Design of Experiments:
Part 1

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Plan for Today

• Discussion of the reading assignment
• History of DOE
• Full factorial designs
  – The design
  – The model
  – Analysis of the sum of squares
  – Hypothesis testing
• Other designs
  – Fractional factorial designs
  – Central composite designs
Statistics as a Catalyst to Learning

- Concerned improvement of a paper helicopter
- Screening experiment (16) \(2^{8-4}_{IV}\)
- Steepest ascent (5)
- Full factorial (16) \(2^4\)
- Sequentially assembled CCD (16+14=30)
- Ridge exploration (16)
- \((16+5+30+16)*4 > 250\) experiments
- Resulted in a 2X increase in flight time vs the starting point design

Factors Considered Initially

TABLE 1: Factor Levels Used in Design I: An Initial $2^S_{IV}$ Screening Experiment.
and FIGURE 1: The Initial Helicopter Design in Box and Liu, 1999.
Screening Design

- What is the objective of screening?
- What is special about this matrix of 1s and -1s?

TABLE 2: Design I: Layout and Data for $2^{8-4}$ Screening Design in Box and Liu, 1999.
Effect Estimates

Image removed due to copyright restrictions.

TABLE 3: Design I: Estimates for a $2^{8-4}$ Screening Design in Box and Liu, 1999.
Normal Probability Plots

• What's the purpose of these graphs?

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FIGURE 2: Design I - Normal Plots for: (a) Location effects from $y$ and (b) Dispersion Effects from $100 \log(s)$ in Box and Liu, 1999.
"Steepest" Ascent

• What does "steep" mean in this context?

Image removed due to copyright restrictions.
FIGURE 4: Data for 5 Helicopters on the path of Steepest Ascent Calculated from Design 1 in Box and Liu, 1999.
Factors Re-Considered

Wing width $w$
Wing length $l$

Wing area $A = lw$
Wing aspect ratio $Q = l/w$

Image removed due to copyright restrictions.
FIGURE 1: The Initial Helicopter Design in Box and Liu, 1999.
Central Composite Design

$2^n$ with center points and axial runs

Enables a model to be fit with all second order polynomial terms included (i.e. $A^2$, $AB$, etc.)

$2^3$ shown here

$2^4$ run by Box
Analysis of Variance

- What would you conclude about lack of fit?
- What is being used as the denominator of $F$?
Thought Questions

• If we “optimize” this thing, what does that mean?
• How were design parameters chosen?
• Were important ones missed?
• What does Box say about variables being recombined to make this process more efficient?
• Is it reasonable to run 248 experiments on a simple design? Under what circumstances?
• What are the key differences between the process described here and system design in industry?
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• Discussion of the reading assignment

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"An experiment is simply a question put to nature … The chief requirement is simplicity: only one question should be asked at a time."


Table III.

<table>
<thead>
<tr>
<th>Plot</th>
<th>Mean yield (Bushels per acre)</th>
<th>Mean annual decrement (Bushels per acre)</th>
<th>Mean annual decrement %</th>
</tr>
</thead>
<tbody>
<tr>
<td>5, no ammonia</td>
<td>14.18 ± 0.44</td>
<td>0.090</td>
<td>63 ± 16</td>
</tr>
<tr>
<td>6, single ammonia</td>
<td>22.58 ± 0.71</td>
<td>0.141</td>
<td>62 ± 19</td>
</tr>
<tr>
<td>7, double ,,</td>
<td>31.37 ± 0.90</td>
<td>0.144</td>
<td>46 ± 15</td>
</tr>
<tr>
<td>8, treble ,,</td>
<td>35.69 ± 0.93</td>
<td>0.092</td>
<td>26 ± 14</td>
</tr>
</tbody>
</table>

“To call in the statistician after the experiment is done may be no more than asking him to perform a post-mortem examination: he may be able to say what the experiment died of.”


