# $2^2$ Factorial Analysis

Can we find which terms are important?

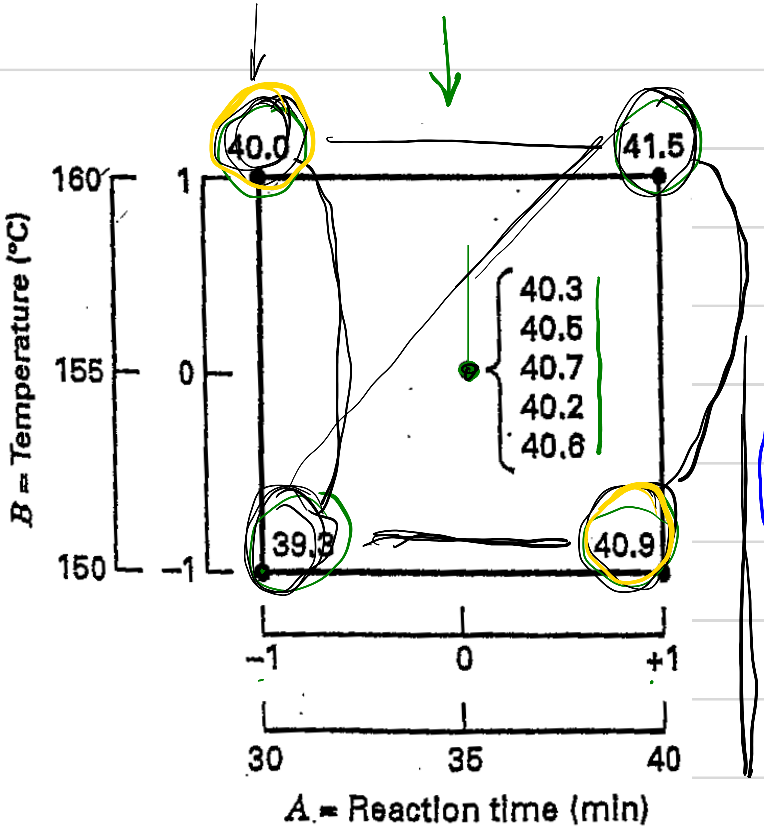
What will be the first-order model?

Will a first-order model be appropriate?

First order model, $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cancel{\beta_{12} x_1 x_2}^{\,0} + \varepsilon$

Obs

predicted, $\boxed{\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2}$




| Natural Variables | | Coded Variables | | Response |
|---|---|---|---|---|
| $\xi_1$ | $\xi_2$ | $x_1$ | $x_2$ | $y$ |
| 30 | 150 | −1 | −1 | 39.3 |
| 30 | 160 | −1 | 1 | 40.0 |
| 40 | 150 | 1 | −1 | 40.9 |
| 40 | 160 | 1 | 1 | 41.5 |
| 35 | 155 | 0 | 0 | 40.3 |
| 35 | 155 | 0 | 0 | 40.5 |
| 35 | 155 | 0 | 0 | 40.7 |
| 35 | 155 | 0 | 0 | 40.2 |
| 35 | 155 | 0 | 0 | 40.6 |

First let's find out (DIY)

$\beta_0, \beta_1, \beta_2, \beta_{12}$

$\beta_0 = \left(\frac{39.3 + 40 + 40.9 + 41.5}{4}\right)$

$= 40.425$

$\beta_1 = \frac{1}{2}(-39.3 - 40.0 + 40.9 + 41.5)$

$= 1.55$

$\beta_2 = \frac{1}{2}(-39.3 + 40 - 40.9 + 41.5)$

$= 0.65$

$\beta_{12} = -0.05$

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

?

can we reduce this to a 1-order model

$$+ \left(\beta_{11} x_1^2 + \beta_{22} x_2^2\right)$$

$SS_T$ , $SS_{mean}$

ANOVA TABLE

| | DF | SS | MS | $F_0$ |
|---|---|---|---|---|
| Total | 9 | | | |
| $x_1$ | 1 | 2.4025 | | 55.87 |
| $x_2$ | 1 | 0.4225 | | 9.83 |
| $x_1 x_2$ | 1 | 0.0025 | | 0.06 |
| mean | 1 | | | |
| $\varepsilon$ | 5-1 | 0.172 | | |
| and | 1 | ? | | |

$$SS_{x_1} = 2\left( (39.65 - 40.425)^2 + (41.2 - 40.425)^2 \right)$$

$$SS_{x_2} = 2\left( (40.1 - 40.425)^2 + (40.75 - 40.425)^2 \right)$$

$$SS_{x_1 x_2} = 2\left( (40.45 - 40.425)^2 + (40.9 - 40.2425)^2 \right)$$

$$= 0.0025$$

$$\varepsilon = (y_1 - \bar{y}_c)^2 + (y_2 - \bar{y}_c)^2 + \cdots + (y_5 - \bar{y}_c)^2$$

$$= (40.3 - 40.46)^2 + (\quad)^2 + \cdots + (40.6 - 40.46)^2$$

$$=$$

Find $SS_{quad} = \frac{n_F n_c (\bar{y}_F - \bar{y}_c)^2}{n_F + n_c} = \frac{4 \times 5 (40.425 - 40.46)^2}{9}$

Another check of the adequacy of the straight-line model is obtained by applying the check for pure quadratic curvature effect described in Section 6-6. Recall that this consists of comparing the average response at the four points in the factorial portion of the design, say $\bar{y}_F = 40.425$, with the average response at the design center, say $\bar{y}_C = 40.46$. If there is quadratic curvature in the true response function, then $\bar{y}_F - \bar{y}_C$ is a measure of this curvature. If $\beta_{11}$ and $\beta_{22}$ are the coefficients of the "pure quadratic" terms $x_1^2$ and $x_2^2$, then $\bar{y}_F - \bar{y}_C$ is an estimate of $\beta_{11} + \beta_{22}$. In our example, an estimate of the pure quadratic term is

$$\begin{aligned}\hat{\beta}_{11} + \hat{\beta}_{22} &= \bar{y}_F - \bar{y}_C \\ &= 40.425 - 40.46 \\ &= -0.035\end{aligned}$$

