7. Response Surface Methodology (Ch.10. Regression Modeling Ch. 11. Response Surface Methodology)

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Introduction

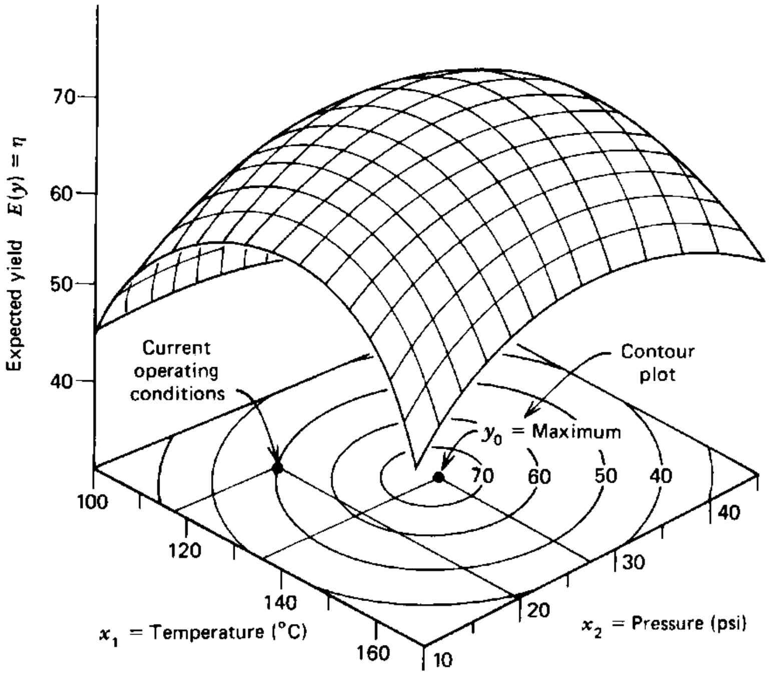
- Response surface methodology, or **RSM**, is a collection of mathematical and statistical techniques in which a response of interest is influenced by several variables and the objective is to optimize this response.
- For example, suppose that a chemical engineer wishes to find the levels of temperature (x_1) and pressure (x_2) that maximize the yield (y) of a process. The process yield is a function of the levels of temperature and pressure, say $y = f(x_1, x_2) + \varepsilon$

  where ε represents the noise or error observed in the response y. Then the surface represented by $\eta = f(x_1, x_2)$, which is called a **response surface**

Objective of RSM

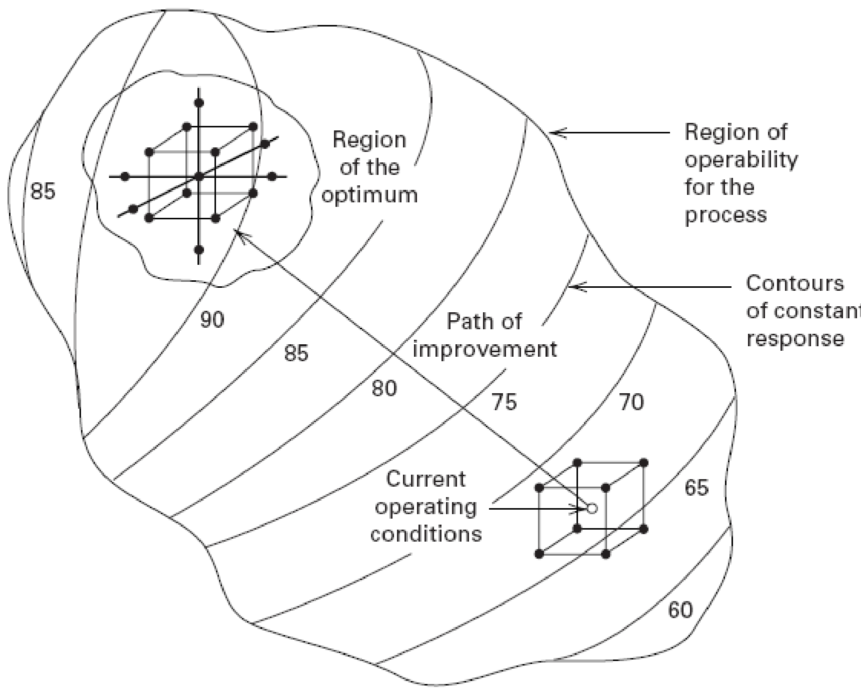
- We usually represent the response surface graphically, where η is plotted versus the levels of x_1 and x_2. To help visualize the shape of a response surface, we often plot the contours of the response surface as well. In the contour plot, lines of constant response are drawn in the x_1, x_2 plane. Each contour corresponds to a particular height of the response surface.
- Objective is to

  optimize the response



Steps in RSM

1. Find a suitable approximation for $y = f(\mathbf{x})$ using Least Square Method using Low-order polynomial}
2. Move towards the region of the optimum
3. When curvature is found find a new approximation for $y = f(\mathbf{x})$ (generally a higher order polynomial) and perform the "Response Surface Analysis"



Response Surface Methodology

For **(1) Screening** and **(2) Steepest ascent,** we use first order model

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

For (3) **Optimization,** we use second order model -

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

Least Square Method

- Least Square Method is typically used for the Estimation of the Parameters (**β**)
- We may write the model equation in terms of the observations

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik} + \epsilon_i$$
$$= \beta_0 + \sum_{j=1}^{k} \beta_j x_{ij} + \epsilon_i \quad i = 1, 2, \ldots, n$$

y	x_1	x_2	...	x_k
y_1	x_{11}	x_{12}	...	x_{1k}
y_2	x_{21}	x_{22}	...	x_{2k}
$\vdots$	$\vdots$	$\vdots$		$\vdots$
y_n	x_{n1}	x_{n2}	...	x_{nk}

- The equation is rewritten in matrix form as follows.

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}, \text{ and } \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

Estimation of the Parameters (β)

- L, the least square estimator to be minimized, is

$$L = \sum_{i=1}^{n} \epsilon_i^2 = \boldsymbol{\epsilon}'\boldsymbol{\epsilon} = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Note that L may be expressed as

$$\begin{aligned} L &= \mathbf{y}'\mathbf{y} - \boldsymbol{\beta}'\mathbf{X}'\mathbf{y} - \mathbf{y}'\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta} \\ &= \mathbf{y}'\mathbf{y} - 2\boldsymbol{\beta}'\mathbf{X}'\mathbf{y} + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta} \end{aligned}$$

- L is minimized by taking derivatives with respect to the model parameters and equating to zero

$$\left.\frac{\partial L}{\partial \boldsymbol{\beta}}\right|_{\hat{\boldsymbol{\beta}}} = -2\mathbf{X}'\mathbf{y} + 2\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{0}$$

$$\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{y}$$

$$\boxed{\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}}$$

Fitted Regression Model

Fitted regression model is $\hat{\mathbf{y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$

In scalar notation the fitted model is

$$\hat{y}_i = \hat{\beta}_0 + \sum_{j=1}^{k} \hat{\beta}_j x_{ij} \qquad i = 1, 2, \ldots, n$$

The residual is $\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}}$

Square sum of residual is

$$SS_E = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} e_i^2 = \mathbf{e}'\mathbf{e}$$

$$= \mathbf{y}'\mathbf{y} - \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y}$$

Validation of Regression Model

Sum of square of total

$$SS_T = \mathbf{y}'\mathbf{y} - \frac{\left(\sum_{i=1}^{n} y_i\right)^2}{n}$$

Sum of square of regression

$$SS_R = SS_T - SS_E$$

Coefficient of multiple determination

$$R^2 = \frac{SS_R}{SS_T} = 1 - \frac{SS_E}{SS_T}$$

Adjusted R^2 statistics

$$R^2_{adj} = 1 - \frac{SS_E/(n-p)}{SS_T/(n-1)}$$

If R^2 and Adjusted R^2 differ dramatically, there is a good chance of including non-significant terms

Example of Least Square Method

■ **TABLE 10.2**

Viscosity Data for Example 10.1 (viscosity in centistokes @ 100°c)

Observation	Temperature (x_1, °C)	Catalyst Feed Rate (x_2, lb/h)	Viscosity
1	80	8	2256
2	93	9	2340
3	100	10	2426
4	82	12	2293
5	90	11	2330
6	99	8	2368
7	81	8	2250
8	96	10	2409
9	94	12	2364
10	93	11	2379
11	97	13	2440
12	95	11	2364
13	100	8	2404
14	85	12	2317
15	86	9	2309
16	87	12	2328

