4. Quadratic Models

- Empirical Models
- Steepest Ascent
- Two-Factor Curved Relationships
- First-Order Designs
- Second-Order Models
- Central Composite Designs
- Sequential Design Strategy
- Box and Behnken Designs
- Orthogonal Polynomials
Empirical Models$^a$

“All Models Are Wrong, Some Models are Useful”$^b$

Suppose that true but unknown relationship between a response $\eta$ and the factors Temperature ($T$), pressure ($P$) and concentration ($C$) was represented by the contour diagram a.

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$^a$BHH2e Chapter 11. $^b$George Box (1979);
Empirical Models

Experimental designs as a $2^3$ factorial design has been used expressed generically in a coded form.

$$x_1 = \pm 1, \quad x_2 = \pm 1, \quad x_3 = \pm 1$$

From the figure you see the Temperature $T$, pressure $P$ and concentration $C$ were coded by

$$x_1 = \frac{T - 172}{20}, \quad x_2 = \frac{P - 100}{25}, \quad x_3 = \frac{C - 36}{15}$$

Thus, $T = 172^\circ C$, $P = 100$ psi and $C = 36\%$ defines the center of the design where $x_1 = x_2 = x_3 = 0$. Suppose that running these experimental trials in random order leads to the fitted model

$$\hat{y} = 53 + 6x_1 - 5x_2 + 7x_3$$

The first-order approximation to the response $\eta$ could be adequate if the main objective was to gain general idea of what was happening in the experimental region and to discover the direction to improve the response. The approximating equation (1) is merely a local graduation function.
Trends and Steepest Ascent

In the fitted model

$$\hat{y} = 53 + 6x_1 - 5x_2 + 7x_3$$

(1)

$b_0 = 53$ is the response at the center of the design, and the first-order coefficients $b_1 = 6, b_2 = -5, b_3 = 7$ are the gradients or rates of change of $\hat{y}$ as $x_1, x_2, x_3$ change. These are the derivatives $\frac{\partial \eta}{\partial x_i}$.

A vector radiating from the center of the design that is normal (orthogonal, perpendicular) to the planar contours (fitted response) indicates the direction of the steepest ascent and its direction is determined by the relative values of the first-order coefficients $(6, -5, 7)$. In the general case of $k$ factors

$$\hat{y} = b_0 + b_1 x_1 + \cdots + b_k x_k$$

the steepest ascent direction is given by the vector

$$\frac{\partial \eta}{\partial x} = \left( \frac{\partial \eta}{\partial x_1}, \ldots, \frac{\partial \eta}{\partial x_k} \right)' = (b_1, \ldots, b_k)'$$
Runs on the Path of Steepest Ascent

In the fitted model

\[ \hat{y} = 53 + 6x_1 - 5x_2 + 7x_3 \]  

(1)

with scaling

\[ x_1 = \frac{T - 172}{20}, \quad x_2 = \frac{P - 100}{25}, \quad x_3 = \frac{C - 36}{15} \]

the steepest ascent path requires relative changes (assuming we are interested on increasing \( T \) by 20\(^\circ\)C):

<table>
<thead>
<tr>
<th>Changes in ( x )'s</th>
<th>Unit Conversion</th>
<th>Planned Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x_1 + 6 )</td>
<td>( T : +6 \times 20 = +120 )</td>
<td>( +120 / 6 = +20.0^\circ C )</td>
</tr>
<tr>
<td>( x_2 - 5 )</td>
<td>( P : -5 \times 25 = -125 )</td>
<td>( -125 / 6 = -20.8 ) psi</td>
</tr>
<tr>
<td>( x_3 + 7 )</td>
<td>( C : +7 \times 15 = +105 )</td>
<td>( -105 / 6 = +17.5% )</td>
</tr>
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</table>

