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DO 2: 09:40 AM – 11:30 PM

Subject Code

18MEO113T - Design of Experiments

Handled by

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Disclaimer

The content prepared in the presentation are from various sources, only used for education purpose. Thanks to all the sources.

Unit 4

Unit 4

Source: *This lecture is prepared primarily based on* ***Chapter 11*** *of "****Design and Analysis of Experiments****" by* ***D C Montgomery****, Wiley, 8^{th} Edition*

Assumptions of Linearity in two-level designs

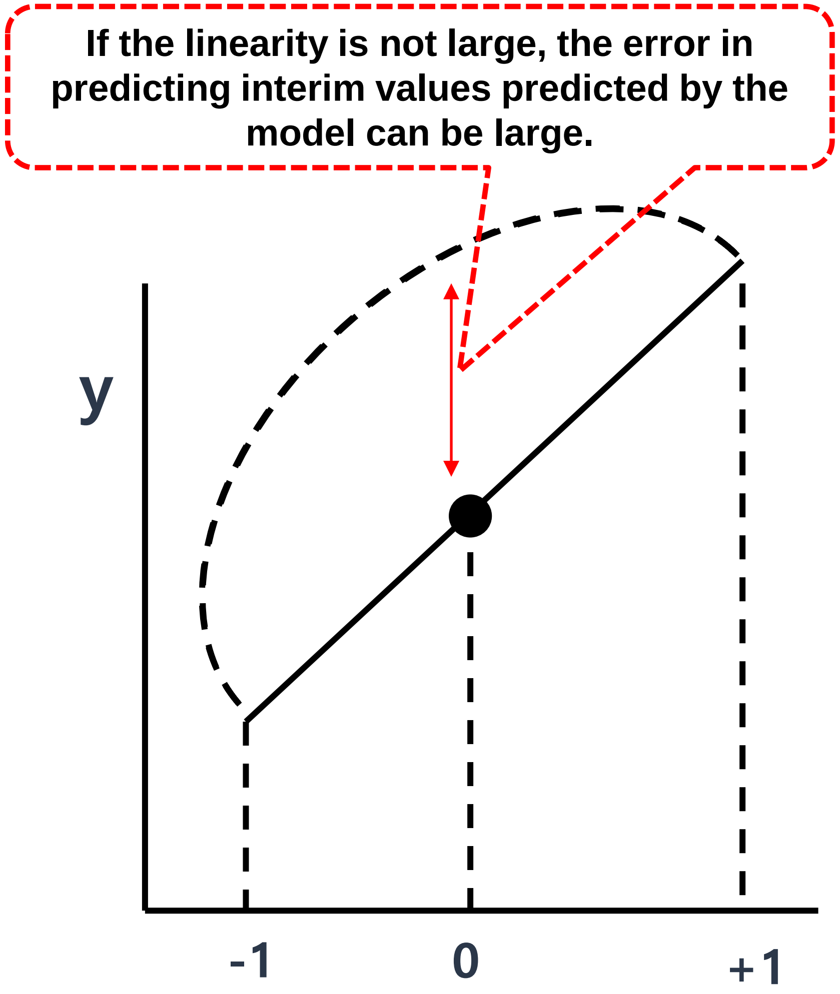
- **In general, significant proportion of experiments are performed with two-level factorials.**
- **Two-level full factorial designs with k factors are denoted as 2^k**
- These models assume linear response
- For example, linear regression model of 2^2 design is:

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

Zi

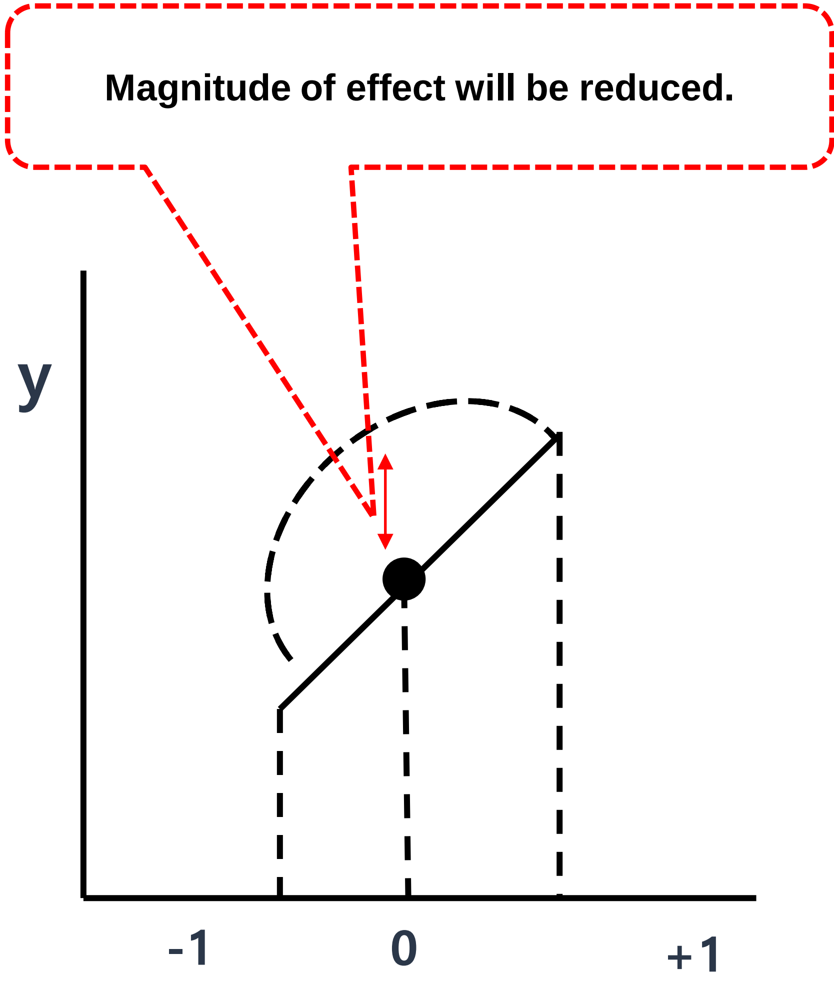
Assumptions of Linearity in two-level designs

- Two-level factorial designs assumes linearity of response
- In reality, the response may not be linear
- The more the curvature or non-linearity, the more will be error in the prediction of interim values.