Example of Least Square Method

EXAMPLE 10.1

Sixteen observations on the viscosity of a polymer (y) and two process variables—reaction temperature (x_1) and catalyst feed rate (x_2)—are shown in Table 10.2. We will fit a multiple linear regression model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$$

to these data. The **X** matrix and **y** vector are

$$\mathbf{X} = \begin{bmatrix} 1 & 80 & 8 \\ 1 & 93 & 9 \\ 1 & 100 & 10 \\ 1 & 82 & 12 \\ 1 & 90 & 11 \\ 1 & 99 & 8 \\ 1 & 81 & 8 \\ 1 & 96 & 10 \\ 1 & 94 & 12 \\ 1 & 93 & 11 \\ 1 & 97 & 13 \\ 1 & 95 & 11 \\ 1 & 100 & 8 \\ 1 & 85 & 12 \\ 1 & 86 & 9 \\ 1 & 87 & 12 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 2256 \\ 2340 \\ 2426 \\ 2293 \\ 2330 \\ 2368 \\ 2250 \\ 2409 \\ 2364 \\ 2379 \\ 2440 \\ 2364 \\ 2404 \\ 2317 \\ 2309 \\ 2328 \end{bmatrix}$$

The $\mathbf{X'X}$ matrix is

$$\mathbf{X'X} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 80 & 93 & \cdots & 87 \\ 8 & 9 & \cdots & 12 \end{bmatrix} \begin{bmatrix} 1 & 80 & 8 \\ 1 & 93 & 9 \\ \vdots & \vdots & \vdots \\ 1 & 87 & 12 \end{bmatrix}$$

$$= \begin{bmatrix} 16 & 1458 & 164 \\ 1458 & 133,560 & 14,946 \\ 164 & 14,946 & 1,726 \end{bmatrix}$$

and the $\mathbf{X'y}$ vector is

$$\mathbf{X'y} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 80 & 93 & \cdots & 87 \\ 8 & 9 & \cdots & 12 \end{bmatrix} \begin{bmatrix} 2256 \\ 2340 \\ \vdots \\ 2328 \end{bmatrix} = \begin{bmatrix} 37,577 \\ 3,429,550 \\ 385,562 \end{bmatrix}$$

The least squares estimate of $\boldsymbol{\beta}$ is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X'X})^{-1}\mathbf{X'y}$$

or

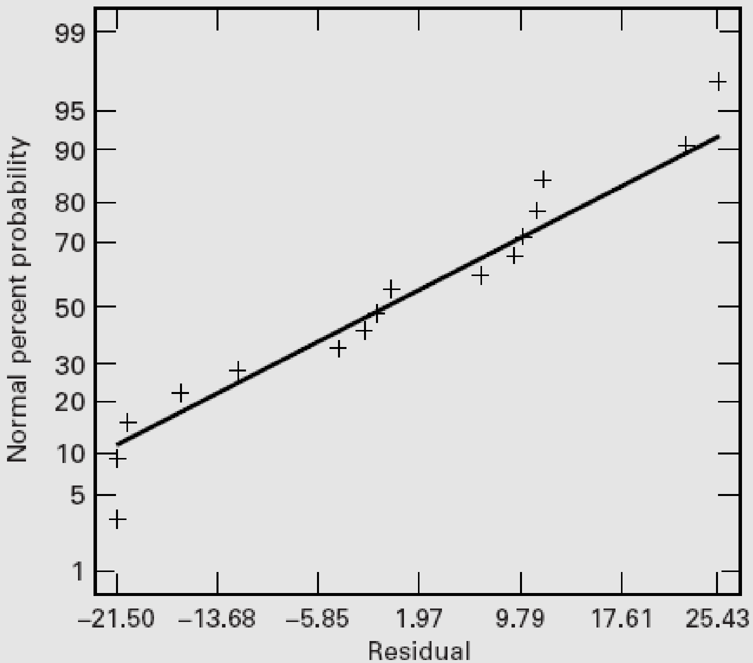
$$\hat{\boldsymbol{\beta}} = \begin{bmatrix} 14.176004 & -0.129746 & -0.223453 \\ -0.129746 & 1.429184 \times 10^{-3} & -4.763947 \times 10^{-5} \\ -0.223453 & -4,763947 \times 10^{-5} & 2.222381 \times 10^{-2} \end{bmatrix} \begin{bmatrix} 37,577 \\ 3,429,550 \\ 385,562 \end{bmatrix} = \begin{bmatrix} 1566.07777 \\ 7.62129 \\ 8.58485 \end{bmatrix}$$

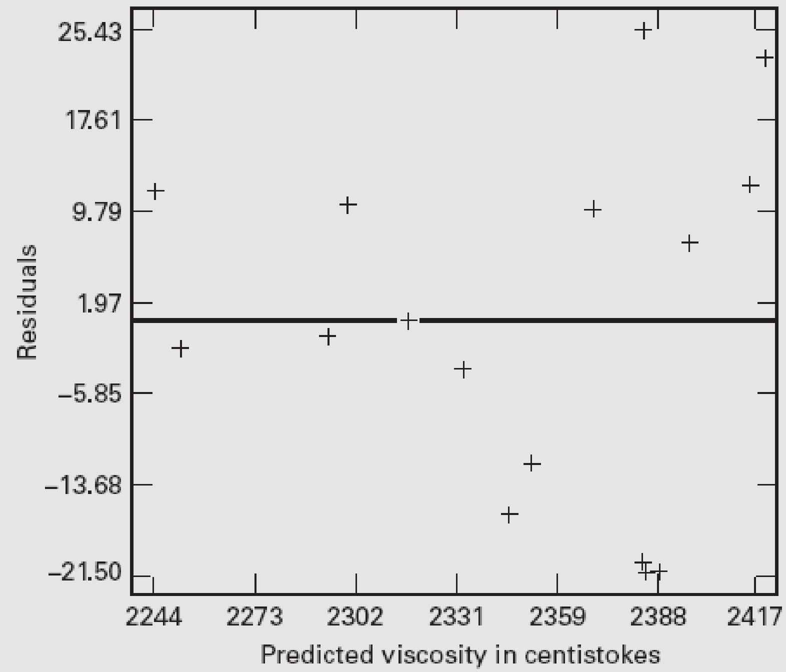
Example of Least Square Method

The least squares fit, with the regression coefficients reported to two decimal places, is

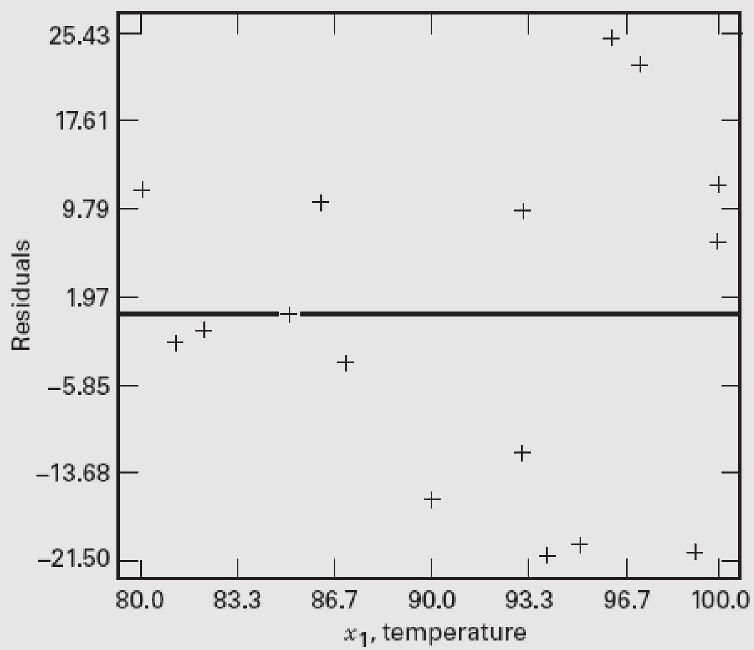
$$\hat{y} = 1566.08 + 7.62x_1 + 8.58x_2$$

The first three columns of Table 10.3 present the actual observations y_i, the predicted or fitted values $\hat{y}_i$, and the residuals. Figure 10.1 is a normal probability plot of the residuals. Plots of the residuals versus the predicted values $\hat{y}_i$ and versus the two variables x_1 and x_2 are shown in Figures 10.2, 10.3, and 10.4, respectively. Just as in designed experiments, residual plotting is an integral part of regression model building. These plots indicate that the variance of the observed viscosity tends to increase with the magnitude of viscosity. Figure 10.3 suggests that the variability in viscosity is increasing as temperature increases.

