomized in block
  – BIBD - one blocking factor, not all trts occur in block
  – Latin square - two blocking factors
Linear Model Construction

- Construct model for $y$ based on structures of experiment

$$ y = \text{design structure components} + \text{treatment structure components} + \text{error structure} $$

- Elements of treatment structure may be fixed or random

- Elements of design structure typically random effects

- As a result, error structure often derived from the interactions of treatment structure by design structure

- This topic focuses on more complex treatment structures
Two-Factor CRD

- In one-factor CRD, trts are often levels of one factor
- More common to be interested in combinations of levels from two (or more) factors
  - Temperature and Pressure
  - Seed variety and Fertilizer
  - Diet and Exercise regimes
- Could treat each combination as a treatment
  - $a$ levels of factor A and $b$ levels of factor B
  - $ab$ total treatments each with $n$ observations
  - Use contrasts to study specific factor effects
HW #3 Example

An experiment is conducted to study the effect of hormones injected into test rats. There are two distinct hormones (C,D) each with two distinct levels. We will consider this to be four different treatments labeled \{C,c,D,d\}. Each treatment is applied to six rats with the response being the amount of glycogen (in mg) in the liver.

<table>
<thead>
<tr>
<th>Treatment</th>
<th>Responses</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>106 101 120 86 132 97</td>
</tr>
<tr>
<td>c</td>
<td>51 98 85 50 111 72</td>
</tr>
<tr>
<td>D</td>
<td>103 84 100 83 110 91</td>
</tr>
<tr>
<td>d</td>
<td>50 66 61 72 85 60</td>
</tr>
</tbody>
</table>

Three contrasts are of interest. They are:

<table>
<thead>
<tr>
<th>Comparison</th>
<th>C</th>
<th>c</th>
<th>D</th>
<th>d</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hormone C vs Hormone D</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>Low level vs High level</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>Equivalence of level effect</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>

Factorial Treatment Structure
HW #3 Example

- These three contrasts are orthogonal so the $SS_{Trt}$ from a one-way ANOVA is separated into sums of squares for each of these contrasts.

- Independent $F$ (or $t$) tests performed to assess these comparisons of interest

- Can we redo the analysis in such a way so that we can study these comparisons without using contrasts?
Factorial Experiment

- Consider treatments as level combinations of two factors
- For this example, each factor has 2 levels
- Treatment structure known as a $2^2$ factorial
  - Factor A: Hormone (C or D)
  - Factor B: Level (L or H)
- In general, a full factorial structure investigates all level combinations of the two factors
- If $a$ levels of Factor A and $b$ levels of Factor B, a single replicate of a factorial involves $ab$ observations
Factorial Experiment

- Design often illustrated in table format or graphically putting one factor on the x-axis and the other factor on the y-axis.

<table>
<thead>
<tr>
<th>Hormone</th>
<th>Low</th>
<th>High</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>xxxx</td>
<td>xxxx</td>
</tr>
<tr>
<td>D</td>
<td>xxxx</td>
<td>xxxx</td>
</tr>
</tbody>
</table>

Factorial Treatment Structure
Statistical Model

- Statistical model (for CRD design structure) is

\[ y_{ijk} = \mu + \tau_i + \beta_j + (\tau \beta)_{ij} + \epsilon_{ijk} \]

\[ \begin{align*}
    & i = 1, 2, \ldots, a \\
    & j = 1, 2, \ldots, b \\
    & k = 1, 2, \ldots, n
\end{align*} \]

- \( \tau_i \) - \( i \)th level effect of factor A (main effect - ignores B)
- \( \beta_j \) - \( j \)th level effect of factor B (main effect - ignores A)
- \((\tau \beta)_{ij}\) - interaction effect of combination \( ij \)
- \((\tau \beta)_{ij}\) explains deviation of means from additive model
- \( \epsilon_{ijk} \sim N(0, \sigma^2) \)
**Model Estimates**

- Under the “sum to zero” parameter constraints:

\[ \hat{\mu} = \bar{y}_{...} \]
\[ \hat{\tau}_i = \bar{y}_{i.} - \bar{y}_{...} \]
\[ \hat{\beta}_j = \bar{y}_{.j} - \bar{y}_{...} \]
\[ (\hat{\tau} \hat{\beta})_{ij} = \bar{y}_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{...} \]

- The predicted value is \( ij \) combination average, so

\[ \hat{y}_{ijk} = \bar{y}_{ij} \text{ and } \hat{\epsilon}_{ijk} = y_{ijk} - \bar{y}_{ij} \]

- We would get the same predicted values and residuals if we combined factors into single treatment factor and used one-way ANOVA
Caution!!