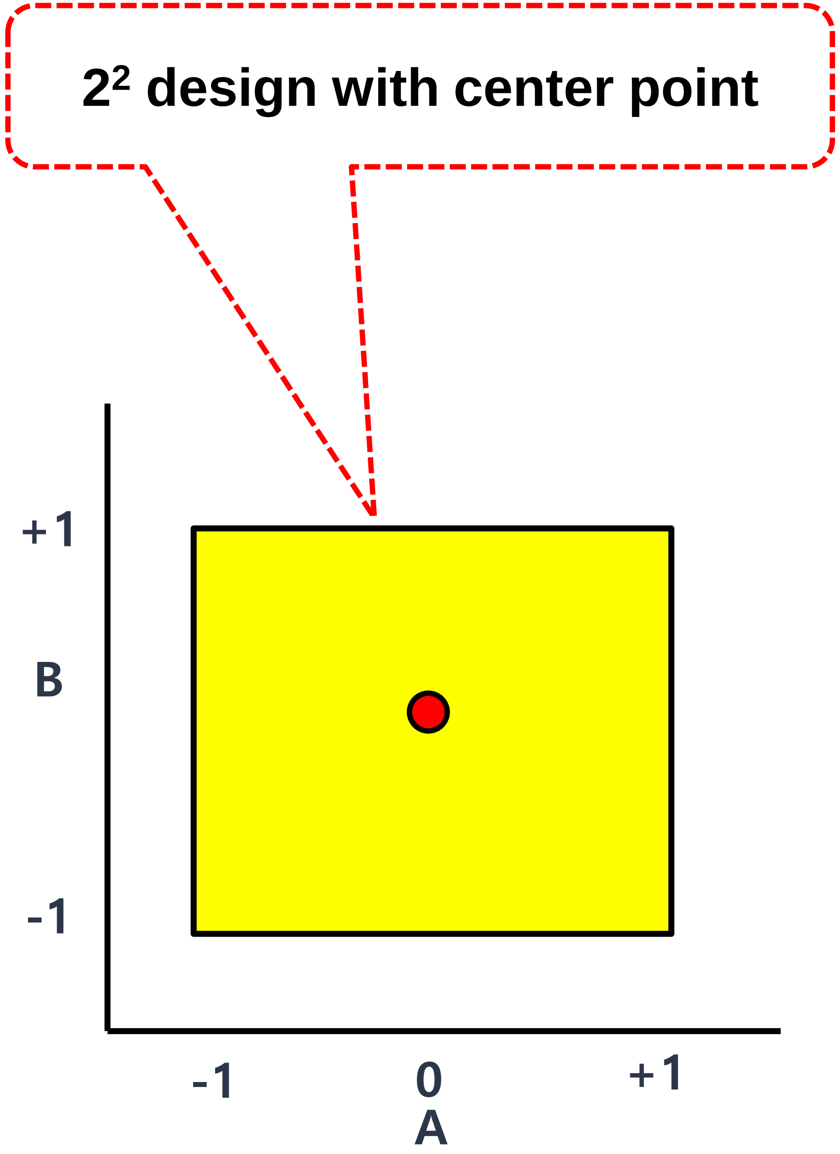
Assumptions of Linearity in two-level designs

- **How to minimize effect of non-linearlity**
- **One possible recommendation is to select levels of the factors as close as possible.**
- **This will help reducing the error. However, it will affect the magnitude of the effect/ response.**



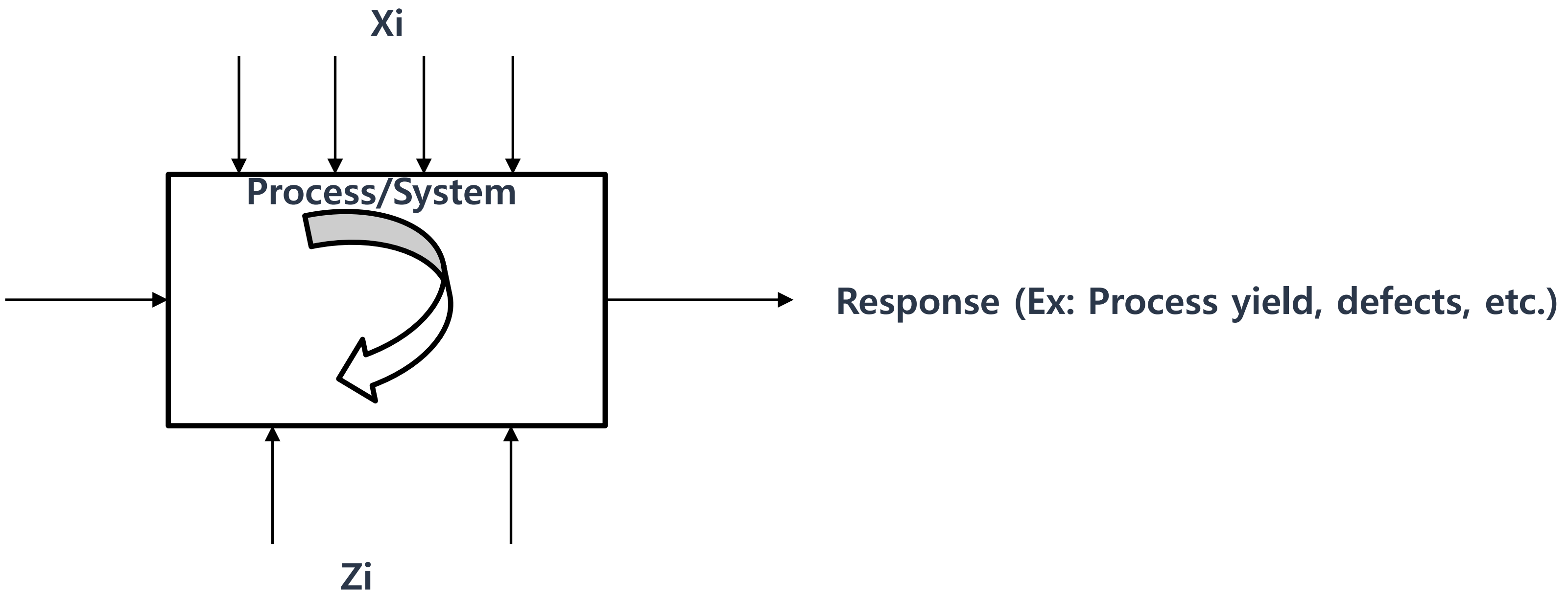
Addition of Center Point

- **Therefore experimenters often add a center point in the design.**
- **The purpose of adding a center point is to validate the assumption of linearity.**
- **If the response at the center point is significantly different than the predicted value on the straight line, then a non linear model will be required to reduce the error. This can be done with a Response Surface Design.**



Background of response surface design

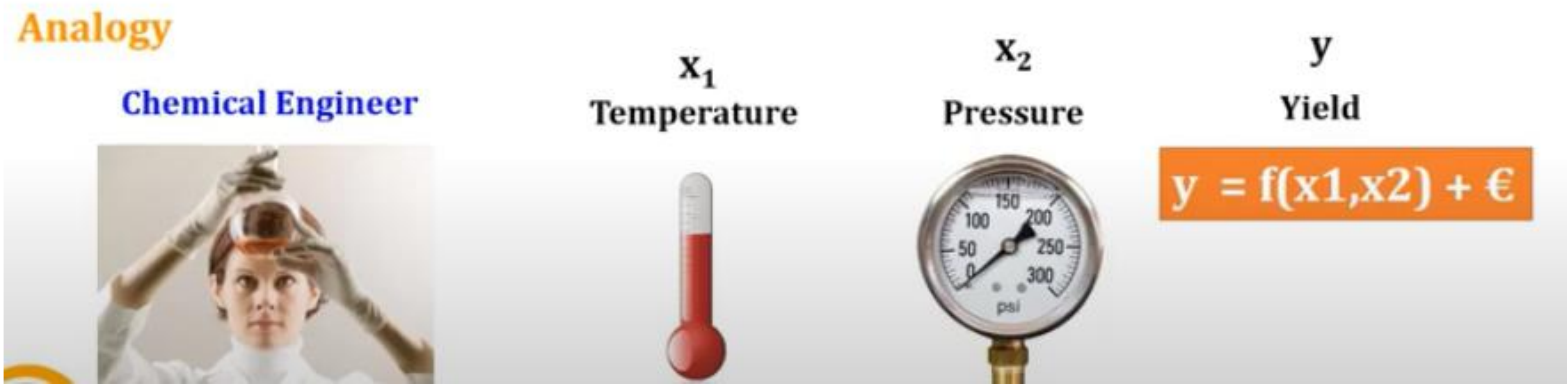
- **Response Surface Methodology, or RSM,** is a **collection of mathematical and statistical techniques** useful for the **modeling** and **analysis** of problems in which a response of interest is influenced by several variables and **the objective is to optimize this response**.



Setting the X in the particular range or zone by that we can able to get the optimal response value.