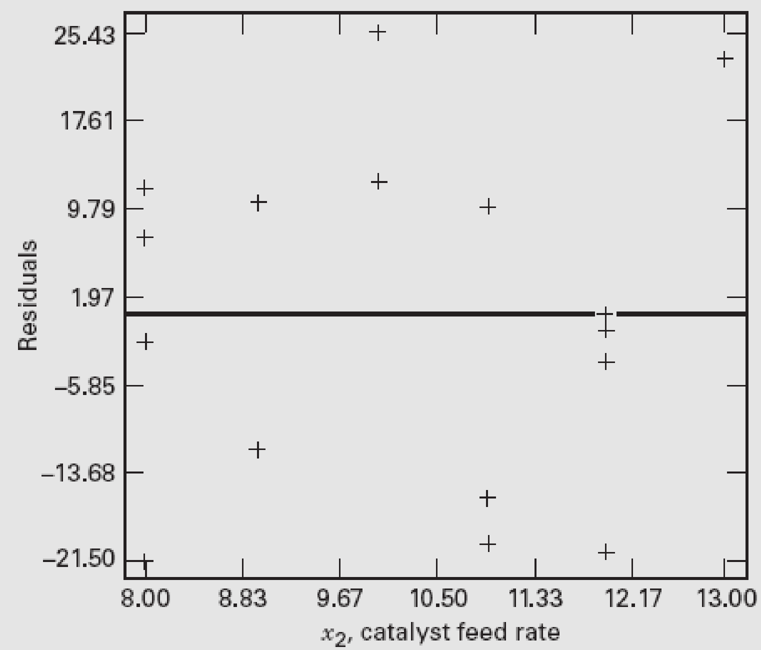




Example of Least Square Method



■ **FIGURE 10.3** Plot of residuals versus x_1 (temperature), Example 10.1



■ **FIGURE 10.4** Plot of residuals versus x_2 (feed rate), Example 10.1

Example of Least Square Method

TABLE 10.4

Minitab Output for the Viscosity Regression Model, Example 10.1

Regression Analysis

The regression equation is

Viscosity = 1566 + 7.62 Temp + 8.58 Feed Rate

Predictor	Coef	Std. Dev.	T	P
Constant	1566.08	61.59	25.43	0.000
Temp	7.6213	0.6184	12.32	0.000
Feed Rat	8.585	2.439	3.52	0.004

S = 16.36   R-Sq = 92.7%   R-Sq (adj) = 91.6%

Analysis of Variance

Source	DF	SS	MS	F	P
Regression	2	44157	22079	82.50	0.000
Residual Error	13	3479	268		
Total	15	47636			

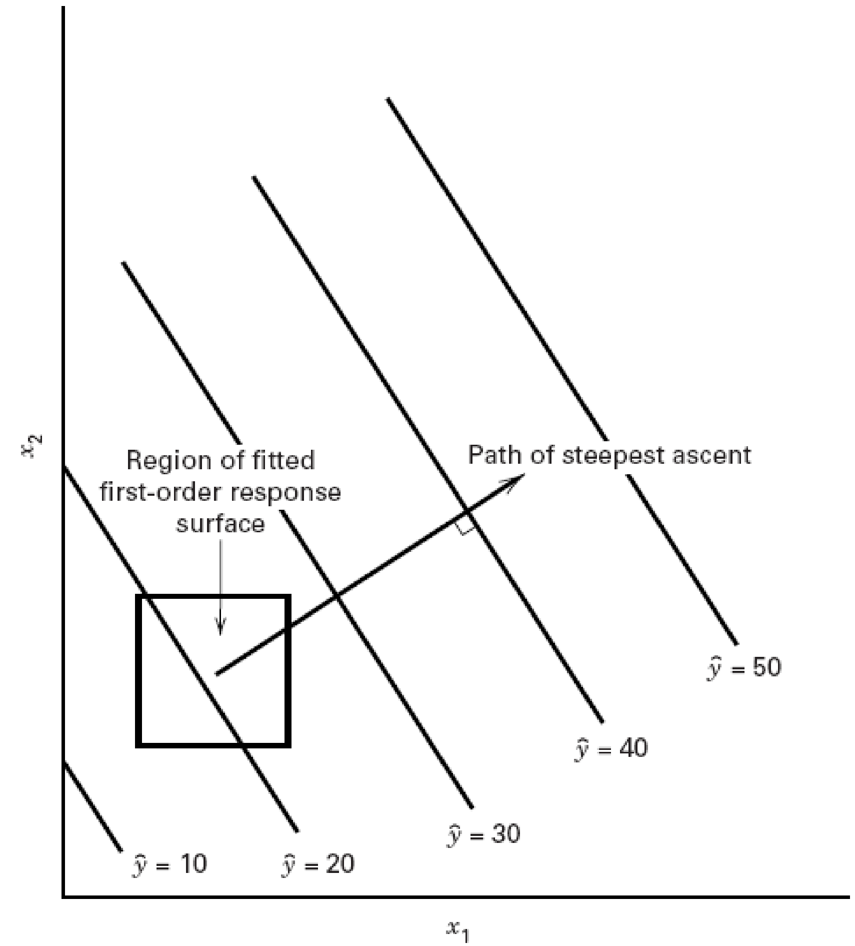
Source	DF	Seq SS
Temp	1	40841
Feed Rat	1	3316

The Method of Steepest Ascent

- A procedure for moving sequentially from an initial "guess" towards to region of the optimum
- Based on the fitted first-order model

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

- Steepest ascent is a gradient procedure



The Method of Steepest Ascent

- Points on the path of steepest ascent are proportional to the magnitudes of the model regression coefficients
- The direction depends on the sign of the regression coefficient
- Step-by-step procedure:

1. Choose a step size in one of the process variables, say Δx_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 Δx_i from coded variables to the natural variables.

Chemical Processing Example

- A chemical engineer is interested in determining the operating conditions that maximize the yield of a process. Two controllable variables influence process yield: reaction time and reaction temperature. The engineer is currently operating the process with a reaction time of 35 minutes and a temperature of 155°F, which result in yields of around 40 percent. Since it is unlikely that this region contains the optimum, she fits a first-order model and applies the method of steepest ascent.
- The engineer decides that the region of exploration for fitting the first-order model should be (30, 40) minutes of reaction time and (150, 160)°F. To simplify the calculations, the independent variables will be coded to the usual (-1, 1) interval.

Chemical Processing Example

- The experimental design is shown in the table. Note that the design used to collect the data is a 2^2 factorial augmented by five center points. Replicates at the center are used to estimate the experimental error and to allow for checking the adequacy of the first-order model. Also, the design is centered about the current operating conditions for the process.

