Unit 7: Orthogonal Array Experiments and Response Surface Methodology

- A modern system of experimental design.
- Orthogonal arrays (sections 8.1-8.2; appendix 8A and 8C).
- Analysis of experiments with complex aliasing (part of sections 9.1-9.4).
- Brief response surface methodology, central composite designs (sections 10.1-10.2).

Two Types of Fractional Factorial Designs

- Regular (2^{n-k}, 3^{n-k} designs):
  columns of the design matrix form a group over a finite field; the interaction between any two columns is among the columns,
  $\Rightarrow$ any two factorial effects are either
  orthogonal or fully aliased.

- Nonregular (mixed-level designs, orthogonal arrays)
  some pairs of factorial effects can be *partially* aliased
  $\Rightarrow$ more complex aliasing pattern. This includes 3^{n-k} designs with linear-quadratic system.

A Modern System of Experimental Design

It has four branches:

- Regular orthogonal arrays (Fisher, Yates, Finney, ...): 2^{n-k}, 3^{n-k} designs, using minimum aberration criterion.
- Nonregular orthogonal designs (Plackett-Burman, Rao, Bose): Plackett-Burman designs, orthogonal arrays.
- Response surface designs (Box): fitting a parametric response surface.
- Optimal designs (Kiefer): optimality driven by specific model/criterion.

Orthogonal Arrays

- In Tables 1 and 2, the design used does not belong to the 2^{k-p} series (Chapter 5) or the 3^{k-p} series (Chapter 6), because the latter would require run size as a power of 2 or 3. These designs belong to the class of orthogonal arrays.
- An **orthogonal array** array $OA(N, s_1^{m_1} \ldots s_\gamma^{m_\gamma}, t)$ of strength t is an $N \times m$ matrix, $m = m_1 + \ldots + m_\gamma$, in which m_i columns have $s_i (\geq 2)$ symbols or levels such that, for any t columns, all possible combinations of symbols appear equally often in the matrix.
- For OA of strength two, the index $t = 2$ is dropped for simplicity.
- An $OA(12, 2^{11})$ is used in Table 1 and an $OA(18, 2^1 3^7)$ is used in Table 2.

Example : $OA(12, 2^{11})$

Table 1: Design Matrix and Lifetime Data, Cast Fatigue Experiment

	Factor											Logged
Run	*A*	*B*	*C*	*D*	*E*	*F*	*G*	8	9	10	11	Lifetime
1	+	+	–	+	+	+	–	–	–	+	–	6.058
2	+	–	+	+	+	–	–	–	+	–	+	4.733
3	–	+	+	+	–	–	–	+	–	+	+	4.625
4	+	+	+	–	–	–	+	–	+	+	–	5.899
5	+	+	–	–	–	+	–	+	+	–	+	7.000
6	+	–	–	–	+	–	+	+	–	+	+	5.752
7	–	–	–	+	–	+	+	–	+	+	+	5.682
8	–	–	+	–	+	+	–	+	+	+	–	6.607
9	–	+	–	+	+	–	+	+	+	–	–	5.818
10	+	–	+	+	–	+	+	+	–	–	–	5.917
11	–	+	+	–	+	+	+	–	–	–	+	5.863
12	–	–	–	–	–	–	–	–	–	–	–	4.809

Example : $OA(18, 2^1 3^7)$

Table 2: Design Matrix and Response Data, Blood Glucose Experiment

	Factor								Mean
Run	*A*	*G*	*B*	*C*	*D*	*E*	*F*	*H*	Reading
1	0	0	0	0	0	0	0	0	97.94
2	0	0	1	1	1	1	1	1	83.40
3	0	0	2	2	2	2	2	2	95.88
4	0	1	0	0	1	1	2	2	88.86
5	0	1	1	1	2	2	0	0	106.58
6	0	1	2	2	0	0	1	1	89.57
7	0	2	0	1	0	2	1	2	91.98
8	0	2	1	2	1	0	2	0	98.41
9	0	2	2	0	2	1	0	1	87.56
10	1	0	0	2	2	1	1	0	88.11
11	1	0	1	0	0	2	2	1	83.81
12	1	0	2	1	1	0	0	2	98.27
13	1	1	0	1	2	0	2	1	115.52
14	1	1	1	2	0	1	0	2	94.89
15	1	1	2	0	1	2	1	0	94.70
16	1	2	0	2	1	2	0	1	121.62
17	1	2	1	0	2	0	1	2	93.86
18	1	2	2	1	0	1	2	0	96.10

