12.1 Response Surface

$x \in \mathbb{R}^k$, we want $\mu(x) = \mathbb{E}(Y \mid X = x)$

$\mu(x) = \text{surface}$

$Y = \text{response}$

We would like to know the whole curve, but we aren’t going to get it from two points. $2^k$ factorials will not give the whole surface.

Next goal: $\mathbb{E}(Y) = \beta_0 + \sum_{j=1}^{k} \beta_j x_j + \sum_{j=1}^{k} \beta_{jj} x_j^2 + \sum_{1 \leq j < l \leq k} \beta_{jl} x_j x_l$

$x \in \mathbb{R}^k \quad \text{3 levels} \rightarrow \text{can fit quadratic}$
Center Point

\[ +1 \quad \cdot \quad \cdot \]
\[ 0 \quad \cdot \quad \cdot \]
\[ -1 \quad \cdot \quad \cdot \]

\[ x_{i1} = \pm x_{i2} \rightarrow x_{i1}^2 = x_{i2}^2 \]
Can estimate \( \beta_{11} + \beta_{22} \), test for curvature

\[ \frac{1}{2} \]

12.2 \( 3^k \) factorial

\[ x_{ij} \in {-1, 0, 1} \]
3\( ^1 \): \( \bar{Y}_{-1}, \bar{Y}_0, \bar{Y}_1 \)
E(Y | X) = \beta_0 + \beta_1 x + \beta_2 x^2 \quad 2 \text{ df, since 3 parameters}

\begin{align*}
\hat{\beta}_1 &= \frac{\bar{Y}_1 - \bar{Y}_{-1}}{2} \\
\hat{\beta}_2 &= \bar{Y}_0 - \frac{\bar{Y}_1 - \bar{Y}_{-1}}{2}
\end{align*}

n = 3^k \quad n \text{ is large, which is a problem since we don't want to do that many observations}

- Can do $3^{k-p}$
- Can do blocks of size $3^p$

$3^3$ factors are A,B,C

<table>
<thead>
<tr>
<th>Source</th>
<th>DF</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>2</td>
</tr>
<tr>
<td>B</td>
<td>2</td>
</tr>
<tr>
<td>C</td>
<td>2</td>
</tr>
<tr>
<td>AB</td>
<td>4</td>
</tr>
<tr>
<td>AC</td>
<td>4</td>
</tr>
<tr>
<td>BC</td>
<td>4</td>
</tr>
<tr>
<td>ABC</td>
<td>8</td>
</tr>
</tbody>
</table>

n = 27

It is not good that most of the degrees of freedom are not in the main effects (only 6 are).

$3^k$'s let us estimate...

- $A_L$
- $A_Q$
- $B_L$
- $B_Q$
- $C_L$
- $C_Q$
- $A_LxB_L$
- $A_LxB_Q$
- ...
- $B_QxC_Q$
- ...
- $A_QxB_QxC_Q$

Care most about Linear:

- Linear
- Quadratic
- Linear x Linear
12.3 Central Composite Design

\[ 2^{k-p} + \text{one at a time} + \text{center points} \]

Need at least resolution \( V \)

\[
\begin{array}{cccc}
\pm 1 & \pm 1 & \ldots & \pm 1 \\
\pm \alpha & 0 & \ldots & 0 \\
0 & \pm \alpha & \ldots & 0 \\
\ldots & \ldots & \ldots & \ldots \\
0 & 0 & \ldots & \pm \alpha \\
0 & 0 & \ldots & 0 \\
\end{array}
\]

Repeat the last row \( n_c \) times to replicate the center point

12.3.1 Picking Range

Wider range is more informative, but phenomenal may go non-quadratic or even unsafe. Try to get \( \hat{\beta}_j, \hat{\beta}_{jj}, \hat{\beta}_{jk} \) uncorrelated.

Regression matrix \( X = \begin{bmatrix} 1 & x_{i1} & \ldots & x_{ik} & x_{i1j} & x_{i2} & \ldots & x_{ilj} - \bar{x}_{ij}^2 & x_{il}^2 - \bar{x}_l^2 & x_{ij}x_{il} \\
\end{bmatrix} \)

12.3.2 Lengthy Derivation

Pick \( \alpha \) to get \( X^TX \) diagonal
Take $\alpha = (\frac{QF}{4})^{1/4}$ where $Q = [(F + T)^{1/2} - F^{1/2}]$ and $F = 2^{k-p}$ $T = 2k + n_c$

$2k =$ number of “star” points $n_c =$ number of center points

When $\alpha = 1$, we are getting a subset of $3^k$.

Usually, $\alpha > 1$.

E.g. $n_c = 1$, $k = 5$, we get $\alpha = 1.60$

\[
\begin{array}{cccc}
  x & \cdot & \cdot & x \\
  -1.6 & -1 & 0 & 1 & 1.6 \\
  114 & 120 & 130 & 140 & 146 \\
\end{array}
\]

\[\hat{y}(x) = \beta_0 + \sum_j \beta_j x_j + \sum_j \beta_{jj} x_j^2 + \sum_{j<l} \beta_{jl} x_j x_l\]

Var($\hat{y}(x)$) = $X(X^TX)^{-1}X^T\sigma^2$ but $X$ has cross terms and squares inside

Most precision inside box, but not quite at center.

Rotatable = $V(\hat{y}(x)) = g(||x||)$

Can sometimes choose $\alpha$ to get rotatability.

12.4 Box Behnken

$k = 3$

\[
\begin{array}{ccc}
  \pm 1 & \pm 1 & 0 \\
  \pm 1 & 0 & \pm 1 \\
  0 & \pm 1 & \pm 1 \\
  0 & 0 & 0 \\
\end{array}
\]

Repeat the last row $n_c$ times to replicate the center point

Only 3 levels per variable.
• All points we choose are on the surface of a sphere, except the center point
• We have a balanced incomplete block of $2^k$ factorials

12.4.1 Blocking of Response Surface Designs
Block designs are tabulated.

Good blocking:
Block variable should be uncorrelated with $\hat{\beta}$s for Quadratic

$$\sum_{i \in BLOCK} x_{ij} x_{il} = 0 \quad 0 \leq j < l \leq k$$
$$\frac{\sum_{i \in BLOCK} x_{ij}^2}{\sum_i x_{ij}^2} = \frac{n_b}{N} = \frac{\text{#pointsinblock}}{\text{#pointsinexperiment}}$$

12.5 Mixtures

$$x_j \geq 0 \quad \sum_{j=1}^{k} x_j = 1$$

Examples:
• $x_j =$ proportion of $i^{th}$ color in paint
• $x_j =$ ratios in recipe
• $x_j =$ ratios in fuel
Linear Model:

\[ y = a_0 + \sum_j a_j x_j = a_0 \sum_j x_j + \sum_j a_j x_j = \sum_j b_j x_j \quad b_j = a_j + a_0 \]

Quadratic Model:

\[ y = \sum_{j=1}^{k} b_j x_j + \sum_{1 \leq j < l \leq k} b_{jl} x_j x_l \]

\[ x_j^2 = x_j(1 - \sum_{l \neq j} x_l) = x_j - \sum_{l \neq j} x_j x_l \]