$\frac{0.325}{0.775} = 0.42$

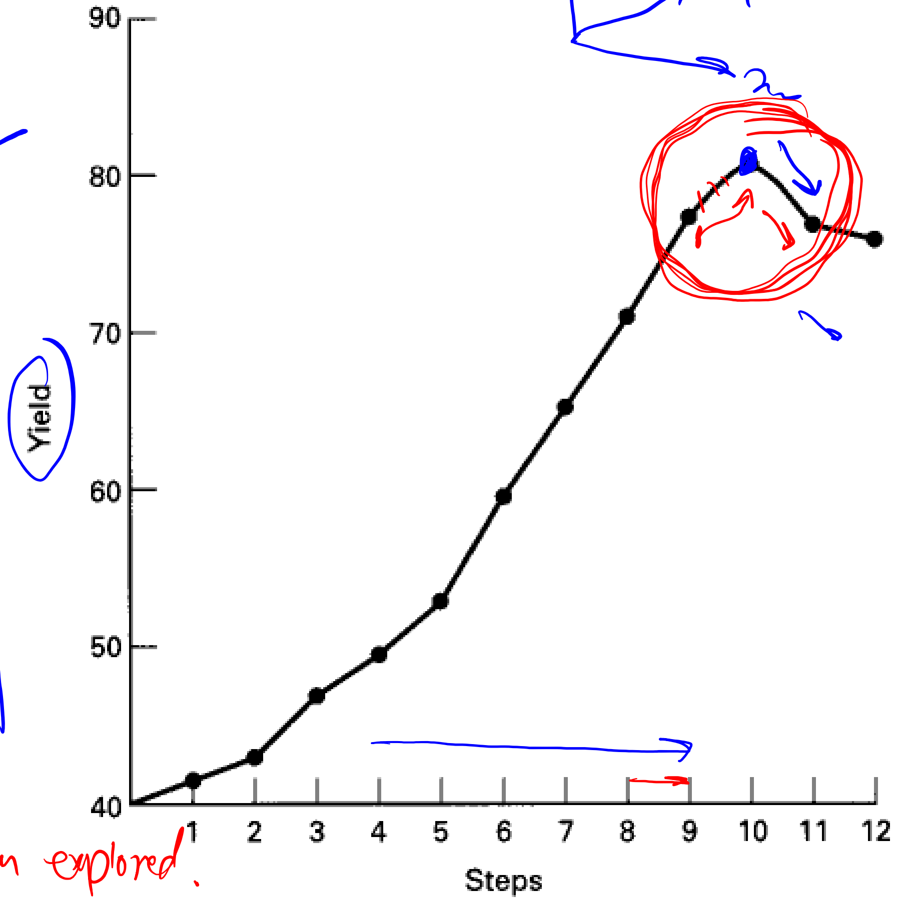
$$\hat{y} = 40.44 + 0.775x_1 + 0.325x_2$$

Only applicable in region explored.

note that $\hat{y} = f(x_1, x_2)$ is a plane

**Table 11-3** Steepest Ascent Experiment for Example 11-1

| Steps | Coded Variables $x_1$ | Coded Variables $x_2$ | Natural Variables $\xi_1$ | Natural Variables $\xi_2$ | Response $y$ |
|---|---|---|---|---|---|
| Origin | 0 | 0 | 35 | 155 | 40.44 |
| Δ | 1.00 | 0.42 | 5 | 2 | |
| Origin + Δ | 1.00 | 0.42 | 40 | 157 | 41.0 |
| Origin + 2Δ | 2.00 | 0.84 | 45 | 159 | 42.9 |
| Origin + 3Δ | 3.00 | 1.26 | 50 | 161 | 47.1 |
| Origin + 4Δ | 4.00 | 1.68 | 55 | 163 | 49.7 |
| Origin + 5Δ | 5.00 | 2.10 | 60 | 165 | 53.8 |
| Origin + 6Δ | 6.00 | 2.52 | 65 | 167 | 59.9 |
| Origin + 7Δ | 7.00 | 2.94 | 70 | 169 | 65.0 |
| Origin + 8Δ | 8.00 | 3.36 | 75 | 171 | 70.4 |
| Origin + 9Δ | 9.00 | 3.78 | 80 | 173 | 77.6 |
| Origin + 10Δ | 10.00 | 4.20 | 85 | 175 | 80.3 |
| Origin + 11Δ | 11.00 | 4.62 | 90 | 179 | 76.2 |
| Origin + 12Δ | 12.00 | 5.04 | 95 | 181 | 75.1 |




**New model needs to be employed around [85, 175]**

they are outside the region you explored.

# New Region of Exploration

Table 11-4 Data for Second First-Order Model

| Natural Variables | | Coded Variables | | Response |
|---|---|---|---|---|
| $\xi_1$ | $\xi_2$ | $x_1$ | $x_2$ | $y$ |
| 80 | 170 | −1 | −1 | 76.5 |
| 80 | 180 | −1 | 1 | 77.0 |
| 90 | 170 | 1 | −1 | 78.0 |
| 90 | 180 | 1 | 1 | 79.5 |
| 85 | 175 | 0 | 0 | 79.9 |
| 85 | 175 | 0 | 0 | 80.3 |
| 85 | 175 | 0 | 0 | 80.0 |
| 85 | 175 | 0 | 0 | 79.7 |
| 85 | 175 | 0 | 0 | 79.8 |

$$\hat{y} = 78.97 + 1.00x_1 + 0.50x_2$$

Table 11-5 Analysis of Variance for the Second First-Order Model

| Source of Variation | Sum of Squares | Degrees of Freedom | Mean Square | $F_0$ |
|---|---|---|---|---|
| Regression | 5.00 | 2 | | |
| Residual | 11.1200 | 6 | | |
| (Interaction) | (0.2500) | 1 | 0.2500 | 4.72 |
| (Pure quadratic) | (10.6580) | 1 | 10.6580 | 201.09 |
| (Pure error) | (0.2120) | 4 | 0.0530 | |
| Total | 16.1200 | 8 | | |

**What does the ANOVA table tell us?**

**Second-order terms are significant. There is a curvature in this region. First order model NOT good enough.**

# General Algorithm

we notice that the *path of steepest ascent is proportional to the signs and magnitudes of the regression coefficients* in the fitted first-order model

$$\hat{y} = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i$$

It is easy to give a general algorithm for determining the coordinates of a point on the path of steepest ascent. Assume that the point $x_1 = x_2 = \ldots = x_k = 0$ is the base or origin point. Then

1. Choose a step size in one of the process variables, say $\Delta x_j$. Usually, we would select the variable we know the most about, or we would select the variable that has the largest absolute regression coefficient $|\hat{\beta}_j|$.