Why Using Orthogonal Array

- **Run size economy.** Suppose 8-11 factors at two levels are to be studied. Using an $OA(12, 2^{11})$ will save 4 runs over a 16-run 2^{k-p} design. Similarly, suppose 5-7 factors at three levels are to be studied. Using an $OA(18, 3^7)$ will save 9 runs over a 27-run 3^{k-p} design.
- **Flexibility.** Many *OA*'s exist for flexible combinations of factor levels. See the collection on next page.

A Result on Run Size of OA

- **Lemma**. For an orthogonal array OA(N, $s_1^{m_1} \cdots s_\gamma^{m_\gamma}$, t), its run size N must be divisible by the least common multiple of $\prod_{i=1}^{\gamma} s_i^{k_i}$ for all possible combinations of k_i with $k_i \leq m_i$ and $\sum_{i=1}^{\gamma} k_i = t$, $i = 1, \ldots, \gamma$.
  Its proof is given on p. 375 of WH.

- **Example of its use**. Suppose an experimenter needs to find an OA(N, $2^2 3^3$) of strength two. Among $2^{k_1} 3^{k_2}$ with $k_1 + k_2 = 2$, there are three possibilities: 2^2, 3^2, and $2 \cdot 3$. Its least common multiple is $4 \times 9 = 36$. Thus the minimal N value is 36.

Useful Orthogonal Arrays

- Collection in Appendix 8A and 8C of WH:

$*OA(12, 2^{11})$	$OA(12, 3^1 2^4)$	$*OA(18, 2^1 3^7)$
$OA(18, 6^1 3^6)$	$OA(20, 2^{19})$	$OA(24, 3^1 2^{16})$
$OA(24, 6^1 2^{14})$	$*OA(36, 2^{11} 3^{12})$	$OA(36, 3^7 6^3)$
$OA(36, 2^8 6^3)$	$OA(48, 2^{11} 4^{12})$	$OA(50, 2^1 5^{11})$
	$OA(54, 2^1 3^{25})$	

  * especially useful

- Learn to choose and use the design tables in the collection.

$OA(18, 2^1 3^7)$ and $OA(18, 6^1 3^6)$

Table 3: $OA(18, 2^1 3^7)$ (columns 1–8) and $OA(18, 6^1 3^6)$ (columns $1'$ and 3–8)

Run	$1'$	1	2	3	4	5	6	7	8
1	0	0	0	0	0	0	0	0	0
2	0	0	0	1	1	1	1	1	1
3	0	0	0	2	2	2	2	2	2
4	1	0	1	0	0	1	1	2	2
5	1	0	1	1	1	2	2	0	0
6	1	0	1	2	2	0	0	1	1
7	2	0	2	0	1	0	2	1	2
8	2	0	2	1	2	1	0	2	0
9	2	0	2	2	0	2	1	0	1
10	3	1	0	0	2	2	1	1	0
11	3	1	0	1	0	0	2	2	1
12	3	1	0	2	1	1	0	0	2
13	4	1	1	0	1	2	0	2	1
14	4	1	1	1	2	0	1	0	2
15	4	1	1	2	0	1	2	1	0
16	5	1	2	0	2	1	2	0	1
17	5	1	2	1	0	2	0	1	2
18	5	1	2	2	1	0	1	2	0