![Table](image)

**Fig. 1.—A Complex Experiment with Winter Oats.**
Say the independent experimental error of observations \((a), (ab),\) et cetera is \(\sigma_\epsilon.\)

We define the main effect estimate \(A\) to be

\[
A = \frac{1}{4}\left[(abc) + (ab) + (ac) + (a) - (b) - (c) - (bc) - (1)\right]
\]

What is the standard deviation of the main effect estimate \(A?\)

1) \(\sigma_A = \frac{1}{2}\sqrt{2}\sigma_\epsilon\)  
2) \(\sigma_A = \frac{1}{4}\sigma_\epsilon\)  
3) \(\sigma_A = \sqrt{8}\sigma_\epsilon\)  
4) \(\sigma_A = \sigma_\epsilon\)
Response Surface Methodology

- A method to seek improvements in a system by sequential investigation and parameter design
  - Variable screening
  - Steepest ascent
  - Fitting polynomial models
  - Empirical optimization

Cross (or Product) Arrays

Robust Parameter Design

“Robust Parameter Design ... is a statistical / engineering methodology that aims at reducing the performance variation of a system (i.e. a product or process) by choosing the setting of its control factors to make it less sensitive to noise variation.”

George Box on Sequential Experimentation

“Because results are usually known quickly, the natural way to experiment is to use information from each group of runs to plan the next …”

“…Statistical training unduly emphasizes mathematics at the expense of science. This has resulted in undue emphasis on “one-shot” statistical procedures… examples are hypothesis testing and alphabetically optimal designs.”

Majority View on “One at a Time”

One way of thinking of the great advances of the science of experimentation in this century is as the final demise of the “one factor at a time” method, although it should be said that there are still organizations which have never heard of factorial experimentation and use up many man hours wandering a crooked path.

My Observations of Industry

• Farming equipment company has reliability problems
• Large blocks of robustness experiments had been planned at outset of the design work
• More than 50% were not finished
• Reasons given
  – Unforseen changes
  – Resource pressure
  – Satisficing

“Well, in the third experiment, we found a solution that met all our needs, so we cancelled the rest of the experiments and moved on to other tasks...”
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Basic Terms in Factorial DOE

• **Response** – the output of the system you are measuring
• **Factor** – an input variable that may affect the response
• **Level** – a specific value a factor may take
• **Trial** – a single instance of the setting of factors and the measurement of the response
• **Replication** – repeated instances of the setting of factors and the measurement of the response
• **Effect** – what happens to the response when factor levels change
• **Interaction** – joint effects of multiple factors
Exhaustive search of the space of 3 discrete 2-level factors is the full factorial $2^3$ experimental design.
## Tabular Representation

<table>
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<tr>
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</table>

A cube has eight vertices

2³ Design
Three Level Factors

8 vertices +
12 edges +
6 faces +
1 center =
27 points

$3^3$ Design
Creating and Randomizing Full Factorials in Matlab

\[
X = \text{fullfact}([4 \ 3]);
\]
\[
r = \text{rand}(1,4*3);
\]
\[
[B, INDEX] = \text{sort}(r);
\]
\[
Xr(1:4*3,:) = X(INDEX,:);
\]
Geometric Growth of Experimental Effort

- $2^n$
- $3^n$
Calculating Main Effects

\[ A \equiv \frac{1}{4} \left[ (abc) + (ab) + (ac) + (a) - (b) - (c) - (bc) - (1) \right] \]
If the standard deviation of \((a), (ab), \text{ et cetera}\) is \(\sigma\), what is the standard deviation of the main effect estimate \(A\)?

\[
A \equiv \frac{1}{4}[(abc) + (ab) + (ac) + (a) - (b) - (c) - (bc) - (1)]
\]

1) \(\sigma\)  2) Less than \(\sigma\)  3) More than \(\sigma\)  4) Not enough info
Factor Effect Plots
Calculating Interactions

\[ AC \equiv \frac{1}{4} [(abc) + (ac) + (b) + (1) - (ab) - (bc) - (c) - (a)] \]
Treatment Effects Model (Two Factors)