Then, equal steps along the steepest ascent path would be

<table>
<thead>
<tr>
<th>Factor</th>
<th>Step 0</th>
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<th>Step 2</th>
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<tr>
<td>( T )</td>
<td>172</td>
<td>192.0</td>
<td>212.0</td>
</tr>
<tr>
<td>( P )</td>
<td>100</td>
<td>79.2</td>
<td>58.4</td>
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<tr>
<td>( C )</td>
<td>36</td>
<td>53.6</td>
<td>71.0</td>
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</table>
One-Factor Curved Relationships

Let the quadratic approximation to the true response $\eta$ be given by the second-order model

$$\hat{y} = b_0 + b_1 x_1 + b_{11} x_1^2$$

Then, the maximum value of the approximating curve is at $x^* = -b_1/2b_{11}$ with $\hat{y}_{\text{max}} = b_0 - b_1^2/4b_{11}$.

**Note:** Remember, such an approximation might be good locally but become inadequate over a larger range. In particular, the fitted quadratic approximation must fall away symmetrically on either side of its maximum.
Two-Factor Curved Relationships: Maxima, Stationary Regions and Related Phenomena

Sometimes the objective of experimentation is to find the levels of several factors that identify a region of greatest interest.

a) Smooth hill; b) Stationary ridge; c) rising (sloping) ridge; and d) minimax (saddle point).
Two-Factor Curved Relationships: Maxima, Stationary Regions and Related Phenomena

a) A maximum:
\[ \hat{y} = 83.69.4x_1 + 7.1x_2 - 7.4x_1^2 - 3.7x_2^2 - 5.8x_1x_2 \]

b) A stationary ridge:
\[ \hat{y} = 83.9+10.2x_1+5.6x_2-6.9x_1^2-2.0x_2^2-7.6x_1x_2 \]

c) A rising ridge
\[ \hat{y} = 82.7+8.8x_1+8.2x_2-7.0x_1^2-2.4x_2^2-7.6x_1x_2 \]

d) A minimax
\[ \hat{y} = 83.6+11.1x_1+4.1x_2-6.5x_1^2-0.4x_2^2-9.4x_1x_2 \]

In the case of \( k \) factors the characterization of the surfaces is done by canonical decomposition.
Experimental Designs

Consider some experimental designs appropriate for fitting the approximating models of first and second order. The problem is to find a pattern of experimental conditions \((x_1, \ldots, x_k)\) that explains the most about the response in the current region of interest.

First-Order Experimental Designs

Consider the first-order model

\[
y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon
\]

and its least squares estimate (LSE)

\[
\hat{y} = b_0 + b_1 x_1 + b_2 x_2
\]
First-Order Experimental Designs

The $2^3$ design, information surface, information contours, and rotatability.
Design Information Function

Since the design is orthogonal the estimated coefficients are distributed independently and so the variance of \( \hat{y} \)

\[
\text{var}(\hat{y}) = \text{var}(b_0) + x_1^2 \text{var}(b_1) + x_2^2 \text{var}(b_2)
\]

where \( \text{var}(b_0) = \text{var}(b_1) = \text{var}(b_2) = \sigma^2/4 \). Thus the standardized variance \( \text{var}(\hat{y})/\sigma^2 \) for \( \hat{y} \) is

\[
\frac{\text{var}(\hat{y})}{\sigma^2} = \frac{1}{4}(1 + x_1^2 + x_2^2) = \frac{1}{4}(1 + r^2)
\]

where \( r^2 = x_1^2 + x_2^2 \) is the distance of the point \((x_1, x_2)\) from the center of the design.

The quantity \( I(\hat{y}) \) defined by

\[
I(\hat{y}) = \frac{\sigma^2}{\text{var}(\hat{y})}
\]

is called the design information function.
Design Information Function

In the case of this example the it is seen that the information function is

\[ I(\hat{y}) = \frac{4}{1 + r^2} \]

The information surface generated by this equation-design is shown in figure c. For this design the information contours are circles for \( I(\hat{y}) = 1, 2, 3, 4 \). The information remains the same whatever the design orientation. The design is called a rotatable design.