$OA(36, 2^{11}3^{12})$

Table 4: $OA(36, 2^{11}3^{12})$

Run	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	1
3	0	0	0	0	0	0	0	0	0	0	0	2	2	2	2	2	2	2	2	2	2	2	2
4	0	0	0	0	0	1	1	1	1	1	1	0	0	0	0	1	1	1	1	2	2	2	2
5	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	2	2	2	2	0	0	0	0
6	0	0	0	0	0	1	1	1	1	1	1	2	2	2	2	0	0	0	0	1	1	1	1
7	0	0	1	1	1	0	0	0	1	1	1	0	0	1	2	0	1	2	2	0	1	1	2
8	0	0	1	1	1	0	0	0	1	1	1	1	1	2	0	1	2	0	0	1	2	2	0
9	0	0	1	1	1	0	0	0	1	1	1	2	2	0	1	2	0	1	1	2	0	0	1
10	0	1	0	1	1	0	1	1	0	0	1	0	0	2	1	0	2	1	2	1	0	2	1
11	0	1	0	1	1	0	1	1	0	0	1	1	1	0	2	1	0	2	0	2	1	0	2
12	0	1	0	1	1	0	1	1	0	0	1	2	2	1	0	2	1	0	1	0	2	1	0
13	0	1	1	0	1	1	0	1	0	1	0	0	1	2	0	2	1	0	2	2	1	0	1
14	0	1	1	0	1	1	0	1	0	1	0	1	2	0	1	0	2	1	0	0	2	1	2
15	0	1	1	0	1	1	0	1	0	1	0	2	0	1	2	1	0	2	1	1	0	2	0
16	0	1	1	1	0	1	1	0	1	0	0	0	1	2	1	0	0	2	1	2	2	1	0
17	0	1	1	1	0	1	1	0	1	0	0	1	2	0	2	1	1	0	2	0	0	2	1
18	0	1	1	1	0	1	1	0	1	0	0	2	0	1	0	2	2	1	0	1	1	0	2

$$OA(36, 2^{11}3^{12})$$

Table 4: Continued

Run	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
19	1	0	1	1	0	0	1	1	0	1	0	0	1	0	2	2	2	0	1	1	0	1	2
20	1	0	1	1	0	0	1	1	0	1	0	1	2	1	0	0	0	1	2	2	1	2	0
21	1	0	1	1	0	0	1	1	0	1	0	2	0	2	1	1	1	2	0	0	2	0	1
22	1	0	1	0	1	1	1	0	0	0	1	0	1	1	2	2	0	1	0	0	2	2	1
23	1	0	1	0	1	1	1	0	0	0	1	1	2	2	0	0	1	2	1	1	0	0	2
24	1	0	1	0	1	1	1	0	0	0	1	2	0	0	1	1	2	0	2	2	1	1	0
25	1	0	0	1	1	1	0	1	1	0	0	0	2	1	0	1	2	2	0	2	0	1	1
26	1	0	0	1	1	1	0	1	1	0	0	1	0	2	1	2	0	0	1	0	1	2	2
27	1	0	0	1	1	1	0	1	1	0	0	2	1	0	2	0	1	1	2	1	2	0	0
28	1	1	1	0	0	0	0	1	1	0	1	0	2	1	1	1	0	0	2	1	2	0	2
29	1	1	1	0	0	0	0	1	1	0	1	1	0	2	2	2	1	1	0	2	0	1	0
30	1	1	1	0	0	0	0	1	1	0	1	2	1	0	0	0	2	2	1	0	1	2	1
31	1	1	0	1	0	1	0	0	0	1	1	0	2	2	2	1	2	1	1	0	1	0	0
32	1	1	0	1	0	1	0	0	0	1	1	1	0	0	0	2	0	2	2	1	2	1	1
33	1	1	0	1	0	1	0	0	0	1	1	2	1	1	1	0	1	0	0	2	0	2	2
34	1	1	0	0	1	0	1	0	1	1	0	0	2	0	1	2	1	2	0	1	1	2	0
35	1	1	0	0	1	0	1	0	1	1	0	1	0	1	2	0	2	0	1	2	2	0	1
36	1	1	0	0	1	0	1	0	1	1	0	2	1	2	0	1	0	1	2	0	0	1	2

Partial and Complex Aliasing

- For the 12-run Plackett-Burman design OA(12,2^{11})

$$E(\hat{\beta}_i) = \beta_i + \frac{1}{3}\sum_{j,k\neq i} \pm\beta_{jk}$$

partial aliasing: coefficient $\pm\frac{1}{3}$

complex aliasing: $45(=\binom{10}{2})$ partial aliases

- Traditionally complex aliasing was considered to be a disadvantage because it leads to many possible models which can be hard to *discriminate*.

