The Fitted Response Surface

Graph the fitted surface and its standard error: response.R
Predicted Yield

Response Surface Methods

Analyzing a Second-Order Response Surface
Response Surface Methods

Analyzing a Second-Order Response Surface
Standard Error

Time

Temperature

78 80 82 84 86 88 90 92

168 170 172 174 176 178 180 182

Response Surface Methods
Analyzing a Second-Order Response Surface
Finding the Optimum

Write the full quadratic model as

\[ \hat{y} = \hat{\beta}_0 + x'\hat{b} + x'\hat{B}x \]

where

\[ x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix}, \quad b = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix}, \quad \text{and} \quad B = \begin{bmatrix} \hat{\beta}_{1,1} & \frac{1}{2}\hat{\beta}_{1,2} & \ldots & \frac{1}{2}\hat{\beta}_{1,k} \\ \frac{1}{2}\hat{\beta}_{1,2} & \hat{\beta}_{2,2} & \ldots & \frac{1}{2}\hat{\beta}_{2,k} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{2}\hat{\beta}_{1,k} & \frac{1}{2}\hat{\beta}_{2,k} & \ldots & \hat{\beta}_{k,k} \end{bmatrix}. \]

The location of the stationary point (maximum, minimum, or saddle-point) is

\[ x_s = -\frac{1}{2}B^{-1}b. \]
In the example

```r
l <- lm(y ~ x1 + x2 + I(x1^2) + I(x2^2) + x1:x2, t11d6)
lc <- coefficients(l)
b <- lc[2:3]
B <- matrix(c(lc[4], lc[6]/2, lc[6]/2, lc[5]), 2, 2)
cat("Stationary point:", -solve(B, b) / 2, "\n")
```

Output

Stationary point: 0.3892304 0.3058466

In engineering units:

\[
\begin{align*}
\xi_1 &= 85 + 5 \times 0.3892304 = 86.94615, \\
\xi_2 &= 175 + 5 \times 0.3058466 = 176.5292.
\end{align*}
\]
We want to round these, but how much?

- 87 and 177?
- 85 and 175?
We can test the hypothesis that the stationary point is $x^{(0)}$: 

- the general quadratic with a stationary point at $x^{(0)}$ is 

$$y = \beta^*_0 + \beta^*_{1,1} \left( x_1 - x_1^{(0)} \right)^2 + \beta^*_{2,2} \left( x_2 - x_2^{(0)} \right)^2$$

$$+ \beta^*_{1,2} \left( x_1 - x_1^{(0)} \right) \left( x_2 - x_2^{(0)} \right) + \epsilon;$$

- fit this as a reduced model, and compare with the full model using the extra sum of squares;

- reduced model has 4 parameters versus 6 in the full model, so test statistic is $F_{2,n-p}$.

Test specific values, or graph the statistic for a grid of values.
Test whether 87, 177 is optimal

\[ x_{10} <- (87 - 85) / 5 \]
\[ x_{20} <- (177 - 175) / 5 \]
\[
\text{summary(aov(y ~ I((x1 - x10)^2) + I((x2 - x20)^2) +}
\text{I((x1 - x10)*(x2 - x20)) + x1 + x2, t11d6))}
\]

Output

<table>
<thead>
<tr>
<th>Df</th>
<th>Sum Sq</th>
<th>Mean Sq</th>
<th>F value</th>
<th>Pr(&gt;F)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I((x1 - x10)^2)</td>
<td>1</td>
<td>18.901</td>
<td>18.901</td>
<td>266.553</td>
</tr>
<tr>
<td>I((x2 - x20)^2)</td>
<td>1</td>
<td>8.681</td>
<td>8.681</td>
<td>122.423</td>
</tr>
<tr>
<td>I((x1 - x10) * (x2 - x20))</td>
<td>1</td>
<td>0.526</td>
<td>0.526</td>
<td>7.415</td>
</tr>
<tr>
<td>x1</td>
<td>1</td>
<td>0.004</td>
<td>0.004</td>
<td>0.057</td>
</tr>
<tr>
<td>x2</td>
<td>1</td>
<td>0.134</td>
<td>0.134</td>
<td>1.895</td>
</tr>
<tr>
<td>Residuals</td>
<td>7</td>
<td>0.496</td>
<td>0.071</td>
<td></td>
</tr>
</tbody>
</table>

---

Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1

\[ F = ((0.004 + 0.134)/2)/0.071 = 0.97, \quad P \approx .5, \quad \text{do not reject} \quad H_0. \]
We can test the same hypothesis without fitting the reduced model:

- the model is

\[ \hat{y}(x_1, x_2) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{1,1} x_1^2 + \beta_{1,2} x_1 x_2 + \beta_{2,2} x_2^2; \]

- so

\[ \frac{\partial \hat{y}}{\partial x_1} = \beta_1 + 2\beta_{1,1} x_1 + \beta_{1,2} x_2, \]

\[ \frac{\partial \hat{y}}{\partial x_2} = \beta_2 + 2\beta_{2,2} x_2 + \beta_{1,2} x_1. \]

So the hypothesis is equivalent to

\[ \beta_1 + 2\beta_{1,1} x_1^{(0)} + \beta_{1,2} x_2^{(0)} = 0, \]

\[ \beta_2 + 2\beta_{2,2} x_2^{(0)} + \beta_{1,2} x_1^{(0)} = 0. \]
That is, $L \left( x^{(0)} \right) \beta = 0$, where

$$L \left( x^{(0)} \right) = \begin{bmatrix} 0 & 1 & 0 & 2x_1^{(0)} & x_2^{(0)} & 0 \\ 0 & 0 & 1 & 0 & x_1^{(0)} & 2x_2^{(0)} \end{bmatrix}$$

and

$$\beta = (\beta_0, \beta_1, \beta_2, \beta_{1,1}, \beta_{1,2}, \beta_{2,2})'.$$

Any hypothesis of this form can be tested as follows:

$$SS_L = (L\hat{\beta})' \left[ L(X'X)^{-1}L' \right]^{-1} (L\hat{\beta})$$

is the sum of squares associated with the hypothesis, $MS_L = SS_L/2$ is the mean square, and $F = MS_L/MS_E$ is the test statistic.
R commands

```
betaHat <- coefficients(l)
V <- summary(l)$cov.unscaled
msE <- summary(l)$sigma^2
L <- rbind(c(0, 1, 0, 2 * x10, 0, x20),
           c(0, 0, 1, 0, 2 * x20, x10))
LbetaHat <- L %*% betaHat
ssL <- sum(LbetaHat * solve(L %*% V %*% t(L), LbetaHat))
msL <- ssL / 2
F <- msL / msE
```

We can calculate $F$ for a grid of $x^{(0)}$ values and graph it.

The region where $F < F_{2,n-p}(\alpha)$ is a $100(1 - \alpha)\%$ confidence region for the optimal settings.
F−Statistic

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F–Statistic Detail

Response Surface Methods
Analyzing a Second-Order Response Surface
We *can* round to 87 and either 176 or 177.

We *cannot* round to 85 and 175.