Background of response surface design

- **RSM,** is a **collection of mathematical and statistical techniques** useful for the **developing, improving, and optimizing processes.**



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

Background of response surface design

- **The difference between a response surface equation and the equation for a factorial design** is the addition of the squared (or quadratic) terms that lets you model curvature in the response, making them useful for:
  - Understanding or mapping a region of a response surface. Response surface equations model how changes in variables affect a response of interest.
  - Finding the levels of variables that optimize a response.
  - Selecting the operating conditions to meet specifications.
- For example, you would like to determine the best conditions for injection-molding a plastic part. You first used a screening or factorial experiment to determine the significant factors (temperature, pressure, cooling rate). You can use a response surface designed experiment to determine the optimal settings for each factor.

Background of response surface design

- **The difference between a response surface equation and the equation for a factorial design**
- A two-level factorial (or fractional factorial) design looks for linear trends, possibly with interactions
  - Does the variable significantly impact the response? In what direction?
  - It helps to define the next experiment.
- Response Surface Methodology (RSM) looks for quadratic or higher order trends
  - Assumes all variable are significant
  - A quadratic response always has a stationary point (minimum or maximum or saddle point)
  - Can be used to optimize a process

Background of response surface design

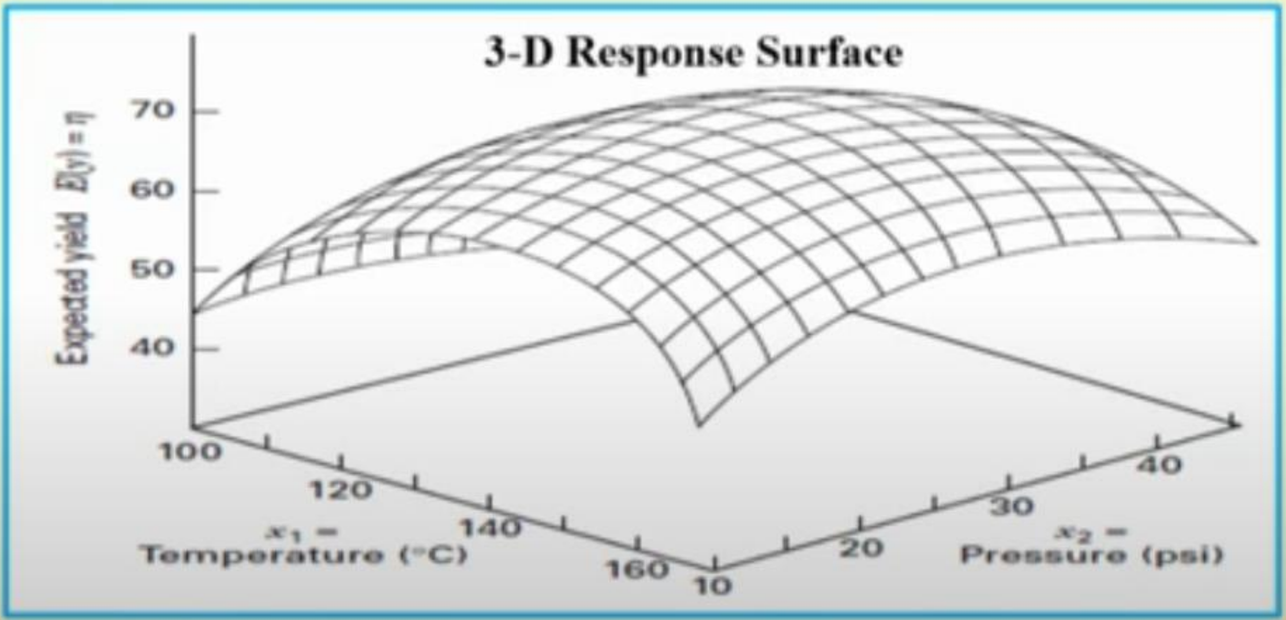
- **RSM:** a collection of mathematical and statistical techniques for the modeling and analysis and the objective is to optimize the response.

- **For example:** Find the **levels of temperature** (x_1) and **pressure** (x_2) that maximize the yield (y) of a process.

$$y = f(x_1, x_2) + \varepsilon$$ (where ε is noise or errors observed in the response y)