Analysis Strategies

- Traditionally experiments with **complex aliasing** were used for **screening** purpose, i.e., estimating main effects only
- A paradigm shift: using effect sparsity/heredity, Hamada-Wu (1992) recognized that complex aliasing can be turned into an advantage for studying interactions
- Analysis methods allow two-factor interactions to be entertained (in addition to main effects). Effective if the number of significant interactions is small. Frequentist method in Section 9.4 and Bayesian method in Section 9.5.

Traditional Approach: Main Effect Analysis

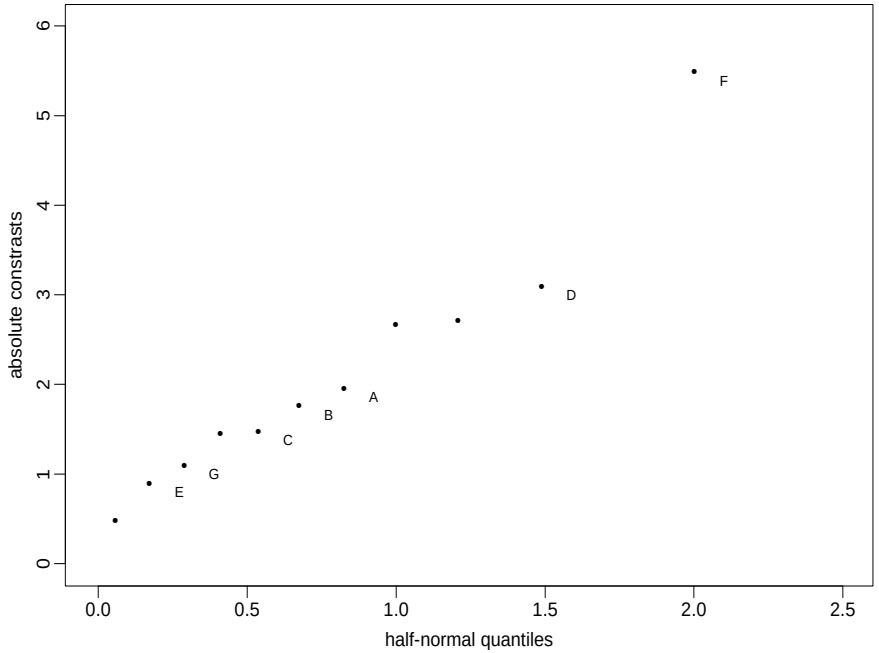

Figure 1: Half-normal plot, cast fatigue experiment.

- Only factor F is significant ($R^2 = 0.45$). Adding the next effect D gives $R^2 = 0.59$, a marginal improvement.

Complex Aliasing

- Consider the cast fatigue experiment. Let the main effect estimate of factor A be $\hat{A} = \bar{y}(A=+) - \bar{y}(A=-)$, etc.
- Assuming no 3fi's or higher, it can be shown that

$$\begin{aligned}
E(\hat{A}) = A \quad &- \frac{1}{3}BC - \frac{1}{3}BD - \frac{1}{3}BE + \frac{1}{3}BF - \frac{1}{3}BG \\
&+ \frac{1}{3}CD - \frac{1}{3}CE - \frac{1}{3}CF + \frac{1}{3}CG + \frac{1}{3}DE \\
&+ \frac{1}{3}DF - \frac{1}{3}DG - \frac{1}{3}EF - \frac{1}{3}EG - \frac{1}{3}FG, \\
E(\hat{B}) = B \quad &- \frac{1}{3}AC - \frac{1}{3}AD - \frac{1}{3}AE + \frac{1}{3}AF - \frac{1}{3}AG \\
&- \frac{1}{3}CD - \frac{1}{3}CE - \frac{1}{3}CF + \frac{1}{3}CG + \frac{1}{3}DE \\
&- \frac{1}{3}DF - \frac{1}{3}DG + \frac{1}{3}EF + \frac{1}{3}EG - \frac{1}{3}FG,
\end{aligned}$$

- Similar complex equations for $\hat{C}$, $\hat{D}$, $\hat{E}$, $\hat{F}$, $\hat{G}$. This relationship is called **complex aliasing**.