Natural variables		Coded variables		Response
ξ_1	ξ_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

$$x = \frac{\xi - (\xi_{\max} + \xi_{\min})/2}{(\xi_{\max} - \xi_{\min})/2}$$

$$x_1 = \frac{(\xi_1 - 35)}{5},$$

$$x_2 = \frac{(\xi_2 - 155)}{5}$$

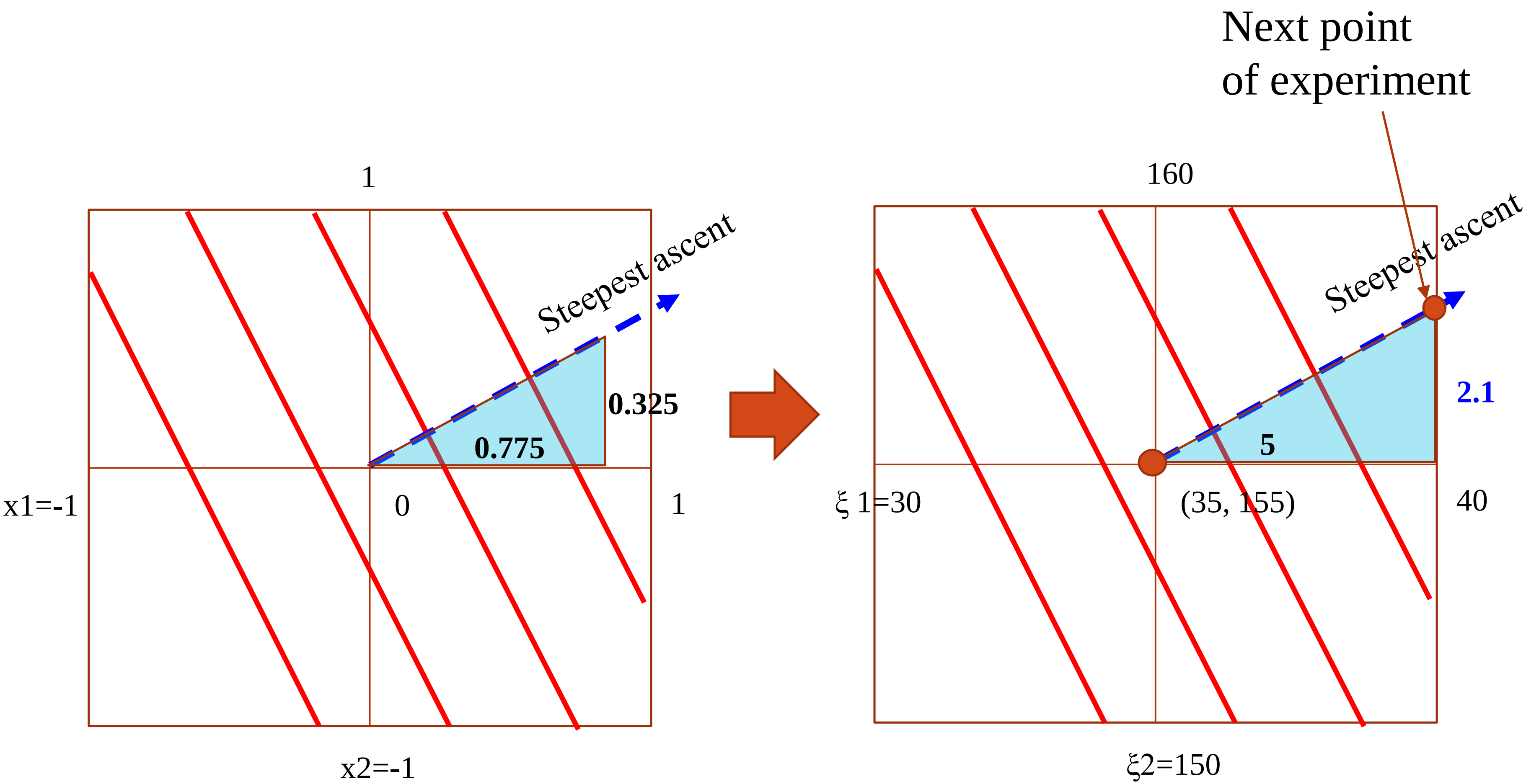
Chemical Processing Example

- A first-order model is $\hat{y} = 40.44 + 0.775x_1 + 0.325x_2$ by Least Square Method
- To move away from the design center, the point ($x_1 = 0$, $x_2 = 0$), along the path of steepest ascent, we would move 0.775 units in the x_1 direction for every 0.325 units in the x_2 direction
- Thus, the path of steepest ascent passes through the point ($x_1 = 0$, $x_2 = 0$) and has a slope 0.325/0.775.
- The engineer decides to use 5 minutes of reaction time as the basic step. Using the relationship of natural and coded variable

$$d\xi_1 = 5dx_1, \qquad d\xi_2 = 5dx_2$$

$$\frac{d\xi_1}{d\xi_2} = \frac{5dx_1}{5dx_2}, \qquad d\xi_2 = \frac{dx_2}{dx_1}(d\xi_1) = \frac{0.325}{0.775} \times (5\text{ min}) = 2.1^\circ F$$

Chemical Processing Example



Coded variable space

Natural variable space

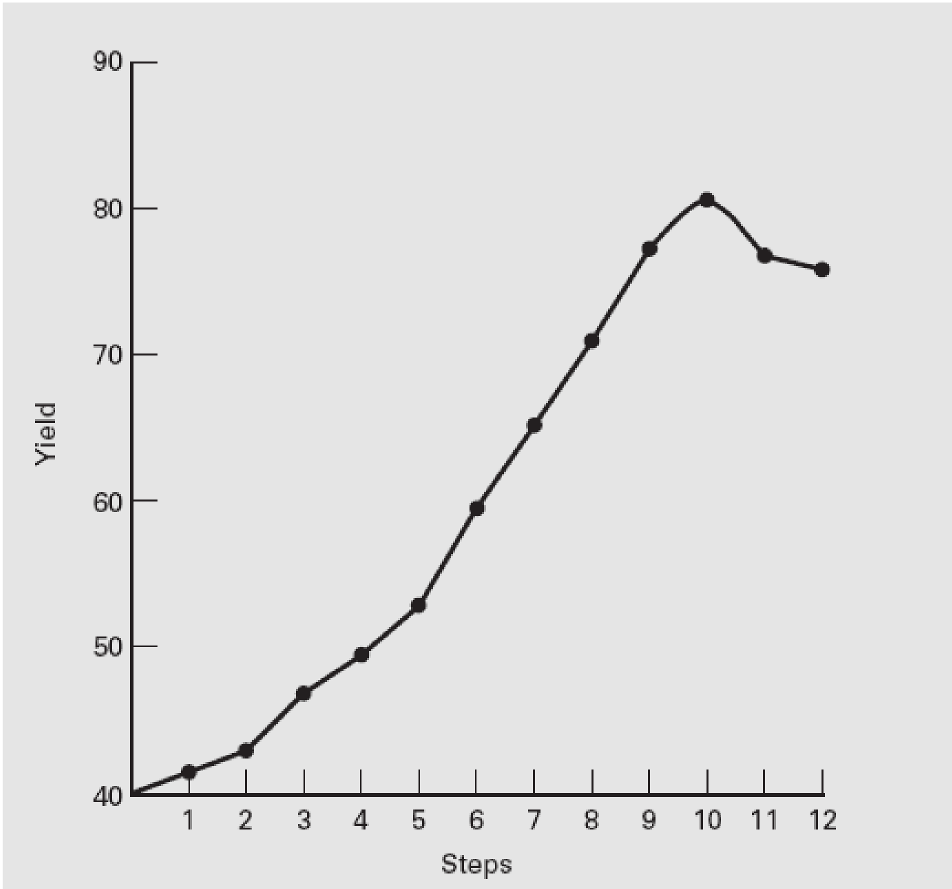
Chemical Processing Example

■ **TABLE 11.3**

Steepest Ascent Experiment for Example 11.1

Steps	**Coded Variables** x_1	x_2	**Natural Variables** ξ_1	ξ_2	**Response** y
Origin	0	0	35	155	
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