- **Expected response:** $E(y) = f(x_1, x_2) = \eta$

Response surface $\eta = f(x_1, x_2)$



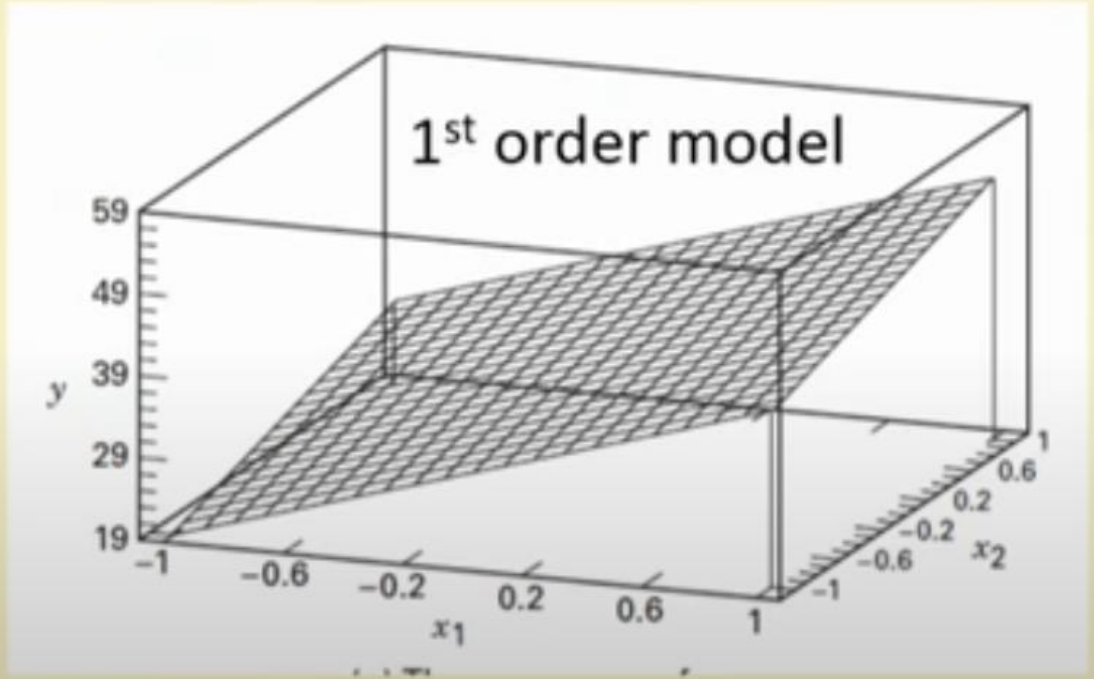
Background of response surface design

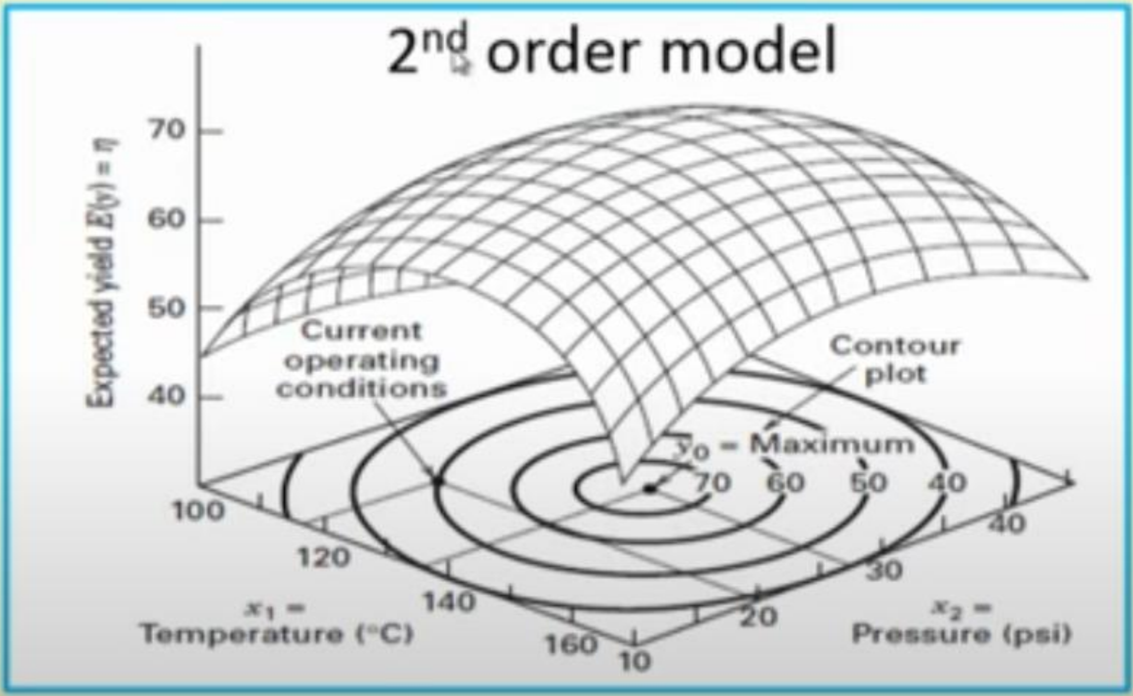
- **First-order model**
  (Linear function of MEs)

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \epsilon$$

- **Second-order model**
  (When there is curvature in the system)

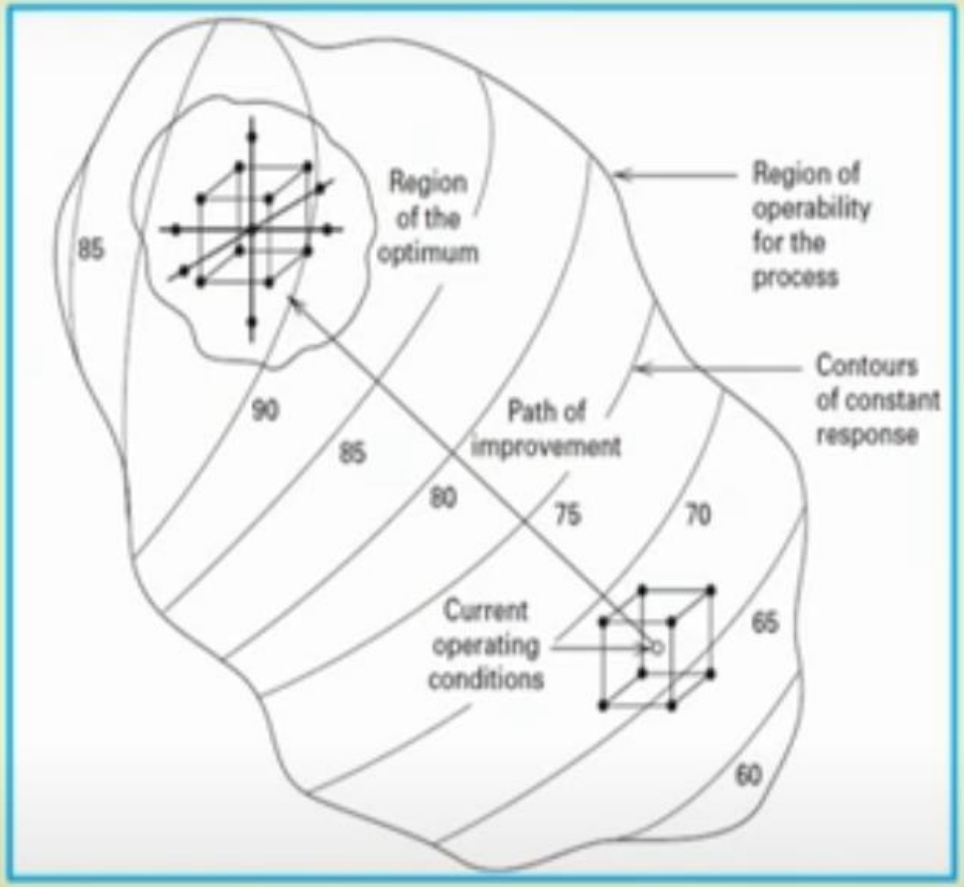
$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j}\sum \beta_{ij} x_i x_j + \epsilon$$





Background of response surface design

- RSM is a **sequential procedure**.
- Finds out the path of improvement toward the **optimum**
- Maximization: **climbing a hill (steepest ascent)**
- Minimization: **descending into a valley (steepest descent)**



The sequential nature of RSM

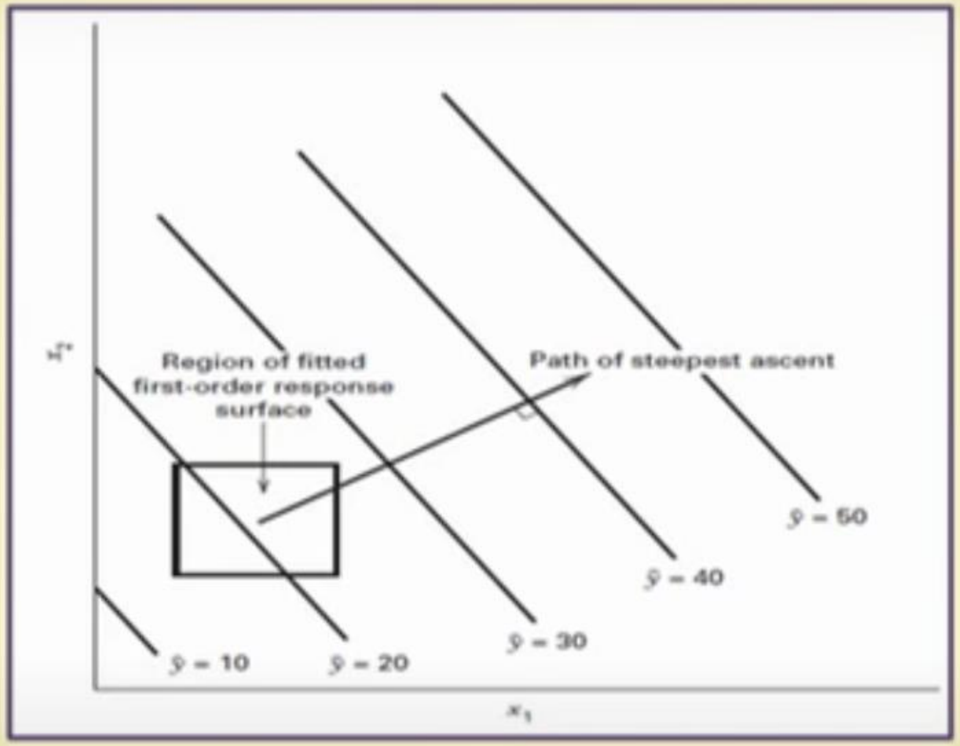
https://online.stat.psu.edu/stat503/lesson/11

Background of response surface design

- **The Method of Steepest Ascent**

Let the fitted first-order model is

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



- **Path of steepest ascent:** The line through the center of the region of interest and normal to the fitted surface

- The steps along the path are proportional to the regression coefficients.
- The actual step size is determined by the experimenter based on process knowledge or other practical considerations.
- Experiments are conducted along the path of steepest ascent until no further increase in response is observed.