Complex Aliasing Simplified by Effect Sparsity

- For the cast fatigue experiment, suppose the true (but unknown) significant effects are A, F, G, AB and FG, which can be justified by effect sparsity. Then the relationships are simplified:

$$
\begin{aligned}
E(\hat{A}) &= A - \frac{1}{3}FG, \\
E(\hat{B}) &= -\frac{1}{3}FG, \\
E(\hat{C}) &= -\frac{1}{3}AB + \frac{1}{3}FG, \\
E(\hat{D}) &= -\frac{1}{3}AB + \frac{1}{3}FG, \\
E(\hat{E}) &= -\frac{1}{3}AB - \frac{1}{3}FG, \\
E(\hat{F}) &= F + \frac{1}{3}AB, \\
E(\hat{G}) &= G - \frac{1}{3}AB,
\end{aligned}
$$

suggesting the viability of estimating significant main effects and 2fi's.

Hamada-Wu Analysis Strategy

1. For each factor X, consider X and all 2fi's XY involving X. Use stepwise regression to identify significant effects. Repeat this for each X and keep the best model.

2. Use stepwise regression to identify significant effects among effects identified in **1** and the main effects.

3. Using effect heredity, consider (i) effects identified in **2** and (ii) 2fi's with at least one parent factor appearing in the main effects in (i). Use stepwise regression to identify significant effects.

4. Iterate between **2** and **3** until model stops changing.

Analysis of Cast Fatigue Experiment

- Since F is significant in the main effect analysis, consider 2fi's involving F. This leads to FG and R^2 is increased to 0.89, almost doubled!
- A better prediction based on

$$\hat{y} = 5.7 + 0.458F - 0.459FG.$$

By choosing G_- and F_+, predicted life is

$$5.7 + 0.458 - 0.459(-1) = 5.7 + 0.92 = 6.62,$$

a 16% increase $(= \frac{0.92}{5.7})$ over the main effect model with F only.

Summary of Analysis Results

- Cast Fatigue Experiment:

$$\begin{aligned} \text{Main effect analysis}: &\quad F \quad (R^2 = 0.45) \\ &\quad F, \quad D \ (R^2 = 0.59) \\ \text{HW analysis}: &\quad F, \quad FG \ (R^2 = 0.89) \\ &\quad F, \quad FG, \ D \ (R^2 = 0.92) \end{aligned}$$

- Blood Glucose Experiment:

$$\begin{aligned} \text{Main effect analysis}: &\quad E_q, \quad F_q \ (R^2 = 0.36) \\ \text{HW analysis}: &\quad B_l, \quad (BH)_{lq}, \ (BH)_{qq} \ (R^2 = 0.89) \end{aligned}$$

Poorman's Response Surface Methodology

- Consider an experiment to study three quantitative factors with up to 5 levels.

Table 5: Factors and Levels, Ranitidine Experiment

Factor	Levels
A. pH	2, 3.42, 5.5, 7.58, 9
B. voltage (kV)	9.9, 14, 20, 26, 30.1
C. α-CD (mM)	0, 2, 5, 8, 10

- The design matrix and the data are given on the next page. The design differs from 2^{k-p} design in two respects :
  - 6 replicates at the center,
  - 6 runs along the three axes.

  It belongs to the class of *central composite designs*.

Ranitidine Experiment

Table 6: Design Matrix and Response Data

Run	Factor *A*	*B*	*C*	CEF	ln CEF
1	−1	−1	−1	17.293	2.850
2	1	−1	−1	45.488	3.817
3	−1	1	−1	10.311	2.333
4	1	1	−1	11757.084	9.372
5	−1	−1	1	16.942	2.830
6	1	−1	1	25.400	3.235
7	−1	1	1	31697.199	10.364
8	1	1	1	12039.201	9.396
9	0	0	−1.67	7.474	2.011
10	0	0	1.67	6.312	1.842
11	0	−1.68	0	11.145	2.411
12	0	1.68	0	6.664	1.897
13	−1.68	0	0	16548.749	9.714
14	1.68	0	0	26351.811	10.179
15	0	0	0	9.854	2.288
16	0	0	0	9.606	2.262
17	0	0	0	8.863	2.182
18	0	0	0	8.783	2.173
19	0	0	0	8.013	2.081
20	0	0	0	8.059	2.087

Central Composite Designs

- General definition in Section 10.7 and designs in Table 10A.1. (Not required for the course).
- A simple CCD is shown graphically on the next page. It has three parts (1) *cube* (or corner) points, (2) *axial* (or star) points, (3) *center* points.