A rotatable design in \( k \) factors the information will be constant for points at the same distance \( r \) from the center of the design where \( r = (x_1^2 + \cdots + x_k^2)^{1/2} \).
Second-Order Models

First-order models do not take account of curvature in the response. To do this, it is needed to fit a second-order model. For $k = 3$ factors

$$\hat{y} = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3 + b_{11} x_1^2 + b_{22} x_2^2 + b_{33} x_3^2 + b_{12} x_1 x_2 + b_{13} x_1 x_3 + b_{23} x_2 x_3$$
Central composite design

To estimate quadratic terms you can enhance an initial full factorial $2^3$ design adding six axial points of the *star* design in next figure. Suppose that a $2^3$ design is coded in the usual way with the vertices of the cube at $(\pm 1, \pm 1, \pm 1)$. Then, the axial points have coordinates $(\pm \alpha, 0, 0)$, $(0, \pm \alpha, 0)$ and $(0, 0, \pm \alpha)$. The center points have coordinates $(0, 0, 0)$. The resulting design is called *central composite design*. The choice of $\alpha$ depends on the number of factors $k$.

![Diagram of central composite design](image)

a) A $2^3$ design with center point; b) star; c) central composite design.
Percent of Yield Example

The effect of the yield example was studied as function of temperature ($T$), concentration ($C$) and reaction time ($t$).

\[
x_1 = \frac{T - 167}{5.0}, \quad x_2 = \frac{C - 27.5}{2.5}, \quad x_3 = \frac{t - 6.5}{1.5}
\]

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<th>run</th>
<th>x1</th>
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<th>x11</th>
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<td>-3.64</td>
<td>-0.98</td>
<td>1.82</td>
<td>60.6</td>
</tr>
</tbody>
</table>
Percent of yield example

After the full factorial $2^3$ (8 runs) part of the central composite design was run the fitted first-order models obtained was

$$\hat{y} = 55.6 + 1.76x_1 + 1.18x_2 - 0.01x_3 - 3.09x_1x_2 - 2.19x_1x_3 - 1.21x_2x_3$$

The star part of the design was run and a second-order model was fitted. From the initial analysis of the first 15 runs led to the confirmatory runs $(16, 17)$ and $(18, 19)$ chosen in a widely different conditions. The fitted model for the 19-run design was

$$\hat{y} = 58.78 + 1.90x_1 + 0.97x_2 + 1.06x_3 - 1.88x_1^2 - 0.69x_2^2 - 0.95x_3^2 - 2.71x_1x_2 - 2.17x_1x_3 - 1.24x_2x_3$$

<table>
<thead>
<tr>
<th>Analysis of Variance Table</th>
</tr>
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<tbody>
<tr>
<td>Response: $y$</td>
</tr>
<tr>
<td>Df</td>
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<tr>
<td>Second-order Model</td>
</tr>
<tr>
<td>Residuals</td>
</tr>
<tr>
<td>Total</td>
</tr>
<tr>
<td>F-ratio = 12.59 / 3.18 = 3.96</td>
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</tbody>
</table>
Percent of yield example

The authors recommend an $F$ greater than 4 times the tabulated significance value for the fitted model to be worth of analysis.

From the contour plots above it appears the existence of a ridge of alternated conditions giving a response close to 60. A fuller understanding of the system can be gained with by *canonical analysis*.
Sequential Design Strategy

First-Order Models. Steepest Ascent Step

If reasonably large estimates of the first-order coefficients were found, you might adapt a try-it-and-see policy and make one or two runs along the steepest ascent path, calculated from these first-order terms. For an ongoing investigation this policy is the preferred approach. But it is possible to check for the linearity before you venture.
A linear check
The quantity $q = \bar{y}_p - \bar{y}_0$ compares the average response $\bar{y}_0$ at the center of the design with the average response of the peripheral part of the fractional factorial design. If $q$ was large, that would suggest that the fitted response was likely curved. $q$ close to 0 would suggest that locally the response is linear or, less likely, that there is a minimax. Suppose that there are $n_p$ peripheral runs and $n_0$ center runs, then

$$\text{se}(q) = \sqrt{\frac{1}{n_p} + \frac{1}{n_0}}$$

C. Daniel called $q$ a measure of “droop” in the region of a minimum.

Adding a second half fraction
To gain further information, a second half fraction could be run as a second block completing the full $2^k$ design.