Chemical Processing Example



Second-Order Models in RSM

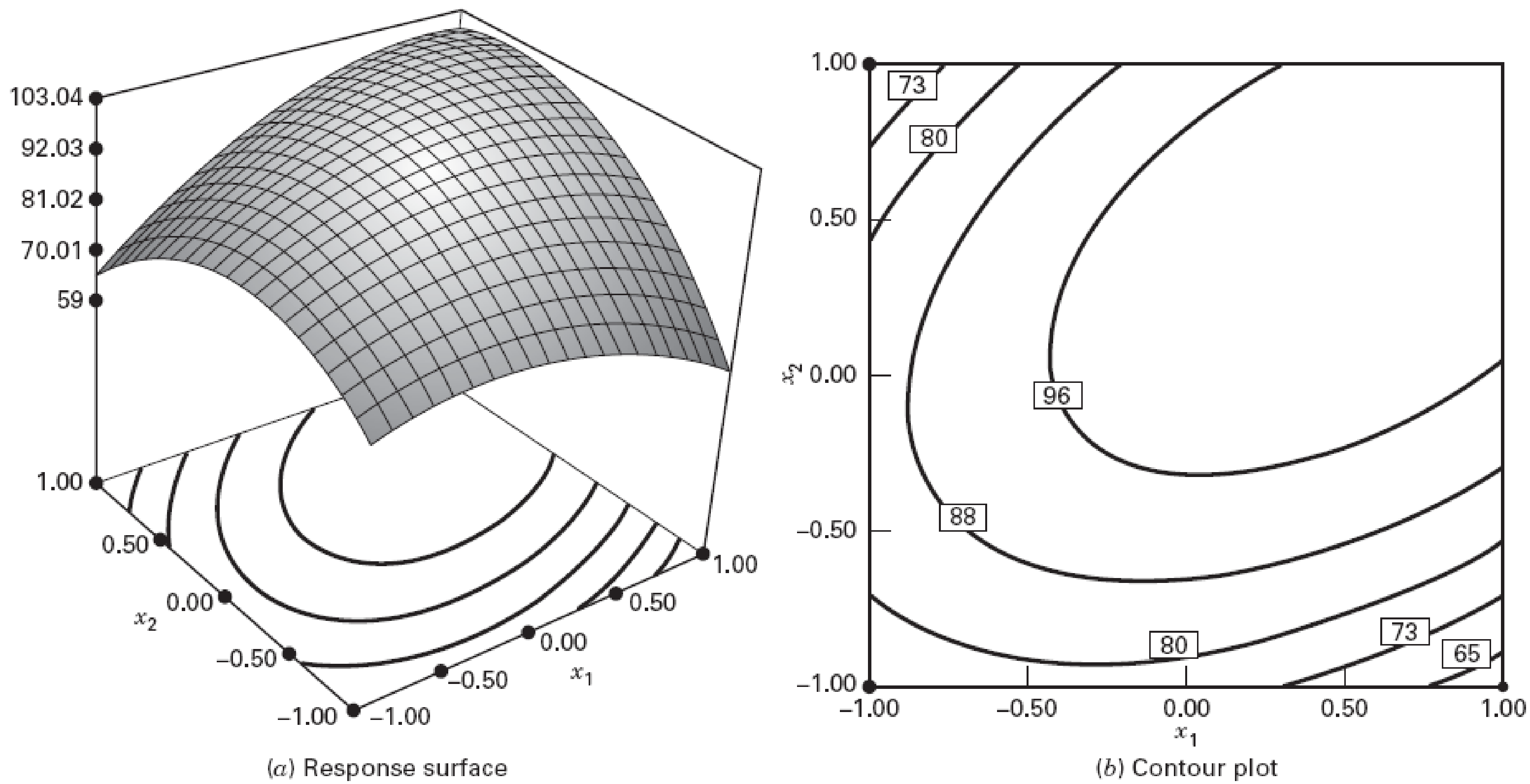
$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j}\sum \beta_{ij} x_i x_j + \varepsilon \qquad \text{or}$$

$$y = \beta_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x} + \varepsilon$$

$$\text{where } \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ .. \\ x_k \end{bmatrix}, \mathbf{b} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ .. \\ \beta_k \end{bmatrix}, \text{ and } \mathbf{B} = \begin{bmatrix} \beta_{11} & \beta_{12}/2 & \dots & \beta_{1k}/2 \\ & \beta_{22} & \dots & \beta_{2k}/2 \\ Sym & & \dots & \dots \\ & & & \beta_{kk} \end{bmatrix}$$

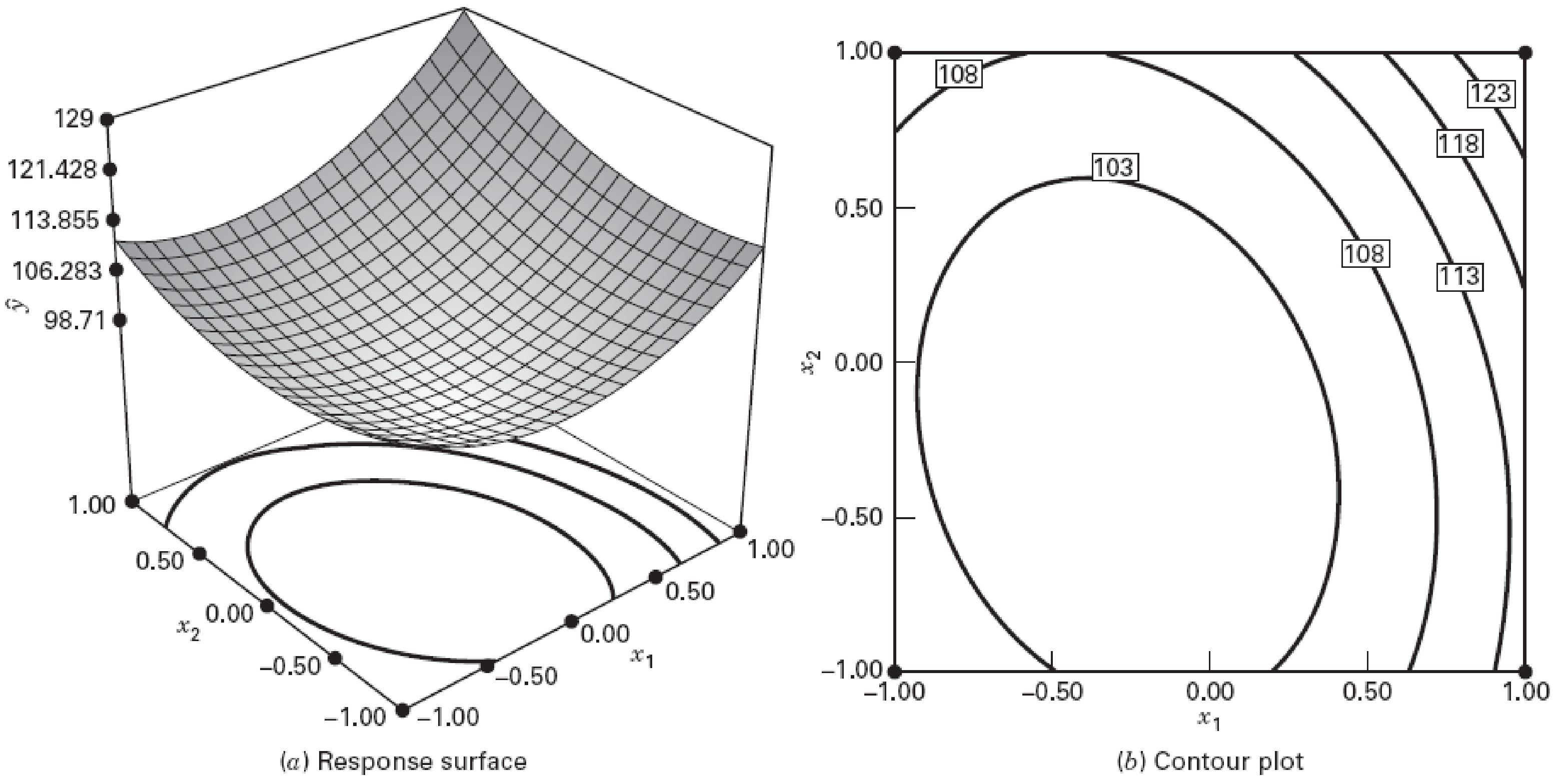
- These models are used widely in practice
- The Taylor series analogy -> Fitting the model is easy, some nice designs are available
- Optimization is easy -> There is a lot of empirical evidence that they work very well