Example 1 (First-order RSM)

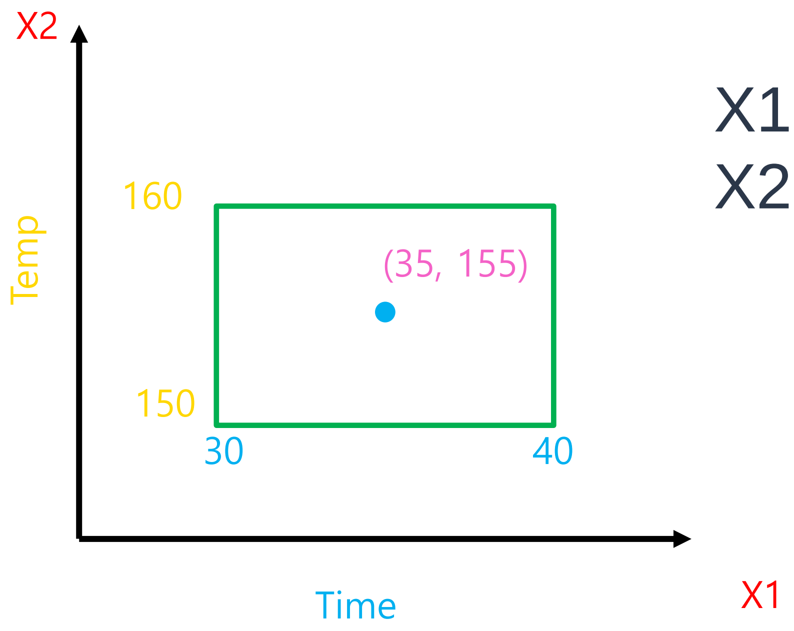
A chemical engineer is interested in determining the operating conditions that maximize the yield of a process. Two controllable variables influence process yield: reaction time and reaction temperature. The engineer is currently operating the process with a reaction time of 35 minutes and a temperature of 155°F, which result in yields of around 40 percent. Because it is unlikely that this region contains the optimum, she fits a first-order model and applies the method of steepest ascent.

Process Data for Fitting the First-Order Model

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

Example 1 (RSM First-order Model)

- Response variable = Process yield = Y = 40%
- Current operating condition:
  - Natural variable (ε_1) = Coded variable (X1) = Reaction time of 35 minutes
  - Natural variable (ε_2) = Coded variable (X2) = Temperature of 155°F



2^K factorial design with center point

X1: High = 40 min (+1); Low = 30 min (-1)
X2: High = 160 F (+1); Low = 150 F (-1)

Example 1 (First-order RSM)

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) Fahrenheit. To simplify the calculations, the independent variables will be coded to the usual (−1, 1) interval. Thus, if ξ_1 denotes the **natural variable** time and ξ_2 denotes the **natural variable** temperature, then the **coded variables** are

$$x_1 = \frac{\xi_1 - 35}{5} \quad \text{and} \quad x_2 = \frac{\xi_2 - 155}{5}$$

The experimental design is shown in Table 11.1. Note that the design used to collect these 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.

A first-order model may be fit to these data by least squares. Employing the methods for two-level designs, we obtain the following model in the coded variables:

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

$$\hat{y} = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i \Rightarrow Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2$$

First-order model (Linear function of MEs) $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \epsilon$

40.44 = Average of all Y observation (β_0)…

$$\beta_1 = \frac{1}{2}(Effect\ of\ X1) = \frac{1}{2}\left(\left(\frac{40.9+41.5}{2}\right) - \left(\frac{39.3+40.0}{2}\right)\right) = 0.775$$

$$\beta_2 = \frac{1}{2}(Effect\ of\ X2) = \frac{1}{2}\left(\left(\frac{40+41.5}{2}\right) - \left(\frac{39.3+40.9}{2}\right)\right) = 0.325$$

Example 1 (First-order RSM)

- In order to check, **whether the first-order model fitted or not**, we have to check the following:

  1. Estimate the Error (based on central point observation)
  2. Test for Interaction ($\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$) whether β_{12} significant or not?
  3. Test for Quadratic effects ($\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2$) whether $\beta_{11} + \beta_{22}$ significant or not?
  4. If step 2 and step 3 is equal to zero, then we can say the first-order model is fit. If not, we have to analysis further.

Example 1 (First-order RSM)

Step 1. Estimate the Error (based on central point observation)

Error = [Sum of square of all the values/responses – (squares of sum of all the values)/n] / n-1

$$\hat{\sigma}^2 = \frac{(40.3)^2 + (40.5)^2 + (40.7)^2 + (40.2)^2 + (40.6)^2 - (202.3)^2/5}{4} = 0.0430$$

The mean square Error (MS_E) = 0.0430

Example 1 (First-order RSM)

Step 2. Test for Interaction Estimate the Error

The first-order model assumes that the variables $x1$ and $x2$ have an **additive effect** on the response. The interaction between the variables would be represented by the coefficient of β_{12} of a cross-product term x1x2 added to the model.

The least squares estimate of this coefficient is just one-half the interaction effect calculated as in an ordinary 2^2 factorial design,

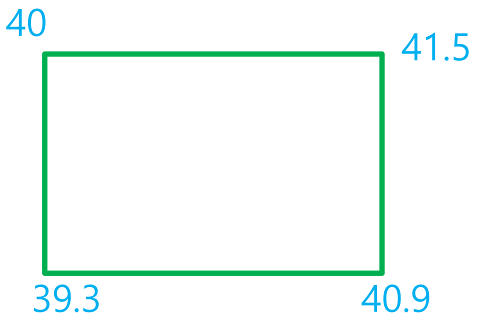
Example 1 (First-order RSM)

Step 2. Test for Interaction Estimate the Error

Test for Interaction ($\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$) whether β_{12} significant or not?

So, Hypothesis H0 = β_{12} = 0

Alternative H1 = $\beta_{12} \neq 0$



β_{12} can be estimated from factorial points.

So Interaction = $\frac{1}{2}$[Average of (39.3+41.5) – Average of (40+40.9)] = - 0.025

(or)

AB = $\frac{1}{2}$(41.5+39.3-40.9-40]

Hence, Interaction = AB/2 = $\frac{1}{4}$(41.5+39.3-40.9-40] = -0.025

Example 1 (First-order RSM)

Step 2. Test for Interaction Estimate the Error

Test for Interaction ($\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$) whether β_{12} significant or not?

Hence, Interaction = -0.025 with DOF = 1

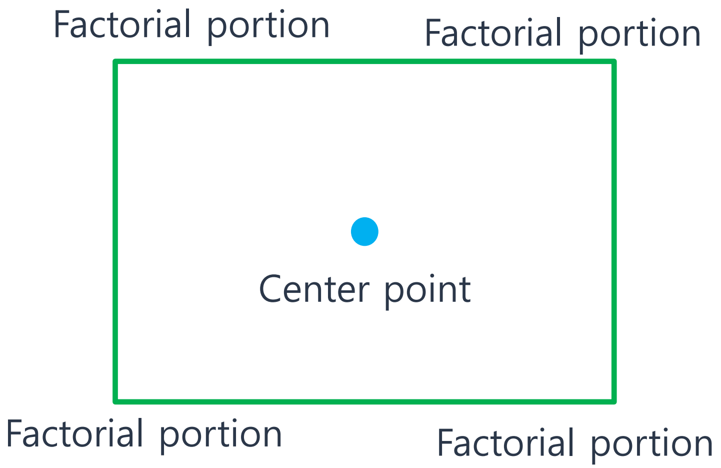
MS_E = 0.0430 with DOF = 4

We have to know whether interaction is significant or not, hence, compare the interaction value with MS_E

F = $\frac{(SS_{x_1 x_2}/DOF)}{MS_E} = \frac{\frac{(-0.1)^2}{4}}{0.0430} = 0.058$…which is small and insignificant or negligible.