- Based on linear model...

\[
\bar{y}_{i..} = \mu + \tau_i + \overline{\beta} + (\tau\beta)_i.
\]

\[
\bar{y}_{i..} - \bar{y}_{i'..} = \tau_i - \tau_{i'} + (\tau\beta)_i - (\tau\beta)_{i'}.
\]

- Difference in Factor A levels depends on \((\tau\beta)\) constraints

- Thus, \(\tau_i - \tau_{i'}\) is non-estimable (if interaction present)

- Caution testing main effects if interaction present

- Should always test interaction first and proceed to main effects only when appropriate!!!
Partitioning the Sum of Squares

• Rewrite each observation as

\[ y_{ijk} = \bar{y}_{..} + (\bar{y}_{i..} - \bar{y}_{..}) + (\bar{y}_{.j.} - \bar{y}_{..}) + (\bar{y}_{ij.} - \bar{y}_{i..} - \bar{y}_{.j.} + \bar{y}_{..}) + (y_{ijk} - \bar{y}_{ij.}) \]

• The total SS \( \sum (y_{ijk} - \bar{y}_{..})^2 \) can be broken up into

\[
bn \sum_i (\bar{y}_{i..} - \bar{y}_{..})^2 +
\]

\[
an \sum_j (\bar{y}_{.j.} - \bar{y}_{..})^2 +
\]

\[
n \sum_i \sum_j (\bar{y}_{ij.} - \bar{y}_{i..} - \bar{y}_{.j.} + \bar{y}_{..})^2 + \ldots
\]

• \( SS_A + SS_B + SS_{AB} + SS_E \)

• Under normality, all SS/\( \sigma^2 \) independent
## Analysis of Variance Table

<table>
<thead>
<tr>
<th>Source of Variation</th>
<th>Sum of Squares</th>
<th>Degrees of Freedom</th>
<th>Mean Square</th>
<th>( F_0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Factor A</td>
<td>( SS_A )</td>
<td>( a - 1 )</td>
<td>( MS_A )</td>
<td>( F_0 )</td>
</tr>
<tr>
<td>Factor B</td>
<td>( SS_B )</td>
<td>( b - 1 )</td>
<td>( MS_B )</td>
<td>( F_0 )</td>
</tr>
<tr>
<td>Interaction</td>
<td>( SS_{AB} )</td>
<td>( (a - 1)(b - 1) )</td>
<td>( MS_{AB} )</td>
<td>( F_0 )</td>
</tr>
<tr>
<td>Error</td>
<td>( SS_E )</td>
<td>( ab(n - 1) )</td>
<td>( MS_E )</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>( SS_T )</td>
<td>( abn - 1 )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
\[ SS_T = \sum \sum \sum y_{ijk}^2 - y_{...}^2 / abn \]
\[ SS_A = \frac{1}{bn} \sum y_{i..}^2 - y_{...}^2 / abn \]
\[ SS_B = \frac{1}{an} \sum y_{.j.}^2 - y_{...}^2 / abn \]
\[ SS_{Sub} = \frac{1}{n} \sum \sum y_{ij.}^2 - y_{...}^2 / abn \]
\[ SS_{AB} = SS_{Sub} - SS_A - SS_B \]
\[ SS_E = \text{Subtraction} \]

\[ df_E > 0 \text{ only if } n > 1. \text{ When } n = 1, \text{ cannot separate interaction from error (confounded). Recall typical RCBD uses } n = 1. \text{ Assuming no interaction in RCBD allows us to estimate error and test for treatment differences.} \]
Hypothesis Testing

• Can show: Fixed Case
  
  \[ E(\text{MS}_E) = \sigma^2 \]
  
  \[ E(\text{MS}_A) = \sigma^2 + bn \sum \tau_i^2 / (a - 1) \]
  
  \[ E(\text{MS}_B) = \sigma^2 + an \sum \beta_j^2 / (b - 1) \]
  
  \[ E(\text{MS}_{AB}) = \sigma^2 + n \sum (\tau \beta)_{ij}^2 / (a - 1)(b - 1) \]

• Use \( F \)-tests to test equality of A, B, and AB effects

\[
F_0 = \frac{SS_A / (a - 1)}{SS_E / (ab(n - 1))}
\]

\[
F_0 = \frac{SS_B / (b - 1)}{SS_E / (ab(n - 1))}
\]

\[
F_0 = \frac{SS_{AB} / (a - 1)(b - 1)}{SS_E / (ab(n - 1))}
\]
Rat Hormone Example

\[ \sum \sum \sum y_{ijk} = 2074 \text{ and } \sum \sum \sum y_{ij}^2 = 191022 \]

\[ y_{12.} = 642, y_{22.} = 571, y_{11.} = 467 \text{ and } y_{21.} = 394 \]

\[ SS_T = 191022 - 2074^2 / 24 = 11793.83 \]

\[ SS_A = (1109^2 + 965^2) / 12 - 2074^2 / 24 = 864.00 \]

\[ SS_B = (861^2 + 1213^2) / 12 - 2074^2 / 24 = 5162.67 \]

\[ SS_{Sub} = (642^2 + 467^2 + 571^2 + 394^2) / 6 - 2074^2 / 24 = 6026.83 \]

\[ SS_{AB} = 6026.83 - 5162.67 - 864.00 = 0.16 \]

\[ SS_E = 11793.83 - 6026.83 = 5767.00 \]

\[ F_{0}^{AB} = (0.16 / 1) / (5767 / 20) \approx 0.0 \text{ (Not Significant)} \]

\[ F_{0}^{A} = (864 / 1) / (5767 / 20) \approx 3.0 \text{ (Not Significant)} \]

\[ F_{0}^{B} = (5162.67 / 1) / (5767 / 20) \approx 17.9 \text{ (Significant)} \]
Comparing Factor Levels