Examples of Second-Order Models



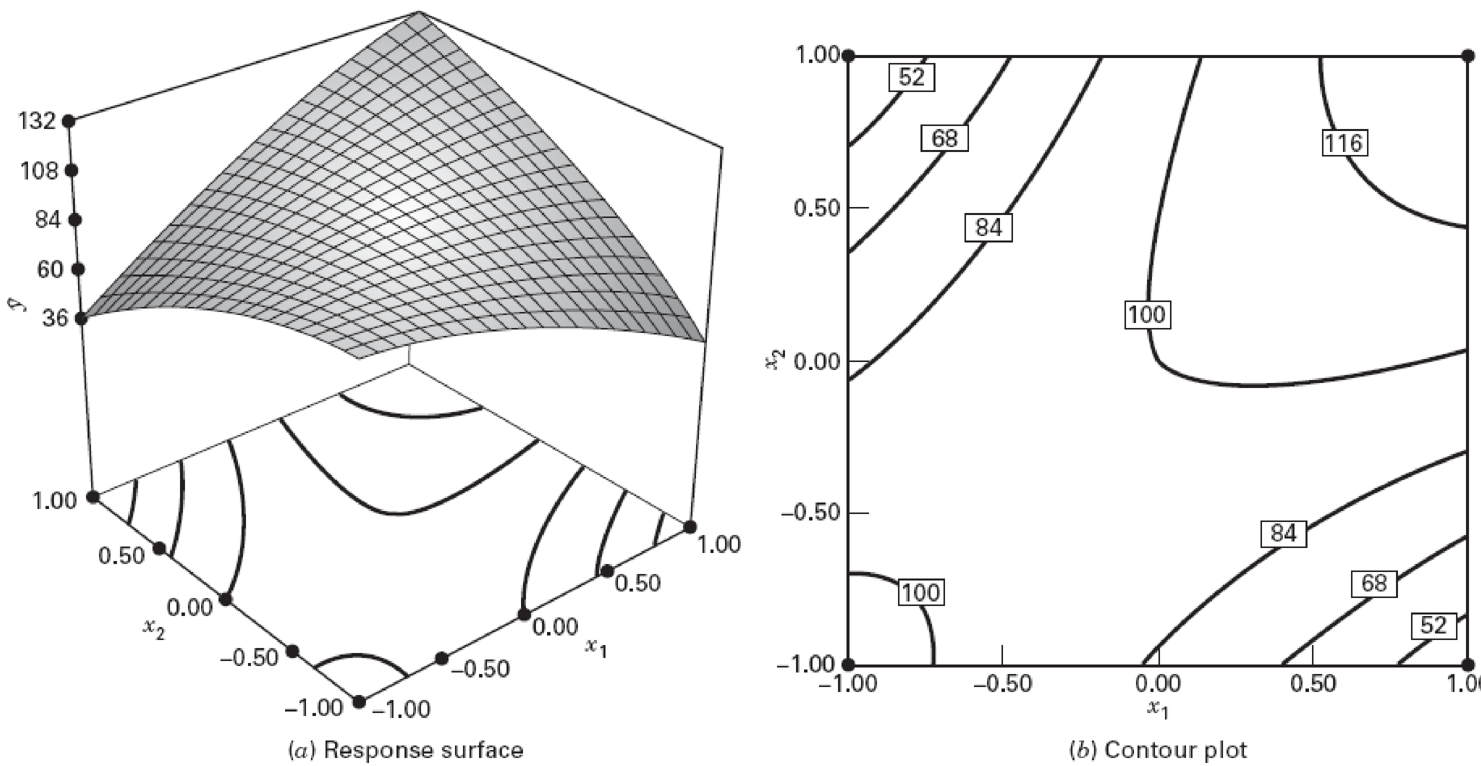
■ **FIGURE 11.6** **Response surface and contour plot illustrating a surface with a maximum**

Examples of Second-Order Models



■ FIGURE 11.7 **Response surface and contour plot illustrating a surface with a minimum**

Examples of Second-Order Models



■ **FIGURE 11.8** **Response surface and contour plot illustrating a saddle point (or minimax)**

Characterization of the Response Surface

- Find out where our stationary point is
- Find what type of surface we have
  - Graphical Analysis
  - Canonical Analysis
- Determine the sensitivity of the response variable to the optimum value
  - Canonical Analysis

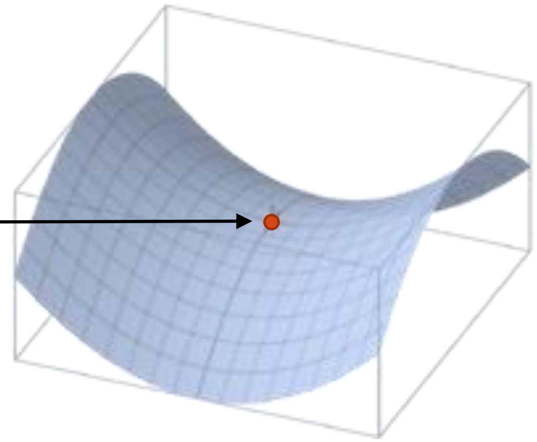
Finding the Stationary Point

- After fitting a second order model take the partial derivatives with respect to the x_i's and set to zero

$$\frac{\partial \hat{y}}{\partial x_1} = \frac{\partial \hat{y}}{\partial x_2} = \cdots = \frac{\partial \hat{y}}{\partial x_k} = 0$$

$$\mathbf{x}_s = \begin{bmatrix} x_{1s} \\ x_{2s} \\ \vdots \\ x_{ks} \end{bmatrix}$$

- Stationary point represents…
  - Maximum Point
  - Minimum Point
  - Saddle Point



Stationary Point

General mathematical solution for the location of the stationary point is obtained as follows.

$$y = \hat{\beta}_0 + \mathbf{x}'\hat{\mathbf{b}} + \mathbf{x}'\hat{\mathbf{B}}\mathbf{x}$$

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

Therefore, Stationary point $x_s = -\frac{1}{2}\hat{\mathbf{B}}^{-1}\hat{\mathbf{b}}$

where $\hat{\mathbf{b}} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ .. \\ \hat{\beta}_k \end{bmatrix}$, and $\hat{\mathbf{B}} = \begin{bmatrix} \hat{\beta}_{11} & \hat{\beta}_{12}/2 & ... & \hat{\beta}_{1k}/2 \\ & \hat{\beta}_{22} & ... & \hat{\beta}_{2k}/2 \\ Sym & & ... & ... \\ & & & \hat{\beta}_{kk} \end{bmatrix}$

Predicted response at the stationary points

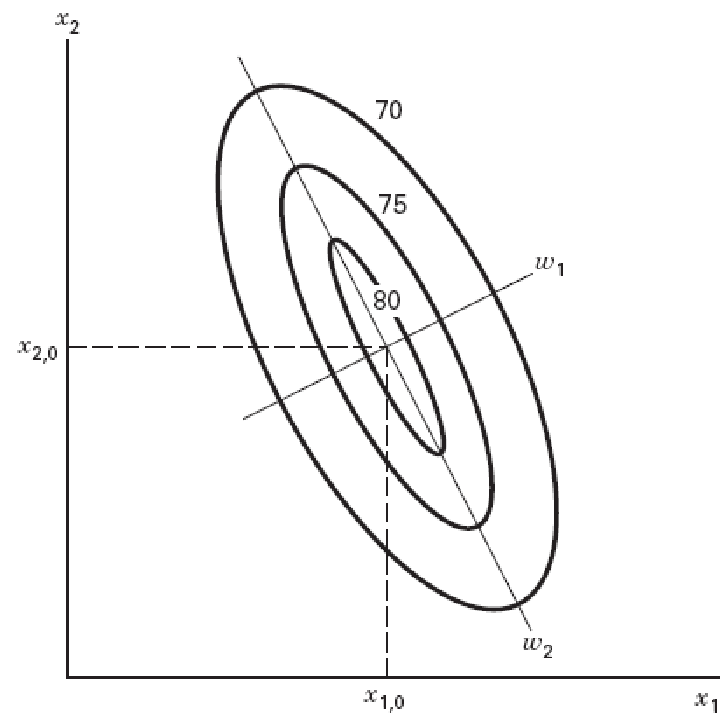
$$\hat{y}_s = \hat{\beta}_0 + \frac{1}{2}\mathbf{x}_s^{'}\mathbf{b}$$

Canonical Analysis

- Used for sensitivity analysis and stationary point identification
- Based on the analysis of a transformed model called: canonical form of the model
- Canonical Model form:
  - $y = y_s + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \ldots + \lambda_k w_k^2$
- $\{\lambda_i\}$ are just the **eigenvalues or characteristic roots** of the matrix **B**.