Adding axial points
If two-factor interactions are relatively large, the design could be further augmented by adding the star design.
Sequential design strategy

Sequential assembly of a design means any procedure where the choice of a further design increment depends upon previous data.

A $2^3$ system with center points and star: central composite.
Choosing $\alpha$ for a Central Composite Design

The choice of the distance $\alpha$ of the axial points from the center of the design involves 2 considerations:

- The nature of the desired information function $I(\hat{y})$. A spherical information function may be obtained by the proper choice of $\alpha$. Then, the design will be rotatable.
- Whether or not you want the cube part of the design and the axial part to be orthogonal blocks.

Orthogonal blocking ensures that in a sequential assembly an inadvertent shift in the level response between running the first part (cube) of the design and the second has no effect on the estimated effects. Suppose $n_c$ the number of runs in the cube and $n_{c0}$ the number of center points added to the first part of the design. Let $n_{\alpha}$ the number of axial points and $n_{\alpha0}$ and $k$ the number of factors.

- For rotatability: $\alpha = \sqrt{n_c}$
- For orthogonal blocking: $\alpha = k \sqrt{\frac{1+n_{\alpha0}/n_\alpha}{1+n_{c0}/n_c}}$
**Choosing $\alpha$ for a Central Composite Design**

<table>
<thead>
<tr>
<th></th>
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<th>$k = 4$</th>
<th>$k = 5^*$</th>
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$\alpha$ for rotatability

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$\alpha$ for orthogonal blocks

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* For $k = 5$ the $2^{5-1}_{IV}$ fraction is considered.
A Noncentral Composite Design

Production of a chemical used in car tires

First eight runs

Coefficients:

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Runs 1–8, 11–13

Coefficients:

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</table>

Stationary point:

\[
\frac{d\hat{y}}{dx} = 0 \implies x_{1s} = -0.53, \quad x_{2s} = -0.22, \quad x_{3s} = -1.32
\]
Box and Behnken Designs

Sometimes it is necessary or desirable that factors be run at only three levels. Box-Behnken designs are incomplete three-level factorials where the experimental points are specifically chosen to allow efficient estimation of the coefficients of a second-order model.

<table>
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<tr>
<th>Three factors</th>
<th>$x_1$</th>
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$^a$BHH2e Sec 11.3
Box and Behnken Designs

### Four factors

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### Five factors

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Box and Behnken Designs

Example \( k = 4 \)

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<th>x20</th>
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</table>

All Data

Fitted model

\[ \hat{y} = 90.7 + 2.1x_{10} - 2.7x_{20} + 1.9x_1 - 2.0x_2 + 1.1x_3 - 3.7x_4 - 1.4x_1^2 - 4.3x_2^2 - 2.2x_3^2 - 2.6x_4^2 - 1.7x_1x_2 - 3.8x_1x_3 + 1.0x_1x_4 - 1.7x_2x_3 - 2.6x_2x_4 - 4.3x_3x_4 \]

Analysis of Variance

<table>
<thead>
<tr>
<th></th>
<th>Df</th>
<th>Sum Sq</th>
<th>Mean Sq</th>
<th>F value</th>
<th>Pr(&gt;F)</th>
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<td>2.12</td>
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</tr>
</tbody>
</table>
Box and Behnken Designs