• For our example, the sample means are

<table>
<thead>
<tr>
<th>Level</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>77.83</td>
<td>65.67</td>
</tr>
<tr>
<td>H</td>
<td>107.00</td>
<td>95.17</td>
</tr>
</tbody>
</table>

• To compare levels of one factor (main effect), we average out the other factor

• Thus, use caution with interpretation if interaction!!!
Comparing Factor Levels

- Comparing Hormone C to Hormone D
  - Average out the level
    \[
    \frac{(77.83 + 107.00)}{2} - \frac{(65.67 + 95.17)}{2} \approx 12.0
    \]

- Comparing Low Level to High Level
  - Average out the hormone
    \[
    \frac{(77.83 + 65.67)}{2} - \frac{(107.00 + 95.17)}{2} \approx -29.335
    \]
Two-Factor Experiment

- Interaction
  - Difference in response of one factor not constant across all levels of the other factor
  - Diff in levels (Hormone C) vs Diff in levels (Hormone D)
    
    \[(107.00 - 77.83) - (95.17 - 65.67) \approx -0.33\]
  
    - If interaction, expect this difference of differences to be away from zero

- Interaction Plot
  
    - Visualize differences in the change in response
    - Is pattern parallel or not?
Interaction Plot for Rat Study

Factorial Treatment Structure

Response

Hormone C

Hormone D

Factor B

L

H
Other Examples of Interaction Plot

- Completely opposite behavior (no Factor 2 main effect?)
Other Examples of Interaction Plot

- Increase but not same amount (still Factor 2 main effect?)
Regression Approach

\[ y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_{12} x_{1i} x_{2i} + \epsilon \]

- \( x_{1i} = 1 \) if Hormone C and \( x_{1i} = -1 \) if Hormone D
- \( x_{2i} = 1 \) if High level and \( x_{2i} = -1 \) if Low Level
- Trt C: \( E(y) = \beta_0 + \beta_1 + \beta_2 + \beta_{12} \), Trt c: \( E(y) = \beta_0 + \beta_1 - \beta_2 - \beta_{12} \)
- Trt D: \( E(y) = \beta_0 - \beta_1 + \beta_2 - \beta_{12} \), Trt d: \( E(y) = \beta_0 - \beta_1 - \beta_2 + \beta_{12} \)
- \( \beta_1 \) estimates Hormone effect
- \( \beta_2 \) estimates Level effect
- \( \beta_{12} \) estimates Interaction
Response Surface Approach

- Used when each treatment factor is quantitative
- Predicts response for other level combinations
- Response surface described for \(-1 \leq x_1, x_2 \leq 1\)
- If $\beta_{12}=0$ then surface is a plane (additive model)
- If $\beta_{12} \neq 0$ then surface “curved” (pgs 185-186)
How to Handle Interaction

• If interaction, can we discuss main effects?
  – In regression, if $\beta_{12} \neq 0$, leave $x_1$ and $x_2$ in model
  – “Main effect” then depends on the level of the other factor
  – Cannot simply average the other factor out (ignore it)
  – Example: opposite behavior $\rightarrow$ main effect “cancels” out

  – Common to compare $\bar{y}_{ij}$’s for each level of $i$ or vice versa
  – Sometimes may be able to discuss “average” main effect
  – Also times when interaction due to only a few combos
    and you can discuss main effect behavior elsewhere
Main effects not interpretable  Can still discuss main effects
Hidden Replication Feature

- **One-factor approach**
  - Can estimate main effects using 3 combinations (C, c, d)
  - Main effect Level: $y_C - y_c$, Main effect Hormone: $y_c - y_d$
  - Must replicate to have variance estimate
  - Cannot estimate interaction without 4th combination
  - If $n = 2$ so $N = 6$, $\text{Var(Effect)} = 2\sigma^2/2 = \sigma^2$

- **Factorial approach**
  - Estimate effects using $N = 4$ observations (C, c, D, d)
  - Have variance estimate if no interaction
  - Main effect Hormone: $.5(y_C + y_c) - .5(y_D + y_d)$
  - $\text{Var(Effect)} = \sigma^2$
  - Replication provides ability to estimate interaction

- **Factorial gives same accuracy with less** ($N = 6$ vs $N = 4$)