2. The step size in the other variables is

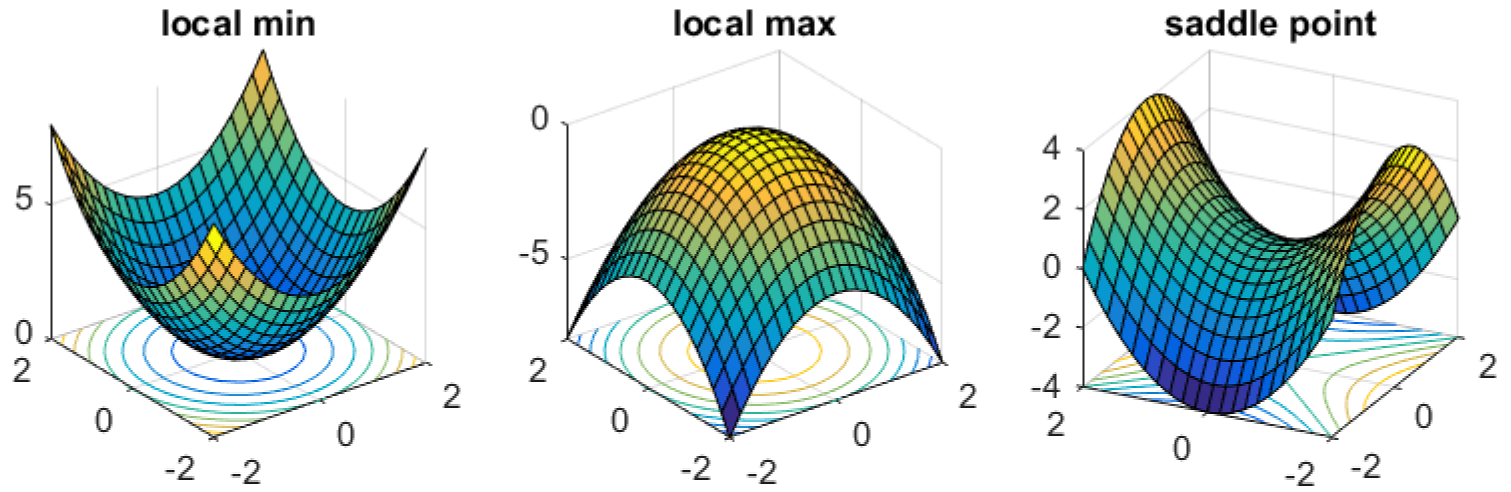
$$\Delta x_i = \frac{\hat{\beta}_i}{\hat{\beta}_j / \Delta x_j} \qquad i = 1, 2, \ldots, k; \qquad i \neq j$$

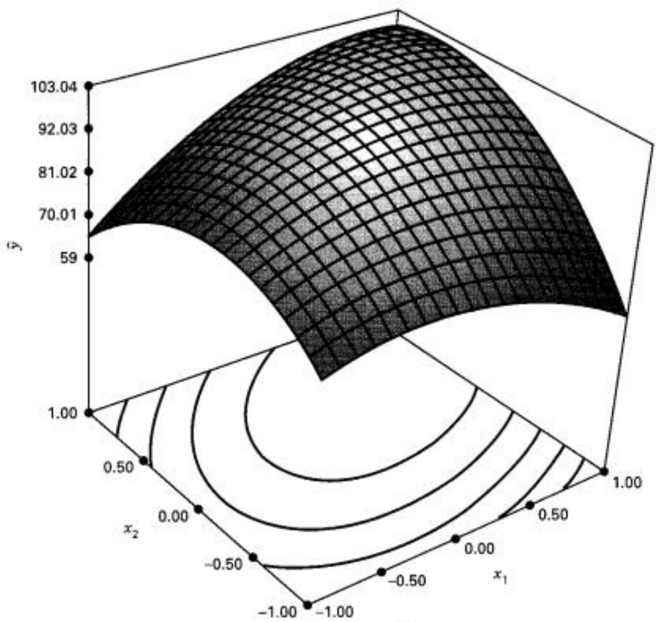
3. Convert the $\Delta x_i$ from coded variables to the natural variables.

# Analysis of Second Order Response Surface

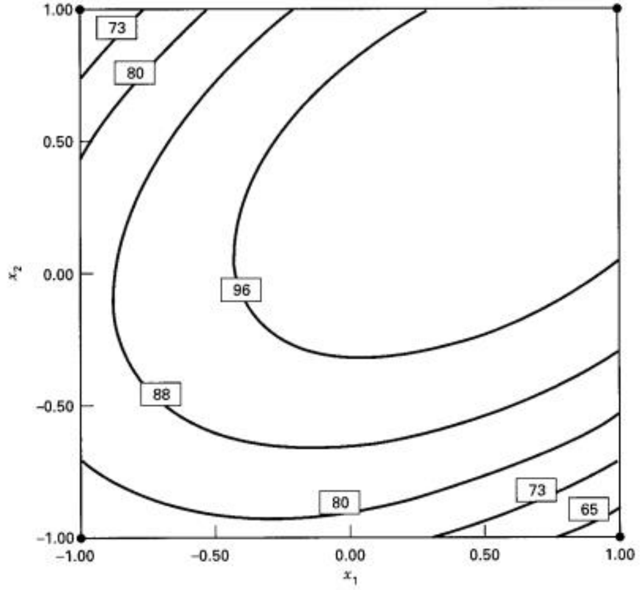
$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum\sum_{i<j} \beta_{ij} x_i x_j + \epsilon$$

- Suppose we want to find the levels of $x_1, x_2, x_3, \ldots, x_k$ that optimize the predicted response
- If such an optimum point exists, then at that point, $\frac{\partial \hat{y}}{\partial x_1} = \frac{\partial \hat{y}}{\partial x_2} = \frac{\partial \hat{y}}{\partial x_3} = \ldots = \frac{\partial \hat{y}}{\partial x_k} = 0$
- This point, say, $x_{1s}, x_{2s}, x_{3s}, \ldots, x_{ks}$ is called a 'stationary point'
- Stationary point could represent a point of maximum response, or minimum response or saddle point.