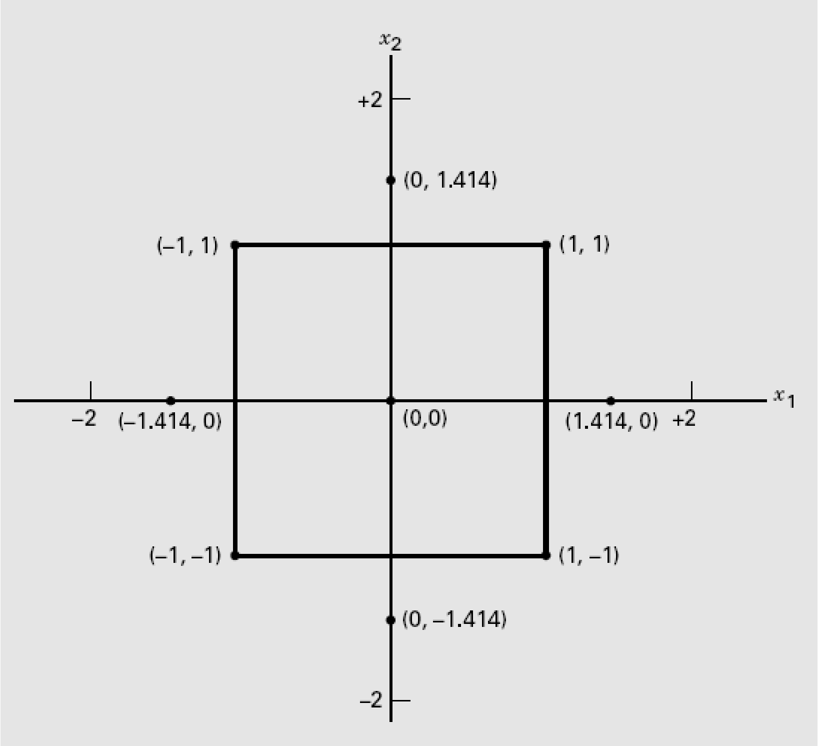
Eigenvalues

- The nature of the response can be determined by the signs and magnitudes of the eigenvalues
  - {e} all positive: a minimum is found
  - {e} all negative: a maximum is found
  - {e} mixed: a saddle point is found
- Eigenvalues can be used to determine the sensitivity of the response with respect to the design factors
- The response surface is steepest in the direction (canonical) corresponding to the largest absolute eigenvalue



Chemical Processing Example

- A second-order model is to be set at the tenth point ($\xi_1 = 85$, $\xi_2 = 175$) in Example 6-1. The experimenter decides to augment the 2^2-and-central-point design in order to have enough points for fitting a second-order model. She obtains four observations at ($x_1 = 0$, $x_2 = \pm 1.414$) and ($x_1 = \pm 1.414$, $x_2 = 0$). The design is displayed in the left figure. (Central Composite Design – CCD)



Chemical Processing Example

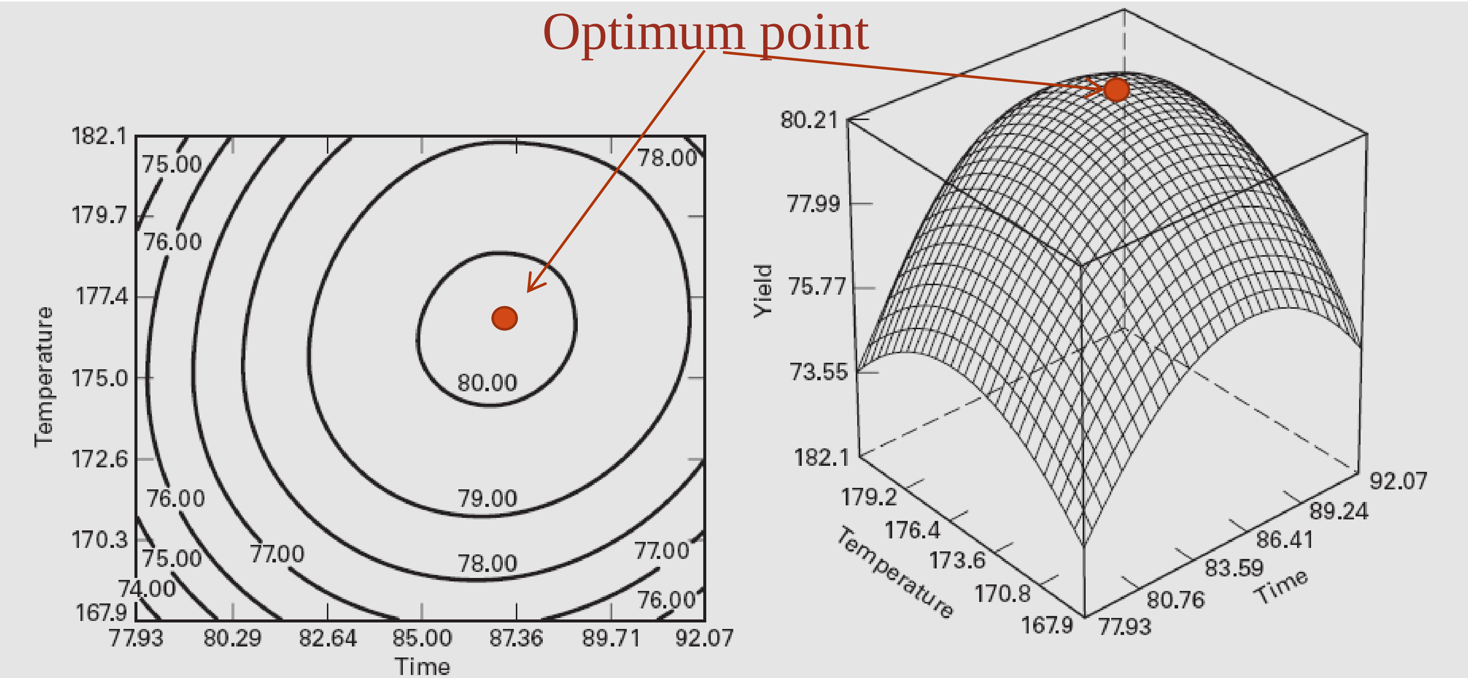
- The complete experiment is shown in the table.

Natural Variables		Coded Variables		Responses		
ξ_1	ξ_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 of Second-order Model

- Using MINITAB, we fist a response surface and to construct the contour plots. The second-order model in terms of the coded variables is

$$\hat{y} = 79.940 + 0.995x_1 + 0.515x_2 - 1.376x_1^2 - 1.001x_2^2 + 0.250x_1x_2$$



(a) The contour plot

(b) The response surface plot

Chemical Processing Example

- Finding the location of the stationary point using the general solution.

$$\mathbf{B} = \begin{bmatrix} -1.376 & 0.125 \\ 0.125 & -1.001 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 0.995 \\ 0.515 \end{bmatrix}$$

So

$$\mathbf{B}^{-1} = \begin{bmatrix} -0.7345 & -0.0917 \\ -0.0917 & -1.0096 \end{bmatrix}$$

The stationary point is

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

$$x_{1s} = 0.389, x_{2s} = 0.306$$

The stationary point in natural variable space is

$$0.389 = \frac{\xi_1 - 85}{5}$$

$$0.306 = \frac{\xi_2 - 175}{5}$$

which yield $\xi_1 = 86.95$ (min), $\xi_2 = 176.53(^{\circ}\mathrm{F})$

Predicted response at the stationary point as $\hat{y}_s = 80.21$.

Chemical Processing Example

- Performing Canonical Analysis.
- The eigenvalues λ_1 and λ_2 are the roots of the determinant equation

$$\mathbf{B} - \lambda\mathbf{I} = 0 \quad \text{or} \quad \begin{vmatrix} -1.377-\lambda & 0.125 \\ 0.125 & -1.0018-\lambda \end{vmatrix} = 0$$

which reduces to

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

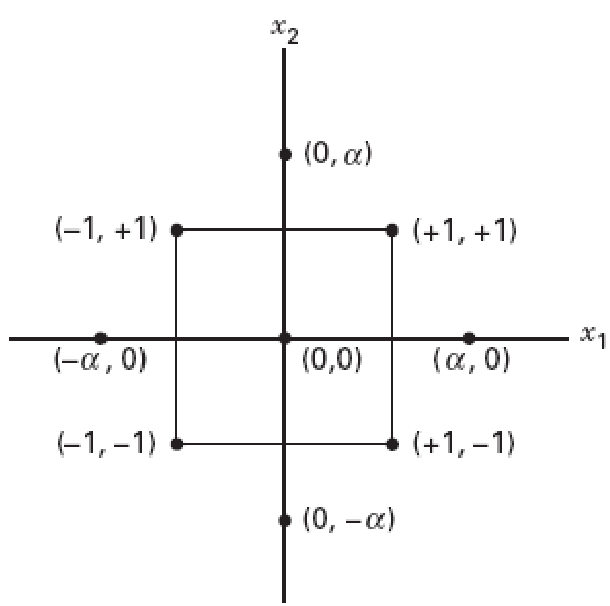
- The roots of this quadratic equation are λ_1 = -0.9641 and λ_2 = -1.4147. Thus, the canonical form of the fitted model is