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

\[ \sum \tau_i = 0 \quad \text{If factor } a \text{ has two levels} \]

\[ \tau_1 + \tau_2 = 0 \]

\[ \tau_1 = -\frac{A}{2} \quad \tau_2 = \frac{A}{2} \]
Treatment Effects Model (Two Factors)

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

interactions – there are of $ab$ these terms

\[
\sum_{i=1}^{a} (\tau\beta)_{ij} = \sum_{j=1}^{b} (\tau\beta)_{ij} = 0
\]

$a+b$ equations but only $a+b-1$ are independent

$(a-1)(b-1)$ DOF
Concept Test

If there are no interactions in this system, then the factor effect plot from this design could look like:

Hold up all cards that apply.
Treatment Effects Model versus the Regression Model

\[ y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon \]

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

- If the factors are **two level** factors
- And they are coded as \((-1,+1)\)
- Then \( \tau_2 = \beta_1 \)  \( \tau_1 = -\beta_1 \)
- And \( (\tau\beta)_{12} = \beta_{12} \)
Recall from the lecture on multiple regression

**Estimation of the Parameters $\beta$**

Assume the model equation

$$y = X\beta + \varepsilon$$

We wish to minimize the sum squared error

$$L = \varepsilon^T \varepsilon = (y - X\beta)^T (y - X\beta)$$

To minimize, we take the derivative and set it equal to zero

$$\frac{\partial L}{\partial \beta} \bigg|_{\hat{\beta}} = -2X^T y + 2X^T X \hat{\beta}$$

The solution is

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

And we define the fitted model

$$\hat{y} = X\hat{\beta}$$
Estimation of the Parameters $\beta$ when $X$ is a $2^k$ design

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

\begin{align*}
(X^T X)_{ij} &= 0 \text{ if } i \neq j & \text{The columns are orthogonal} \\
(X^T X)_{ij} &= n2^k \text{ if } i = j \\
(X^T X)^{-1} &= \frac{1}{n2^k} I
\end{align*}
Breakdown of Sum Squares

“Grand Total Sum of Squares”

SS due to mean

\[ SS = N \bar{y}^2 \]

“Total Sum of Squares”

\[ SS_T = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{k=1}^{n} (y_{ijk} - \bar{y})^2 \]

\[ SS_E = \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{k=1}^{n} (y_{ijk})^2 \]

\[ SS_A = bn \sum_{i=1}^{a} (\bar{y}_{i..} - \bar{y}_{..})^2 \]

\[ SS_{AB} = n \sum_{i=1}^{a} \sum_{j=1}^{b} (\bar{y}_{ij.} - \bar{y}_{i..} - \bar{y}_{..j} + \bar{y}_{..})^2 \]

\[ SS_B = an \sum_{j=1}^{b} (\bar{y}_{.j} - \bar{y}_{..})^2 \]
Breakdown of DOF

\[ abn \]
number of \( y \) values

1
due to the mean

\[ abn-1 \]
total sum of squares

\[ a-1 \]
for factor \( A \)

\[ b-1 \]
for factor \( B \)

\[ (a-1)(b-1) \]
for interaction \( AB \)

\[ ab(n-1) \]
for error
Hypothesis Tests in Factorial Exp

• Equality of treatment effects due to factor $A$ or due to factor $B$

\[ H_0 : \tau_1 = \tau_2 = \ldots = \tau_a = 0 \quad \text{and} \quad H_0 : \beta_1 = \beta_2 = \ldots = \beta_b = 0 \]

\[ H_1 : \tau_i \neq 0 \text{ for at least one } i \quad \text{and} \quad H_1 : \beta_i \neq 0 \text{ for at least one } i \]

• Test statistic

\[ F_0 = \frac{MS_A}{MS_E} \quad \text{and} \quad F_0 = \frac{MS_B}{MS_E} \]

• Criterion for rejecting $H_0$

\[ F_0 > F_{\alpha,a-1,ab(n-1)} \quad \text{and} \quad F_0 > F_{\alpha,b-1,ab(n-1)} \]
Hypothesis Tests in Factorial Exp