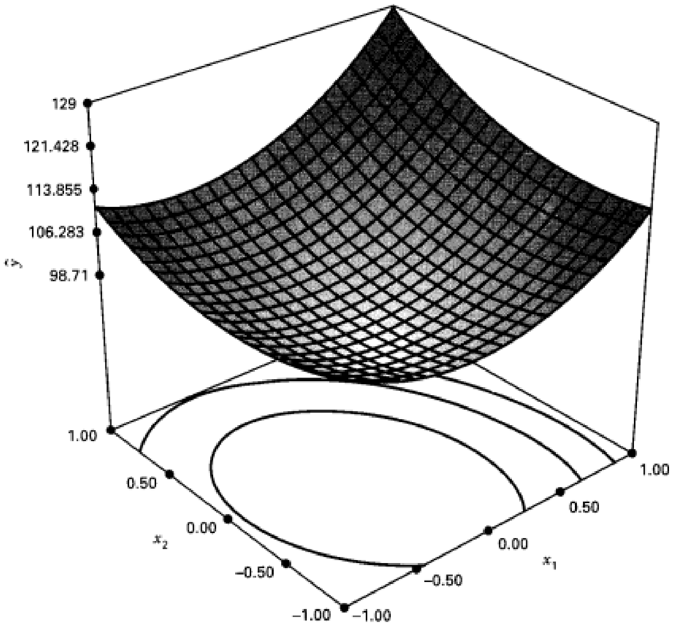




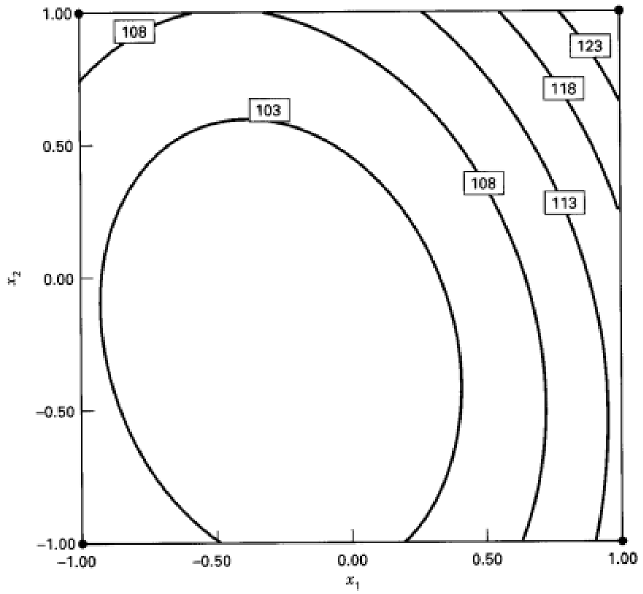

(a) Response surface



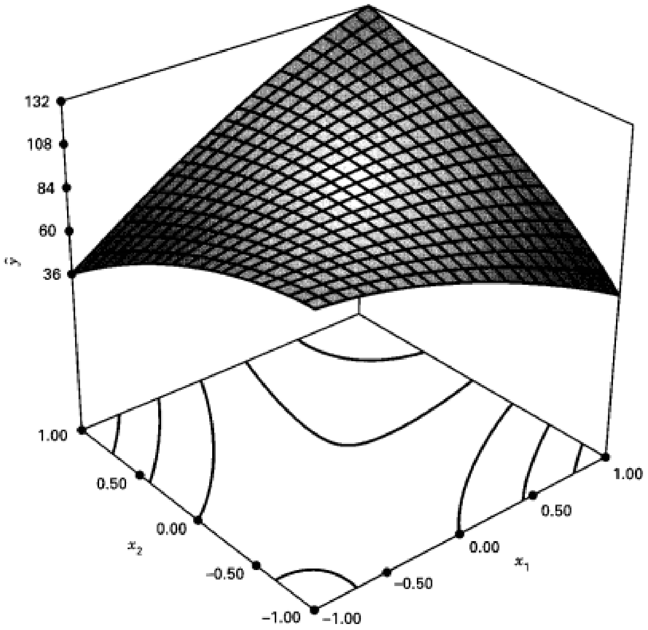

(b) Contour plot



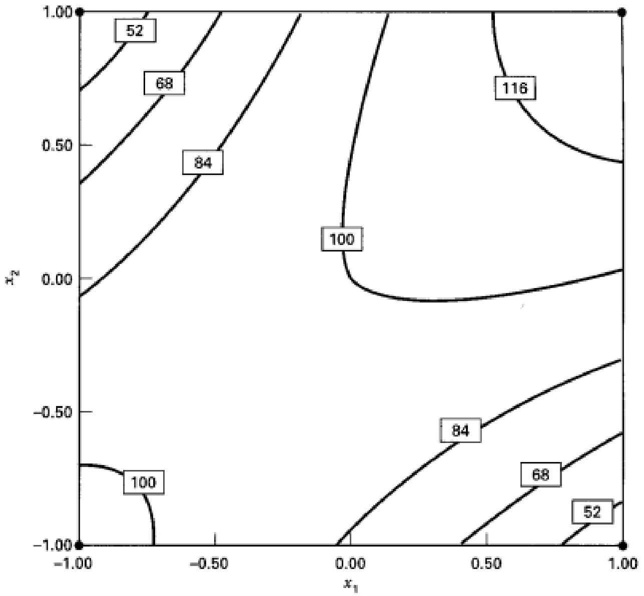

(a) Response surface




(b) Contour plot




(a) Response surface




(b) Contour plot

# Finding the Stationary Point

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j}\sum \beta_{ij} x_i x_j + \epsilon$$

We may obtain a general mathematical solution for the location of the stationary point. Writing the second-order model in matrix notation, we have

$$\hat{y} = \hat{\beta}_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x} \tag{11-5}$$

where

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix}_{k\times 1} \quad \mathbf{b} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix}_{k\times 1} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} \hat{\beta}_{11}, & \hat{\beta}_{12}/2, & \ldots, & \hat{\beta}_{1k}/2 \\ & \hat{\beta}_{22}, & \ldots, & \hat{\beta}_{2k}/2 \\ & & \ddots & \\ \text{sym.} & & & \hat{\beta}_{kk} \end{bmatrix}_{k\times k}$$

That is, $\mathbf{b}$ is a $(k \times 1)$ vector of the first-order regression coefficients and $\mathbf{B}$ is a $(k \times k)$ symmetric matrix whose main diagonal elements are the *pure* quadratic coefficients $(\hat{\beta}_{ii})$ and whose off-diagonal elements are one-half the *mixed* quadratic coefficients $(\hat{\beta}_{ij}, i \neq j)$. The derivative of $\hat{y}$ with respect to the elements of the vector $\mathbf{x}$ equated to $\mathbf{0}$ is

$$\frac{\partial \hat{y}}{\partial \mathbf{x}} = \mathbf{b} + 2\mathbf{B}\mathbf{x} = \mathbf{0} \tag{11-6}$$

The stationary point is the solution to Equation 11-6, or

$$\boxed{\mathbf{x}_s = -\tfrac{1}{2}\mathbf{B}^{-1}\mathbf{b}} \tag{11-7}$$

Furthermore, by substituting Equation 11-7 into Equation 11-5, we can find the predicted response at the stationary point as

$y$ at $x_s$ $\Rightarrow$

$$\hat{y}_s = \hat{\beta}_0 + \tfrac{1}{2}\mathbf{x}_s'\mathbf{b} \tag{11-8}$$

$x' = x^T$

$$\hat{y} = \hat{\beta}_0 + \sum \hat{\beta}_i x_i + \sum \hat{\beta}_{ii} x_i^2 + \sum\sum \hat{\beta}_{ij} x_i x_j$$