Example $k = 4$

Observations 10 and 13 removed

Fitted Model

$$\hat{y} = 91.2 + 2.1x_{10} - 3.8x_{20} + 2.6x_1 - 2.0x_2 + 1.1x_3 - 3.0x_4$$
$$-2.2x_1^2 - 3.9x_2^2 - 1.8x_3^2 - 3.4x_4^2$$
$$-1.7x_1x_2 - 3.8x_1x_3 - 1.5x_1x_4 - 1.7x_2x_3 - 2.7x_2x_4 - 4.3x_3x_4$$

Analysis of Variance

<table>
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<tr>
<th></th>
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Response: y
Orthogonal Polynomials

Laser-Assisted Manufacturing

*Problem:* The experiment dealt with the laser-assisted manufacturing of a thermoplastic composite. The experimental factor is laser power at 40, 50 and 60 watts. The response is bond strength of the composite measure by a short-beam-shear test.

<table>
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<th>Laser Power (w)</th>
<th>40</th>
<th>50</th>
<th>60</th>
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<tbody>
<tr>
<td></td>
<td>25.66</td>
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<td>35.66</td>
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</tbody>
</table>

\(^a\)Wu and Hamada (2000) Sec. 1.8
Orthogonal Polynomials

Laser-Assisted Manufacturing

Coefficients:

|            | Estimate | Std. Error | t value | Pr(>|t|) |
|------------|----------|------------|---------|----------|
| (Intercept)| 24.770   | 1.817      | 13.633  | 9.67e-06 |
| Power50    | 6.573    | 2.570      | 2.558   | 0.04301  |
| Power60    | 12.213   | 2.570      | 4.753   | 0.00315  |

Residual standard error: 3.147 on 6 degrees of freedom
Multiple R-Squared: 0.7905, Adjusted R-squared: 0.7206
F-statistic: 11.32 on 2 and 6 DF, p-value: 0.009198

Analysis of Variance Table

Response: strength

<table>
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<th>Mean Sq</th>
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<th>Pr(&gt;F)</th>
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<td>Total</td>
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<td>283.606</td>
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<td></td>
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</table>
Orthogonal Polynomials

Laser-Assisted Manufacturing

When the experimental factor is *quantitative* and the levels *equidistant* we can further investigate whether the factor has linear or quadratic effects over the response. In our example, we can decompose the 2 df of *Power* into *linear* and a *quadratic contrasts*.

**Contrast Vectors**

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<tr>
<td>Quadratic</td>
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<td>+1</td>
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**Design Matrices**

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<th>Orthogonal Polynomial</th>
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</thead>
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Orthogonal Polynomials

Laser-Assisted Manufacturing

Coefficients:

|            | Estimate | Std. Error | t value | Pr(>|t|) |
|------------|----------|------------|---------|----------|
| (Intercept)| 31.032   | 1.049      | 29.583  | 9.9e-08  |
| Power.L    | 8.636    | 1.817      | 4.753   | 0.00315  |
| Power.Q    | -0.381   | 1.817      | -0.210  | 0.84083  |

Residual standard error: 3.147 on 6 degrees of freedom
Multiple R-Squared: 0.7905,    Adjusted R-squared: 0.7206
F-statistic: 11.32 on 2 and 6 DF,  p-value: 0.009198

Analysis of Variance Table
Response: strength

<table>
<thead>
<tr>
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<th>Df</th>
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<th>F value</th>
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**Conclusion:** Factor *Power* has significant *linear* effect on the strength but not quadratic.
Orthogonal Polynomials

Coefficients of Orthogonal Contrast Vectors

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<td>1</td>
<td>1</td>
<td>+1</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$L^2$</td>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
</tbody>
</table>

where $k =$ number of factor levels; $P_i =$ contrast vector of the $i$th degree orthogonal polynomial; and $L^2$ the squared length for $P_i$.

The contrasts (polynomials) are orthogonal in the sense that $\sum c_{ui} c_{vi} = 0$.

For other applications of orthogonal polynomials in design of experiments see, e. g., Bisgaard and Steinberg (1997).