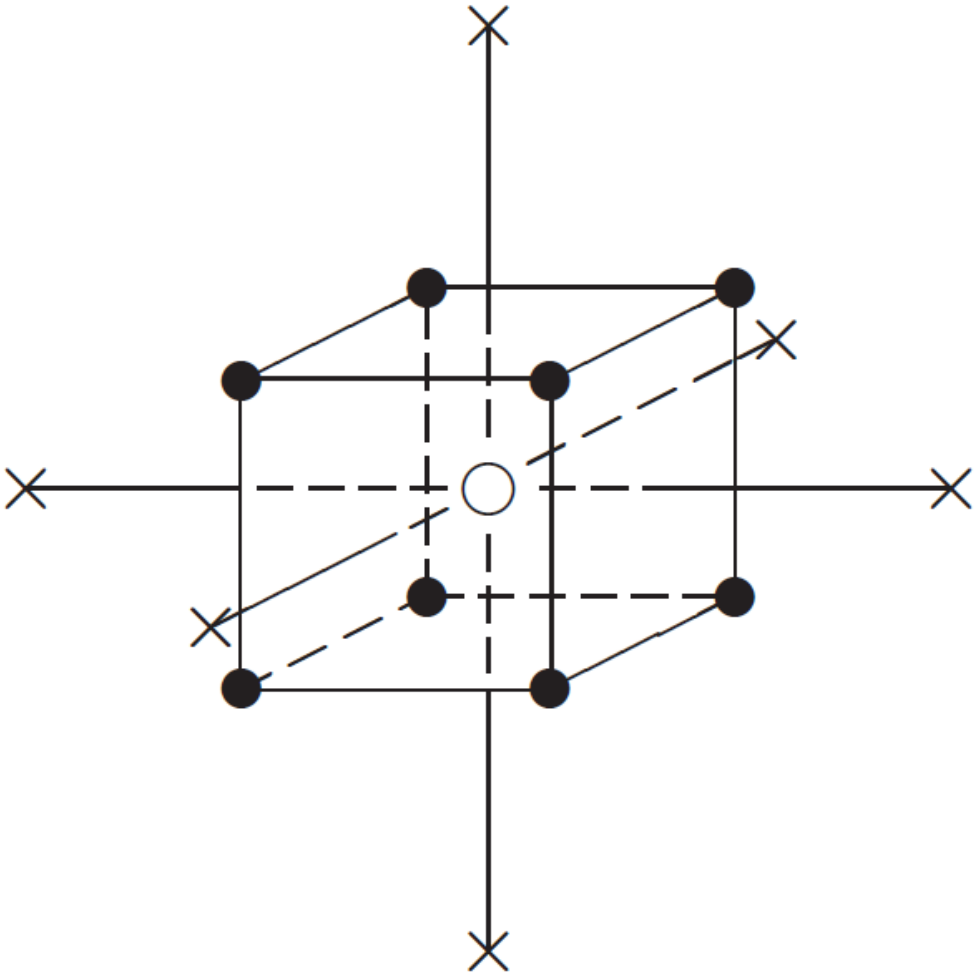

Figure 2: A Central Composite Design in Three Dimensions [cube point (dot), star point (cross), center point (circle)].

Sequential Nature of RSM

1. **Screening Experiment :** When many variables are considered, some are likely to be inert. Use *a* 2^{k-p} *design or an OA.* If the experimental region is far from the optimum, use the **first-order model**

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \varepsilon, \tag{1}$$

   to fit the data.

2. Based on the fitted model, find the steepest ascent direction and perform a search along this direction (called **steepest ascent search**).

   Steps 1 and 2 may be repeated until reaching the optimum region (e.g. peak of the surface).

Sequential Nature of RSM (Contd.)

3. To capture the curvature effects, use a **second-order design** (like the central composite design). Fit a **second-order model**

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i<j}^{k} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \varepsilon \qquad (2)$$

   to data. Use the fitted model (with insignificant terms dropped) to do *contour plots* and find the *optimum* conditions.

   A graphical illustration of these steps is given on next page.

Sequential Exploration of Response Surface