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \hat{\beta}_{12} x_1 x_2 + \hat{\beta}_{11} x_1^2 + \hat{\beta}_{22} x_2^2$$

$$\hat{y} = \hat{\beta}_0 + \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T_{1\times 2} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix}_{2\times 1} + \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T_{1\times 2} \begin{bmatrix} \beta_{11} & \beta_{12}/2 \\ \beta_{12}/2 & \beta_{22} \end{bmatrix}_{2\times 2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{2\times 1}$$

$$= \hat{\beta}_0 + [x_1 \; x_2]\begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + [x_1 \; x_2]\Big( \quad \Big)\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

We know that, at stationary point

$$\frac{\partial \hat{y}}{\partial x_i} = 0 \quad \text{at} \quad x = x_s$$

$$\boxed{x_s = -\frac{1}{2} B^{-1} b}$$

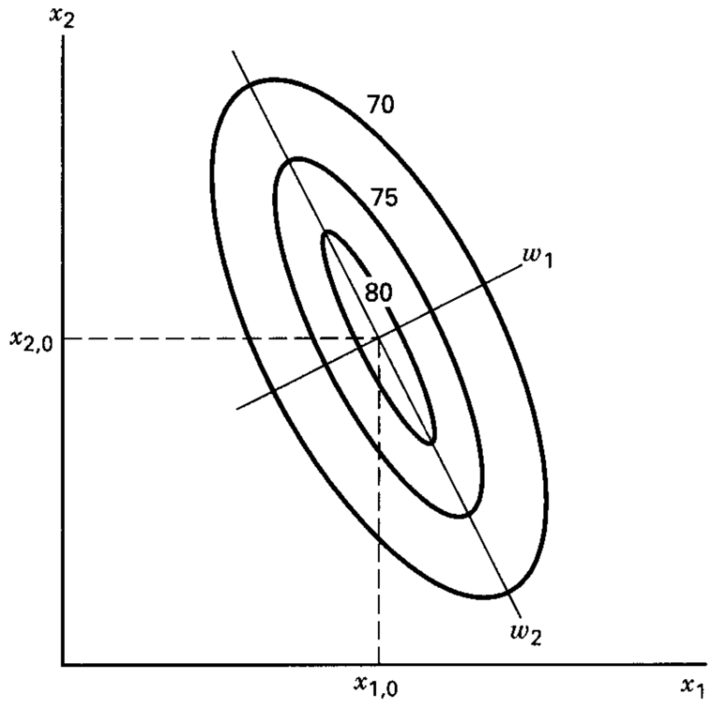
$x = x_s \rightarrow$ 11.5

# Characterizing the Response Surface

- Once we find the stationary point ($x_s$), we would like to characterize the response surface near it – to find out whether that point is maximum, minimum or a saddle
- How can we do that? – by finding the relative sensitivity of the response to $x_1, x_2, x_3, \ldots, x_k$
- This can be done by examining the contour plot – easy if there are only 2/3 independent variables
- What to do when there are more variables? -> **"Canonical Analysis"**

## Canonical Analysis

- To characterize the region near $x_s$,
  1. We shift our origin to xs, and
  2. Rotate our axes until they are parallel to the principal axes of the fitted response surface



# Canonical Form

- After the transformation, we can show that the original equation of the surface

Change of variable

$x_i \rightarrow w_i$

?

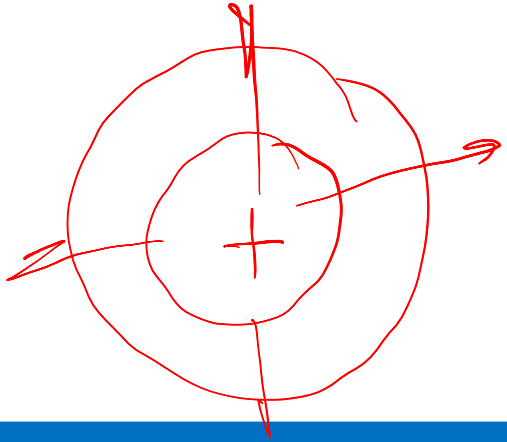
$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum\sum_{i<j} \beta_{ij} x_i x_j \quad = \hat{\beta}_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x} \qquad (1)$$

takes the form of

$$\hat{y} = \hat{y}_s + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \cdots + \lambda_k w_k^2 \qquad (2)$$

Canonical Form of Eq (1)

- Here, $w_i$ are the new (transformed) independent variables, and $\lambda_i$ are the constants
- This is called 'Canonical Form' of the model.
- $\lambda_i$ are the eigen values of matrix **B**

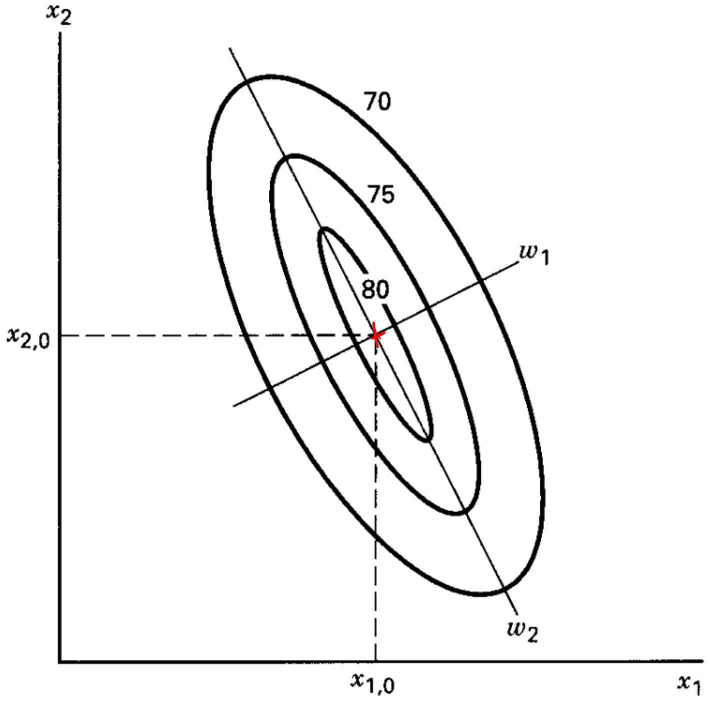


$$\mathbf{B} = \begin{bmatrix} \hat{\beta}_{11}, & \hat{\beta}_{12}/2, \ldots, & \hat{\beta}_{1k}/2 \\ & \hat{\beta}_{22}, \ldots, & \hat{\beta}_{2k}/2 \\ & \ddots & \\ \text{sym.} & & \hat{\beta}_{kk} \end{bmatrix}$$

$k \times k$

# Characterization using Canonical Form

The nature of the response surface can be determined from the stationary point and the *signs* and *magnitudes* of the $\{\lambda_i\}$. First, suppose that the stationary point is within the region of exploration for fitting the second-order model. If the $\{\lambda_i\}$ are all positive, $\mathbf{x}_s$ is a point of minimum response; if the $\{\lambda_i\}$ are all negative, $\mathbf{x}_s$ is a point of maximum response; and if the $\{\lambda_i\}$ have different signs, $\mathbf{x}_s$ is a saddle point. Furthermore, the surface is steepest in the $w_i$ direction for which $|\lambda_i|$ is the greatest. For example, Figure 11-9 depicts a system for which $\mathbf{x}_s$ is a maximum ($\lambda_1$ and $\lambda_2$ are negative) with $|\lambda_1| > |\lambda_2|$.