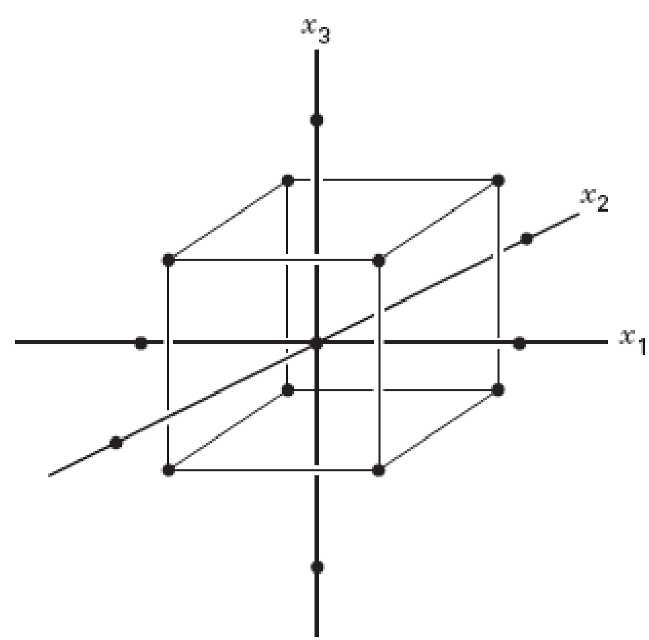
$$\hat{y} = 80.21 - 0.9641w_1^2 - 1.4147w_2^2$$

- Since both λ_1 and λ_2 are negative, we conclude that the stationary point is a maximum.

Central Composite Design - CCD

- The **central composite design or CCD** is the most popular class of designs used for fitting the second-order models. Generally, the CCD consists of a 2^k factorial with n_j runs, $2k$ axial or star runs, and n_c center runs. Figure shows the CCD for $k = 2$ and $k = 3$ factors.





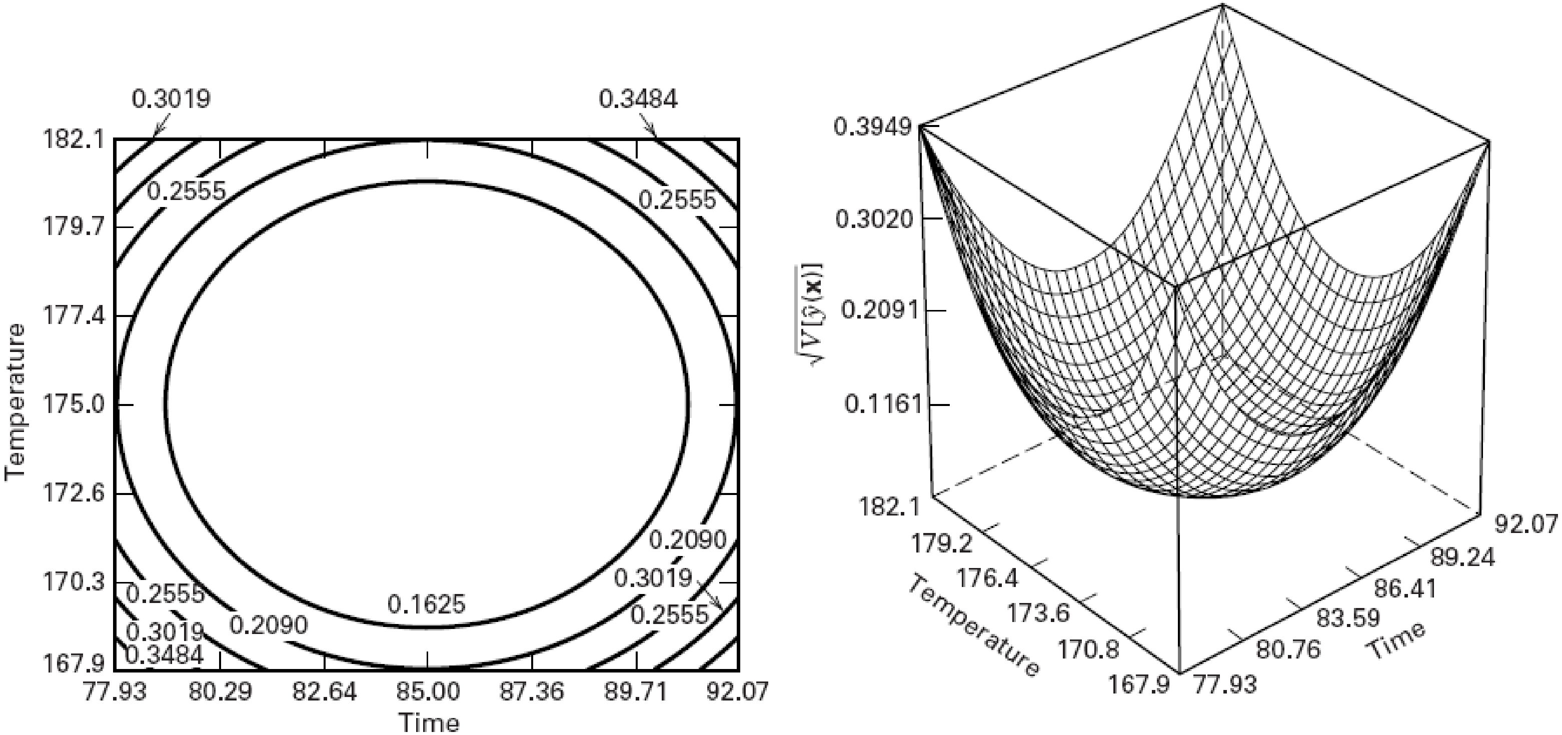
Central Composite Design

- The practical deployment of a CCD often arises through **sequential experimentation.** A 2^k design is first used to fit a first-order model. If this model has exhibited lack of fit, and the axial runs are then added to allow the quadratic terms to be incorporated into the model. The CCD is a very efficient design for fitting the second-order model.
- There are two parameters in the CCD design that must be specified; the **distance** α of the axial runs from the design center, and the **number of center points** n_c. Generally, three to five center runs are recommended.
- The distance α should ensure that a second-order response surface design be **rotable.**

The Rotatable CCD

$$\alpha = F^{1/4}$$

$$where \quad F = 2^k$$



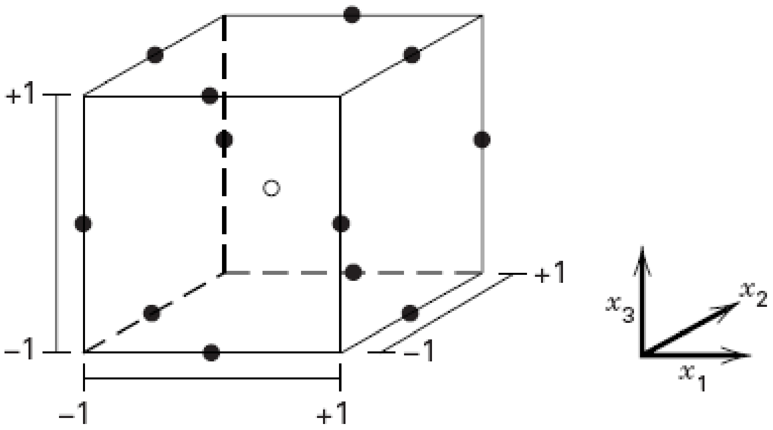
(a) Contours of $\sqrt{V[\hat{y}(\mathbf{x})]}$

(b) The response surface plot

The Box-Behnken Design

■ **TABLE 11.8**
A Three-Variable Box–Behnken Design

Run	x_1	x_2	x_3
1	−1	−1	0
2	−1	1	0
3	1	−1	0
4	1	1	0
5	−1	0	−1
6	−1	0	1
7	1	0	−1
8	1	0	1
9	0	−1	−1
10	0	−1	1
11	0	1	−1
12	0	1	1
13	0	0	0
14	0	0	0
15	0	0	0



■ **FIGURE 11.22** **A Box–Behnken design for three factors**