Example 1 (First-order RSM)

- **Step 3: Test for Quadratic effects whether $\beta_{11} + \beta_{22}$ significant or not?**



whether $\beta_{11} + \beta_{22} = YF \; - YC$

$= 40.425 – 40.46 = -0.035$

Hypothesis H0 = $\beta_{11} + \beta_{22} = \; 0$

Alternative H1 =$\beta_{11} + \beta_{22} \neq 0$

$$SS_{\text{Pure Quadratic}} = \frac{n_F n_C (\bar{y}_F - \bar{y}_C)^2}{n_F + n_C} = \frac{(4)(5)(-0.035)^2}{4+5} = 0.0027$$

$$F = \frac{SS_{\text{Pure Quadratic}}}{\hat{\sigma}^2} = \frac{0.0027}{0.0430} = 0.063$$

0.063…which is small, hence, there is no indication of a pure quadratic effect.

So, quadratic effect not there…interaction effect not there…hence, the first-order model is fit one.

Example 1 (First-order RSM)

■ **TABLE 11.2**

Analysis of Variance for the First-Order Model

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	*P*-Value
Model (β_1, β_2)	2.8250	2	1.4125	47.83	0.0002
Residual	0.1772	6			
(Interaction)	(0.0025)	1	0.0025	0.058	0.8215
(Pure quadratic)	(0.0027)	1	0.0027	0.063	0.8142
(Pure error)	(0.1720)	4	0.0430		
Total	3.0022	8			

Example 1 (First-order RSM)

- Hence, we can say $\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$ is fit one…..
- However, we need to ensure whether the parameters β_1 and β_2 is significant….by doing **Test of Parameter Estimates**..
- For that, we need to identify the variance of β_i….i.e., V(β_i)

V(β_i) = $\frac{MS_E}{4}$

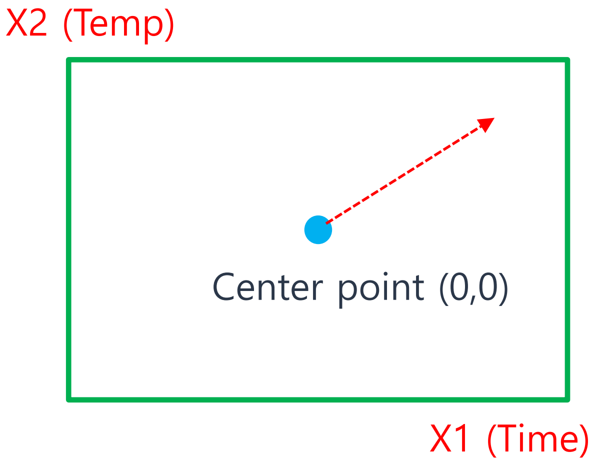
$\hat{y} = 40.44 + 0.775x_1 + 0.325x_2$

SE(β_i) = $\sqrt{\frac{MS_E}{4}} = \sqrt{\frac{0.0430}{4}} = \mathbf{0.1}$

Both regression coefficients and are large relative to their standard errors. At this point, we have no reason to question the adequacy of the first-order model.

Example 1 (First-order RSM)

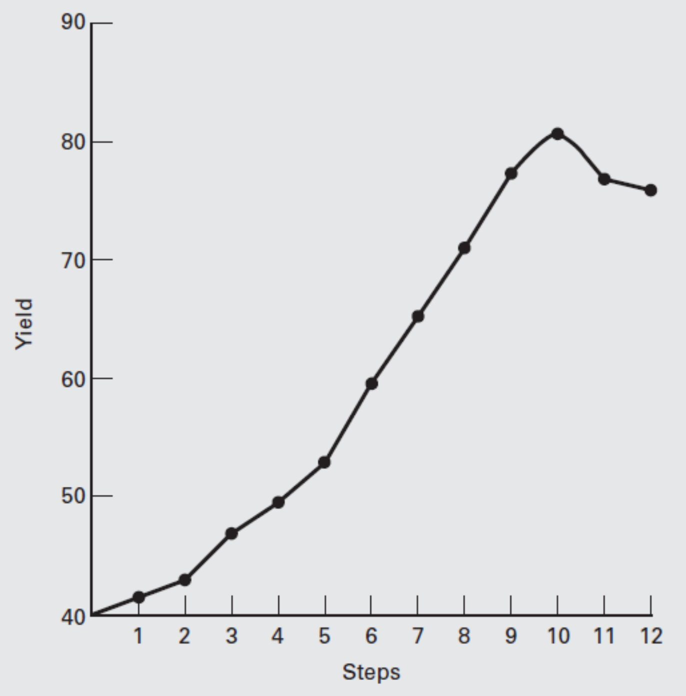
To move away from the design center—the point ($x_1 = 0$, $x_2 = 0$)—along the path of steepest ascent, we would move 0.775 units in the x_1 direction for every 0.325 units in the x_2 direction. Thus, the path of steepest ascent passes through the point ($x_1 = 0$, $x_2 = 0$) and has a slope 0.325/0.775. The engineer decides to use 5 minutes of reaction time as the basic step size. Using the relationship between ξ_1 and x_1, we see that 5 minutes of reaction time is equivalent to a step in the *coded* variable x_1 of $\Delta x_1 = 1$. Therefore, the steps along the path of steepest ascent are $\Delta x_1 = 1.0000$ and $\Delta x_2 = (0.325/0.775) = 0.42$.



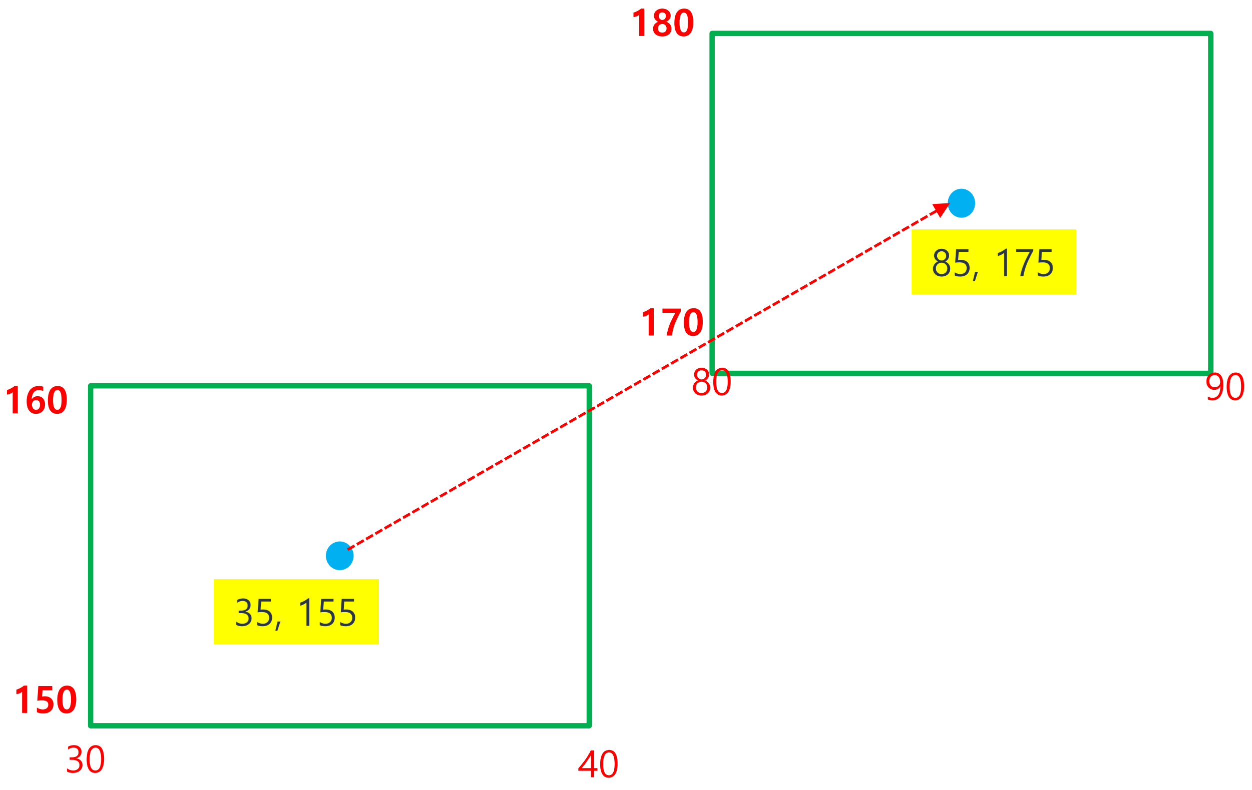
Steepest Ascent Experiment for Example 11.1