# Example

We will continue the analysis of the chemical process in Example 11-1. A second-order model in the variables $x_1$ and $x_2$ cannot be fit using the design in Table 11-4. The experimenter decides to augment this design with enough points to fit a second-order model.[1] She obtains four observations at ($x_1 = 0$, $x_2 = \pm 1.414$) and ($x_1 = \pm 1.414$, $x_2 = 0$). The complete experiment is shown in Table 11-6 (page 442), and the design is displayed in Figure 11-10 (on the next page). This design is called a **central composite design** (or a CCD)

$$x_1 = \frac{\xi_1 - 85}{5} \qquad x_2 = \frac{\xi_2 - 175}{5}$$

time temp

Time, Temp

| Natural Variables | | Coded Variables | | Responses | | |
|---|---|---|---|---|---|---|
| $\xi_1$ | $\xi_2$ | $x_1$ | $x_2$ | $y_1$ (yield) | $y_2$ (viscosity) | $y_3$ (molecular weight) |
| 80 | 170 | −1 | −1 | 76.5 | 62 | 2940 |
| 80 | 180 | −1 | 1 | 77.0 | 60 | 3470 |
| 90 | 170 | 1 | −1 | 78.0 | 66 | 3680 |
| 90 | 180 | 1 | 1 | 79.5 | 59 | 3890 |
| 85 | 175 | 0 | 0 | 79.9 | 72 | 3480 |
| 85 | 175 | 0 | 0 | 80.3 | 69 | 3200 |
| 85 | 175 | 0 | 0 | 80.0 | 68 | 3410 |
| 85 | 175 | 0 | 0 | 79.7 | 70 | 3290 |
| 85 | 175 | 0 | 0 | 79.8 | 71 | 3500 |
| 92.07 | 175 | 1.414 | 0 | 78.4 | 68 | 3360 |
| 77.93 | 175 | −1.414 | 0 | 75.6 | 71 | 3020 |
| 85 | 182.07 | 0 | 1.414 | 78.5 | 58 | 3630 |
| 85 | 167.93 | 0 | −1.414 | 77.0 | 57 | 3150 |

# Example: Second Order Model

**Final Equation in Terms of Coded Factors:**

$$\begin{aligned} \text{yield} = \\ &+79.94 \\ &+0.99 * A \\ &+0.52 * B \\ &-1.38 * A^2 \\ &-1.00 * B^2 \\ &+0.25 * A * B \end{aligned}$$

**Final Equation in Terms of Actual Factors:**

$$\begin{aligned} \text{yield} = \\ &-1430.52285 \\ &+7.80749 * \text{time} \\ &+13.27053 * \text{temp} \\ &-0.055050 * \text{time}^2 \\ &-0.040050 * \text{temp}^2 \\ &+0.010000 * \text{time} * \text{temp} \end{aligned}$$

Response: yield

ANOVA for Response Surface Quadratic Model

Analysis of variance table [Partial sum of squares]

| Source | Sum of Squares | DF | Mean Square | F Value |
|---|---|---|---|---|
| Model | 28.25 | 5 | 5.65 | 79.85 |
| *A* | *7.92* | *1* | *7.92* | *111.93* |
| *B* | *2.12* | *1* | *2.12* | *30.01* |
| *$A^2$* | *13.18* | *1* | *13.18* | *186.22* |
| *$B^2$* | *6.97* | *1* | *6.97* | *98.56* |
| *AB* | *0.25* | *1* | *0.25* | *3.53* |
| Residual | 0.50 | 7 | 0.071 | |
| *Lack of Fit* | *0.28* | *3* | *0.094* | *1.78* |
| *Pure Error* | *0.21* | *4* | *0.053* | |
| Cor Total | 28.74 | 12 | | |

**How do we find the stationary point?**

$$y = \underbrace{\beta_0}_{79.94} + \underbrace{\beta_1}_{0.99} x_1 + \underbrace{\beta_2}_{0.52} x_2 + \underbrace{\beta_{11}}_{-1.38} x_1^2 + \underbrace{\beta_{22}}_{-1.00} x_2^2 + \underbrace{\beta_{12}}_{0.25} x_1 x_2$$

# Example: Stationary Point

We may obtain a general mathematical solution for the location of the stationary point. Writing the second-order model in matrix notation, we have

$$\hat{y} = \hat{\beta}_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x} \tag{11-5}$$

where

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} \qquad \text{and} \qquad \mathbf{B} = \begin{bmatrix} \hat{\beta}_{11}, & \hat{\beta}_{12}/2, \ldots, & \hat{\beta}_{1k}/2 \\ & \hat{\beta}_{22}, \ldots, & \hat{\beta}_{2k}/2 \\ & & \ddots \\ \text{sym.} & & \hat{\beta}_{kk} \end{bmatrix}$$

That is, $\mathbf{b}$ is a $(k \times 1)$ vector of the first-order regression coefficients and $\mathbf{B}$ is a $(k \times k)$ symmetric matrix whose main diagonal elements are the *pure* quadratic coefficients $(\hat{\beta}_{ii})$ and whose off-diagonal elements are one-half the *mixed* quadratic coefficients $(\hat{\beta}_{ij}, i \neq j)$. The derivative of $\hat{y}$ with respect to the elements of the vector $\mathbf{x}$ equated to $\mathbf{0}$ is

$$\frac{\partial \hat{y}}{\partial \mathbf{x}} = \mathbf{b} + 2\mathbf{B}\mathbf{x} = \mathbf{0} \tag{11-6}$$