• Significance of $AB$ interactions

\[ H_0 : \tau \beta_{ij} = 0 \text{ for all } i, j \]
\[ H_1 : \text{at least one } \tau \beta_{ij} \neq 0 \]

• Test statistic

\[ F_0 = \frac{MS_{AB}}{MS_E} \]

• Criterion for rejecting $H_0$

\[ F_0 > F_{\alpha,(a-1)(b-),ab(n-1)} \]
Example 5-1 – Battery Life

FF = fullfact([3 3]);
X = [FF; FF; FF; FF];
Y = [130 150 138 34 136 174 20 25 96 155 188 110 40 122
120 70 70 104 74 159 168 80 106 150 82 58 82 180 126 160
75 115 139 58 45 60];

[p, table, stats] = anovan(Y, {X(:,1), X(:,2)}, 'interaction');

hold off; hold on
for i = 1:3; for j = 1:3;
    intplt(i,j) = (1/4)*sum(Y.*(X(:,1) == j).*(X(:,2) == i));
end
plot([15 70 125], intplt(:,i)); end
Regression – Battery Life

FF = fullfact([3 3]);
A = FF(:,1)-2;  B = FF(:,2)-2;  ones(1:3*3)=1;
R = [ones' A B A.*A B.*B A.*B ];
X = [R; R; R; R];
Y = [130 150 138 34 136 174  20  25 96 155 188 110 40 122
120 70 70 104 74 159 168 80 106 150 82 58 82 180 126 160
75 115 139 58 45 60]';

[b,bint,r,rint,stats] = regress(Y,X,0.05);
[t,m] = meshgrid(-1:.1:1,-1:.1:1);
Yhat = b(1)+b(2)*t+b(3)*m+b(4)*t.*t+b(5)*r;
hold off; h=plot3(t,m,Yhat);
hold on; scatter3(X(:,2),X(:,3),Y);

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Fractional factorial designs
Fractional Factorial Experiments

Cuboidal Representation

This is the $2^{3-1}$ fractional factorial.
## Fractional Factorial Experiments

### Tabular Representation

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<th>C</th>
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<th>E</th>
<th>F</th>
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<th>FG=-A</th>
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2⁷⁻⁴ Design Resolution III.

Two-way interactions are aliased with main effects.
Fractional Factorial Experiments

Cuboidal Representation

\[ A = \frac{1}{2} \left[ (ab) + (ac) - (1) - (bc) \right] \]
One at a Time Experiments

If the standard deviation of \((a)\) and \((1)\) is \(\sigma\), what is the standard deviation of \(A\)?

Provides resolution of individual factor effects
But the effects may be biased

\[ A \approx (a) - (1) \]
Efficiency

• The variance for OFAT is $\sqrt{2\sigma}$ using 4 experiments
• The standard deviation for $2^3{-1}$ was $\sigma$ using 4 experiments
• The inverse ratio of variance per unit is considered a measure of relative efficiency

$$\frac{\left[\sqrt{2\sigma}\right]^2}{\left[\sigma\right]^2} = \frac{4}{4} = 2$$

• The $2^3{-1}$ is considered 2 times more efficient than the OFAT
Overview Research

Concept Design

Adaptive Experimentation and Robust Design

Outreach to K-12

PBS show “Design Squad”

Complex Systems

Methodology Validation

\[
\Pr(\beta_i x_i^* x_i^* > \beta_i) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\exp\left(-\frac{1}{2} \frac{x_i}{\sigma_{\text{INT}}}^2\right)}{\sigma_{\text{INT}} \sqrt{\sigma_{\text{INT}}^2 + (n-2)\sigma_{\text{INT}}^2}} dx_i dx_i
\]
Next Steps

- Friday 27 April
  - Recitation to support the term project
- Monday 30 April
  - Design of Experiments: Part 2
- Wednesday 2 May
  - Design of Computer Experiments
- Friday 4 May
  - Exam review
- Monday 7 May – Frey at NSF
- Wednesday 9 May – Exam #2