	Coded Variables		Natural Variables		Response
Steps	x_1	x_2	ξ_1	ξ_2	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

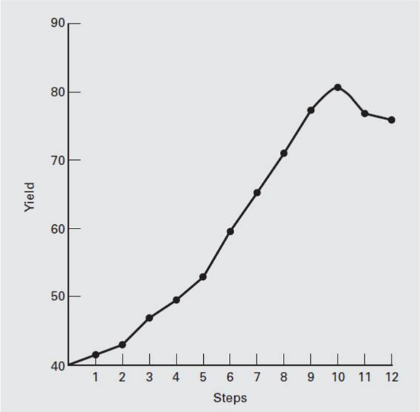
Example 1 (First-order RSM)



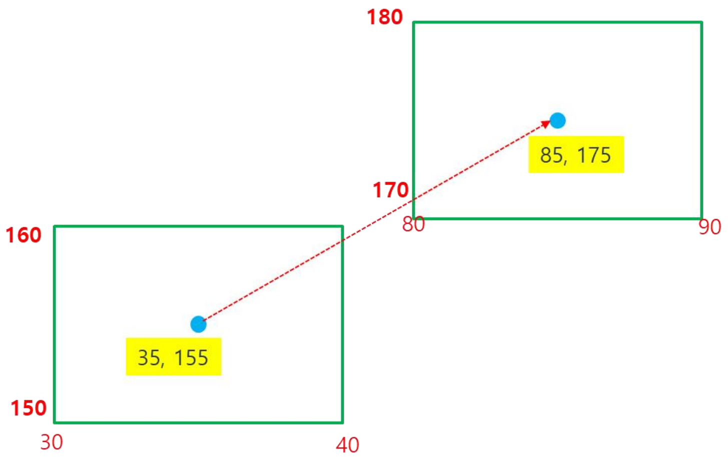
■ FIGURE 11.5 Yield versus steps along the path of steepest ascent for Example 11.1



Example 1 (First-order RSM)



■ **FIGURE 11.5** Yield versus steps along the path of steepest ascent for Example 11.1



Data for Second First-Order Model

Natural Variables		Coded Variables		Response
ξ_1	ξ_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

- The Figure shows the yield at each step along the path of steepest ascent. Increases in response are observed through the tenth step; however, all steps beyond this point result in a decrease in yield. Therefore, another first-order model should be fit in the general vicinity of the point ($\xi_1 = 85, \xi_2 = 175$).
- A new first-order model is fit around the point ($\xi_1 = 85, \xi_2 = 175$). The region of exploration for ξ_1 is [80, 90], and it is [170, 180] for ξ_2.

$$x_1 = \frac{\xi_1 - 85}{5} \quad \text{and} \quad x_2 = \frac{\xi_2 - 175}{5}$$

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

78.97 = Average of all Y observation (β_0)…

$$\beta_1 = \frac{1}{2}(Effect\ of\ X1) = \frac{1}{2}\left(\left(\frac{78+79.5}{2}\right) - \left(\frac{76.5+77}{2}\right)\right) = 1$$

$$\beta_2 = \frac{1}{2}(Effect\ of\ X2) = \frac{1}{2}\left(\left(\frac{77+79.5}{2}\right) - \left(\frac{376.5+78}{2}\right)\right) = 0.5$$

Example 1 (First-order RSM)

The analysis of variance for this model, including the interaction and pure quadratic term checks, is shown in Table 11.5. The interaction and pure quadratic checks imply that the first-order model is not an adequate approximation. This curvature in the true surface may indicate that we are near the optimum. At this point, additional analysis must be done to locate the optimum more precisely.

Analysis of Variance for the Second First-Order Model

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Square	F_0	P-Value	
Regression	5.00	2				
Residual	11.1200	6				
(Interaction)	(0.2500)	1	0.2500	4.72	0.0955	← Insignificant
(Pure quadratic)	(10.6580)	1	10.6580	201.09	0.0001	← Significant
(Pure error)	(0.2120)	4	0.0530			
Total	16.1200	8				

Findings:

- The **interaction** and **pure quadratic checks** imply that the **first-order model is not an adequate approximation**
- This **curvature in the true surface may indicate that we are near the optimum**

Analysis of a Second-Order Response Surface

When the experimenter is relatively close to the optimum, a model that incorporates curvature is usually required to approximate the response. In most cases, the second-order model

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j}\sum \beta_{ij} x_i x_j + \epsilon \qquad \textbf{(11.4)}$$

is adequate. In this section, we will show how to use this fitted model to find the optimum set of operating conditions for the x's and to characterize the nature of the response surface.

Analysis of a Second-Order Response Surface

11.3.1 Location of the Stationary Point

Suppose we wish to find the levels of $x_1, x_2, \ldots, x_k$ that optimize the predicted response. This point, if it exists, will be the set of $x_1, x_2, \ldots, x_k$ for which the partial derivatives $\partial\hat{y}/\partial x_1 = \partial\hat{y}/\partial x_2 = \cdots = \partial\hat{y}/\partial x_k = 0$. This point, say $x_{1,s}, x_{2,s}, \ldots, x_{k,s}$, is called the **stationary point**. The stationary point could represent a point of **maximum response**, a point of **minimum response**, or a **saddle point**. These three possibilities are shown in Figures 11.6, 11.7, and 11.8.

Contour plots play a very important role in the study of the response surface. By generating contour plots using computer software for response surface analysis, the experimenter can usually characterize the shape of the surface and locate the optimum with reasonable precision.