The stationary point is the solution to Equation 11-6, or

$$\mathbf{x}_s = -\tfrac{1}{2}\mathbf{B}^{-1}\mathbf{b} \tag{11-7}$$

Furthermore, by substituting Equation 11-7 into Equation 11-5, we can find the predicted response at the stationary point as

$$\hat{y}_s = \hat{\beta}_0 + \tfrac{1}{2}\mathbf{x}_s'\mathbf{b} \tag{11-8}$$

**Final Equation in Terms of Coded Factors:**

yield =
+79.94
+0.99 * A
+0.52 * B
−1.38 * $A^2$
−1.00 * $B^2$
+0.25 * A * B

**Final Equation in Terms of Actual Factors:**

yield =
−1430.52285
+7.80749 * time
+13.27053 * temp
−0.055050 * $\text{time}^2$
−0.040050 * $\text{temp}^2$
+0.010000 * time * temp

$$\mathbf{b} = \begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} -1.376 & 0.1250 \\ 0.1250 & -1.001 \end{bmatrix}$$

and from Equation 11-7 the stationary point is

$$\mathbf{x}_s = -\tfrac{1}{2}\mathbf{B}^{-1}\mathbf{b}$$

$$= -\tfrac{1}{2}\begin{bmatrix} -0.7345 & -0.0917 \\ -0.0917 & -1.0096 \end{bmatrix}\begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} = \begin{bmatrix} 0.389 \\ 0.306 \end{bmatrix}$$

# Example: Stationary Point

We may obtain a general mathematical solution for the location of the stationary point. Writing the second-order model in matrix notation, we have

$$\hat{y} = \hat{\beta}_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x} \tag{11-5}$$

where

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} \qquad \text{and} \qquad \mathbf{B} = \begin{bmatrix} \hat{\beta}_{11}, & \hat{\beta}_{12}/2, \ldots, & \hat{\beta}_{1k}/2 \\ & \hat{\beta}_{22}, \ldots, & \hat{\beta}_{2k}/2 \\ & & \ddots \\ \text{sym.} & & \hat{\beta}_{kk} \end{bmatrix}$$

That is, $\mathbf{b}$ is a $(k \times 1)$ vector of the first-order regression coefficients and $\mathbf{B}$ is a $(k \times k)$ symmetric matrix whose main diagonal elements are the *pure* quadratic coefficients $(\hat{\beta}_{ii})$ and whose off-diagonal elements are one-half the *mixed* quadratic coefficients $(\hat{\beta}_{ij}, i \neq j)$. The derivative of $\hat{y}$ with respect to the elements of the vector $\mathbf{x}$ equated to $\mathbf{0}$ is

$$\frac{\partial \hat{y}}{\partial \mathbf{x}} = \mathbf{b} + 2\mathbf{B}\mathbf{x} = \mathbf{0} \tag{11-6}$$

The stationary point is the solution to Equation 11-6, or

$$\mathbf{x}_s = -\tfrac{1}{2}\mathbf{B}^{-1}\mathbf{b} \tag{11-7}$$

Furthermore, by substituting Equation 11-7 into Equation 11-5, we can find the predicted response at the stationary point as

$$\hat{y}_s = \hat{\beta}_0 + \tfrac{1}{2}\mathbf{x}_s'\mathbf{b} \tag{11-8}$$

**Final Equation in Terms of Coded Factors:**

yield =
+79.94
+0.99 * A
+0.52 * B
−1.38 * $A^2$
−1.00 * $B^2$
+0.25 * A * B

**Final Equation in Terms of Actual Factors:**

yield =
−1430.52285
+7.80749 * time
+13.27053 * temp
−0.055050 * $\text{time}^2$
−0.040050 * $\text{temp}^2$
+0.010000 * time * temp

$$\mathbf{b} = \begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} -1.376 & 0.1250 \\ 0.1250 & -1.001 \end{bmatrix}$$

and from Equation 11-7 the stationary point is

$$\mathbf{x}_s = -\tfrac{1}{2}\mathbf{B}^{-1}\mathbf{b} = -\tfrac{1}{2}\begin{bmatrix} -0.7345 & -0.0917 \\ -0.0917 & -1.0096 \end{bmatrix}\begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} = \begin{bmatrix} 0.389 \\ 0.306 \end{bmatrix}$$

# Example: Canonical Form

$$\mathbf{b} = \begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} -1.376 & 0.1250 \\ 0.1250 & -1.001 \end{bmatrix}$$

and from Equation 11-7 the stationary point is

$$\mathbf{x}_s = -\tfrac{1}{2}\mathbf{B}^{-1}\mathbf{b}$$

$$= -\tfrac{1}{2}\begin{bmatrix} -0.7345 & -0.0917 \\ -0.0917 & -1.0096 \end{bmatrix}\begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} = \begin{bmatrix} 0.389 \\ 0.306 \end{bmatrix}$$

for eigen vector $\bar{x}_\lambda$

$$B\,\bar{x}_\lambda = \lambda\,\bar{x}_\lambda$$

$$\Rightarrow [B - \lambda I]\,\bar{x}_\lambda = 0$$

$$\Rightarrow \boxed{|B - \lambda I| = 0} \rightarrow \text{gives us ie eigenvalues}$$

Find Eigen values and Eigen vectors of B

$B = [\ ]_{k\times k}$ if this is a tranformation

$B\,\bar{x} = \bar{z}$

$[\ ]_{k\times k}[\ ]_{k\times 1} = [\ ]_{k\times 1}$

eigen vectors are those who do NOT change dir under B

$$B\,\bar{x} = \lambda\,\bar{x}$$

# Example: Canonical Form

$$\mathbf{b} = \begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} -1.376 & 0.1250 \\ 0.1250 & -1.001 \end{bmatrix}$$

and from Equation 11-7 the stationary point is

$$\mathbf{x}_s = -\tfrac{1}{2}\mathbf{B}^{-1}\mathbf{b}$$

$$= -\tfrac{1}{2}\begin{bmatrix} -0.7345 & -0.0917 \\ -0.0917 & -1.0096 \end{bmatrix}\begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix} = \begin{bmatrix} 0.389 \\ 0.306 \end{bmatrix}$$

$$\hat{y} = \beta_0 + \Sigma \beta_i x_i + \Sigma \beta_{ii} x_i^2 + \Sigma \beta_{ij} x_i x_j$$

$$\hat{y} = \hat{y}_s + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \cdots + \lambda_k w_k^2$$

Thus, canonical form of original eq.

$$\boxed{\hat{y} = 80.21 - 0.9641\, w_1^2 - 1.4147\, w_2^2}$$

$$|\mathbf{B} - \lambda\mathbf{I}| = 0$$

$$\begin{vmatrix} -1.376 - \lambda & 0.1250 \\ 0.1250 & -1.001 - \lambda \end{vmatrix} = 0$$

"maxima"

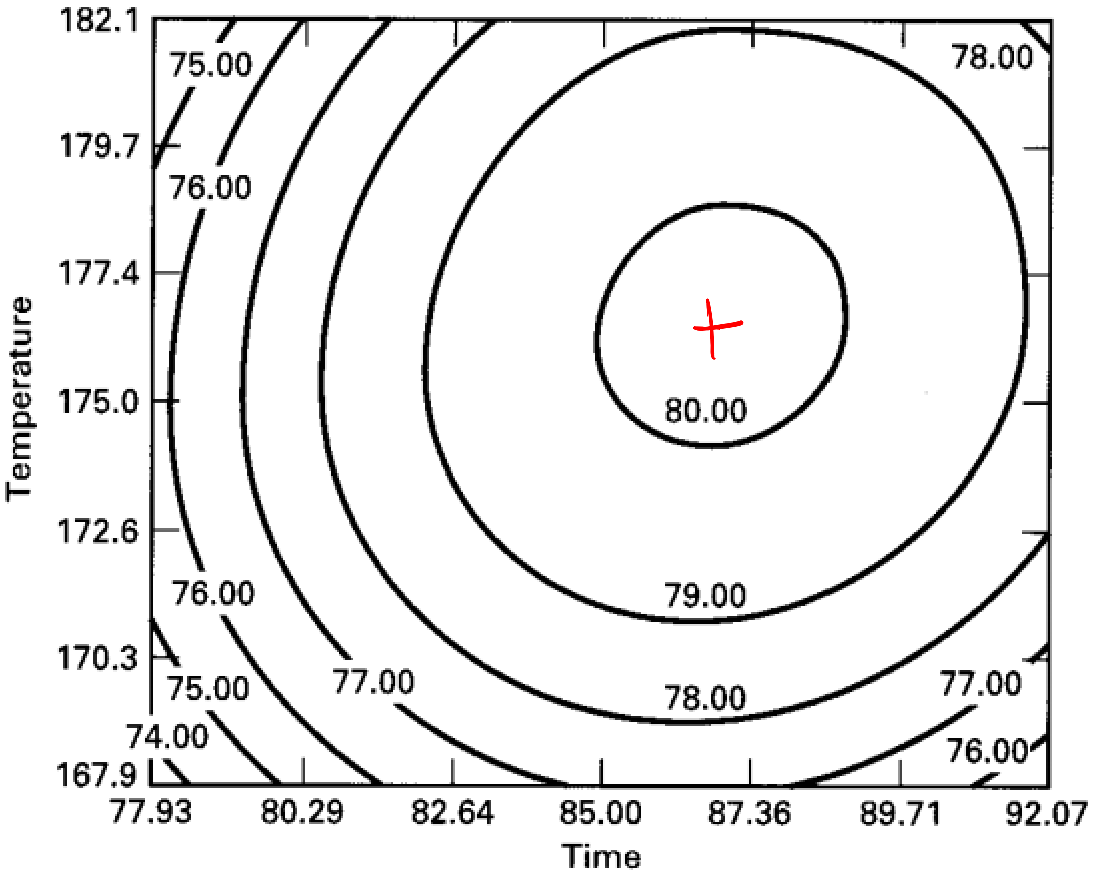
which reduces to

$$\lambda^2 + 2.3788\lambda + 1.3639 = 0$$

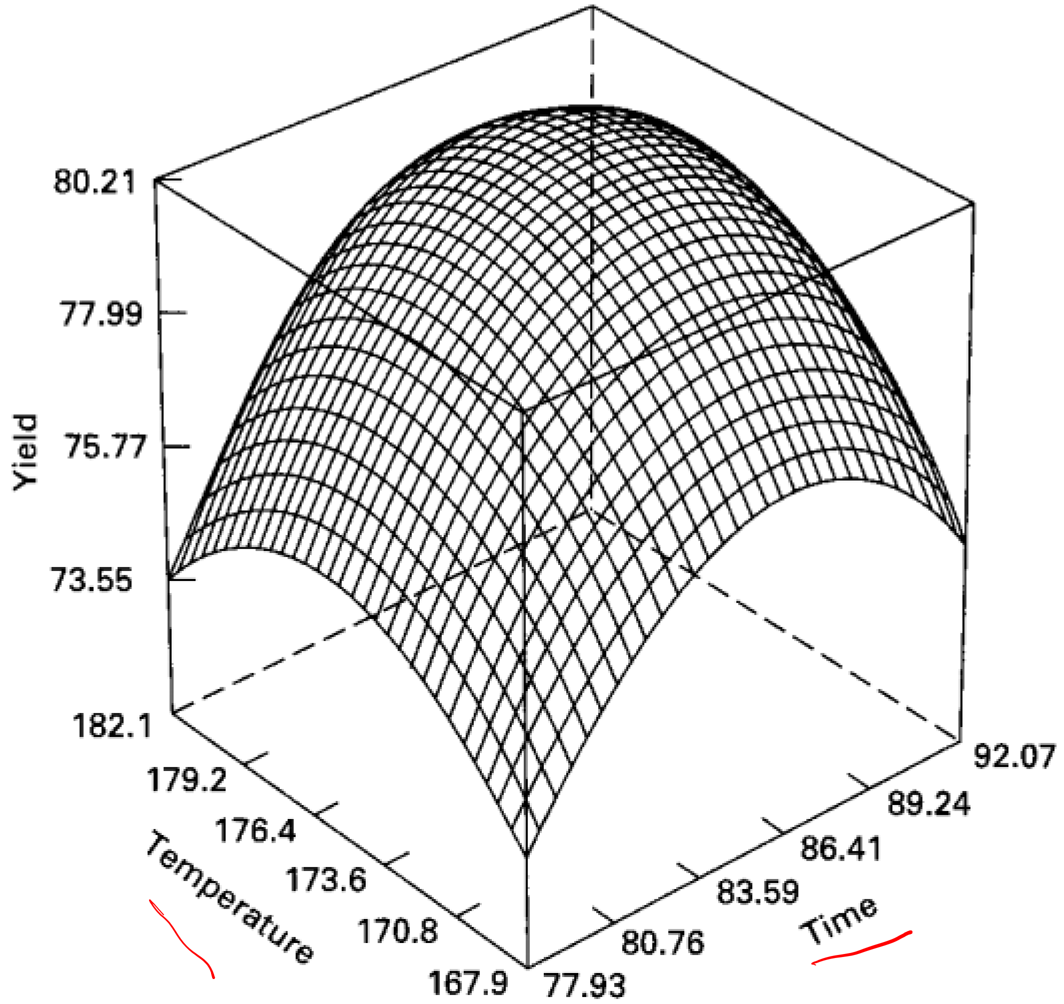
The roots of this quadratic equation are $\lambda_1 = -0.9641$ and $\lambda_2 = -1.4147$. Thus, the canonical form of the fitted model is

$$\hat{y} = 80.21 - 0.9641 w_1^2 - 1.4147 w_2^2$$

# Example: Contour Plot




(a) The contour plot




(b) The response surface plot