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

$$\hat{y} = \hat{\beta}_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x} \qquad \textbf{(11.5)}$$

Analysis of a Second-Order Response Surface

where

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

That is, **b** is a ($k \times 1$) vector of the first-order regression coefficients and **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 **x** equated to **0** is

$$\frac{\partial \hat{y}}{\partial \mathbf{x}} = \mathbf{b} + 2\mathbf{B}\mathbf{x} = \mathbf{0} \tag{11.6}$$

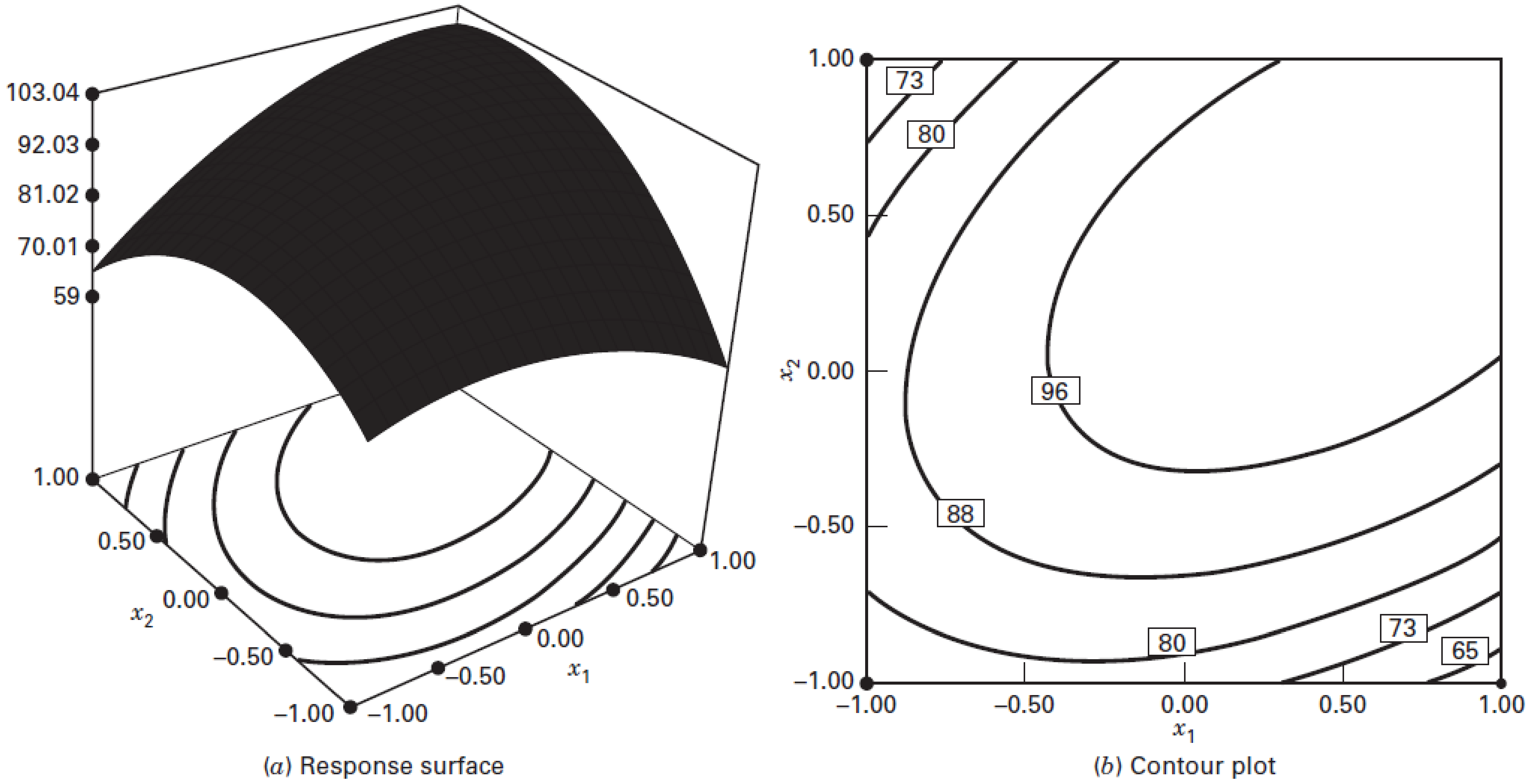
The stationary point is the solution to Equation 11.6, or

$$\mathbf{x}_s = -\frac{1}{2}\mathbf{B}^{-1}\mathbf{b} \tag{11.7}$$

Furthermore, by substituting Equation 11.7 into Equation 11.5, we can find the predicted response at the stationary point as

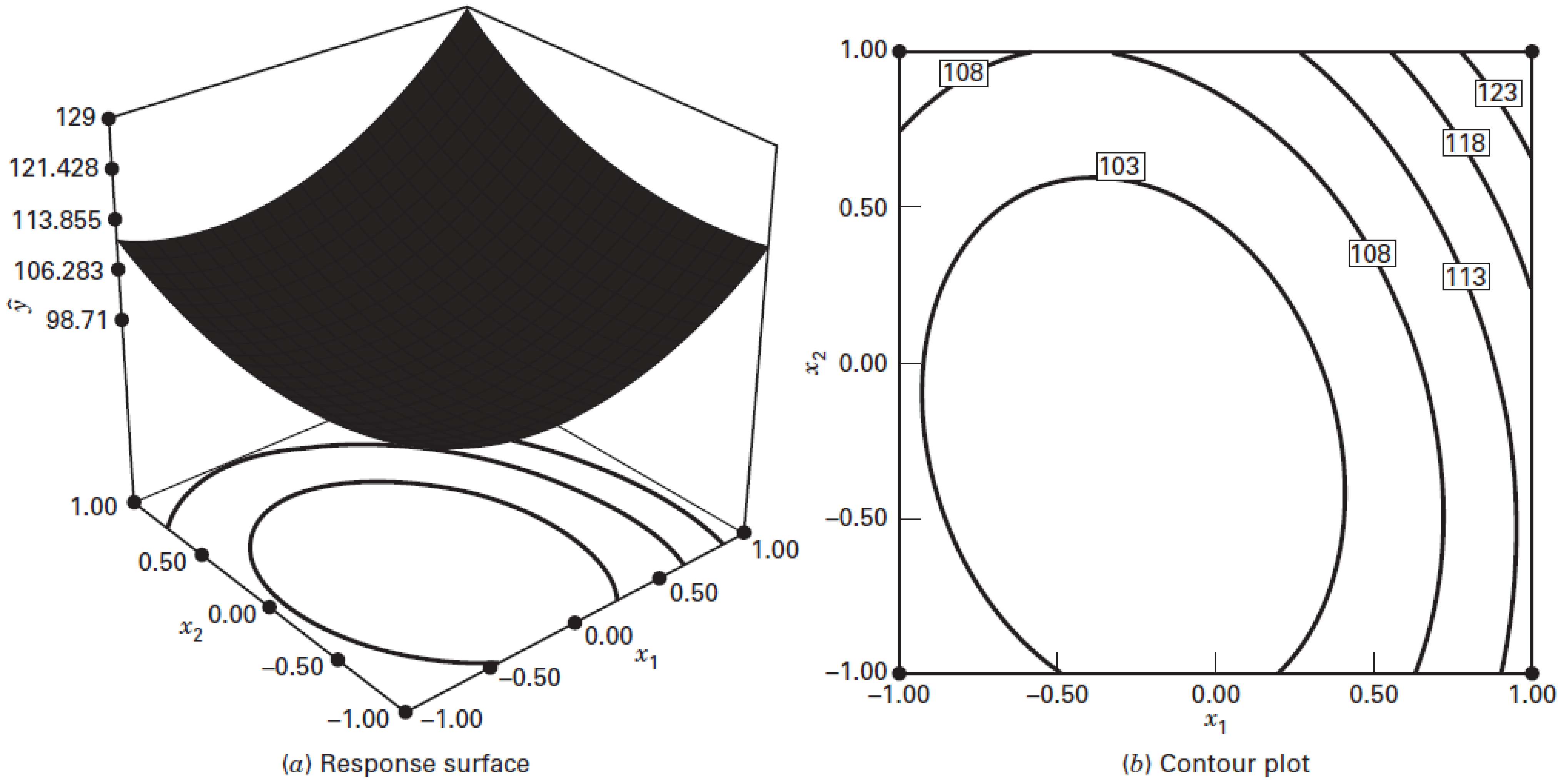
$$\hat{y}_s = \hat{\beta}_0 + \frac{1}{2}\mathbf{x}_s'\mathbf{b} \tag{11.8}$$

Analysis of a Second-Order Response Surface



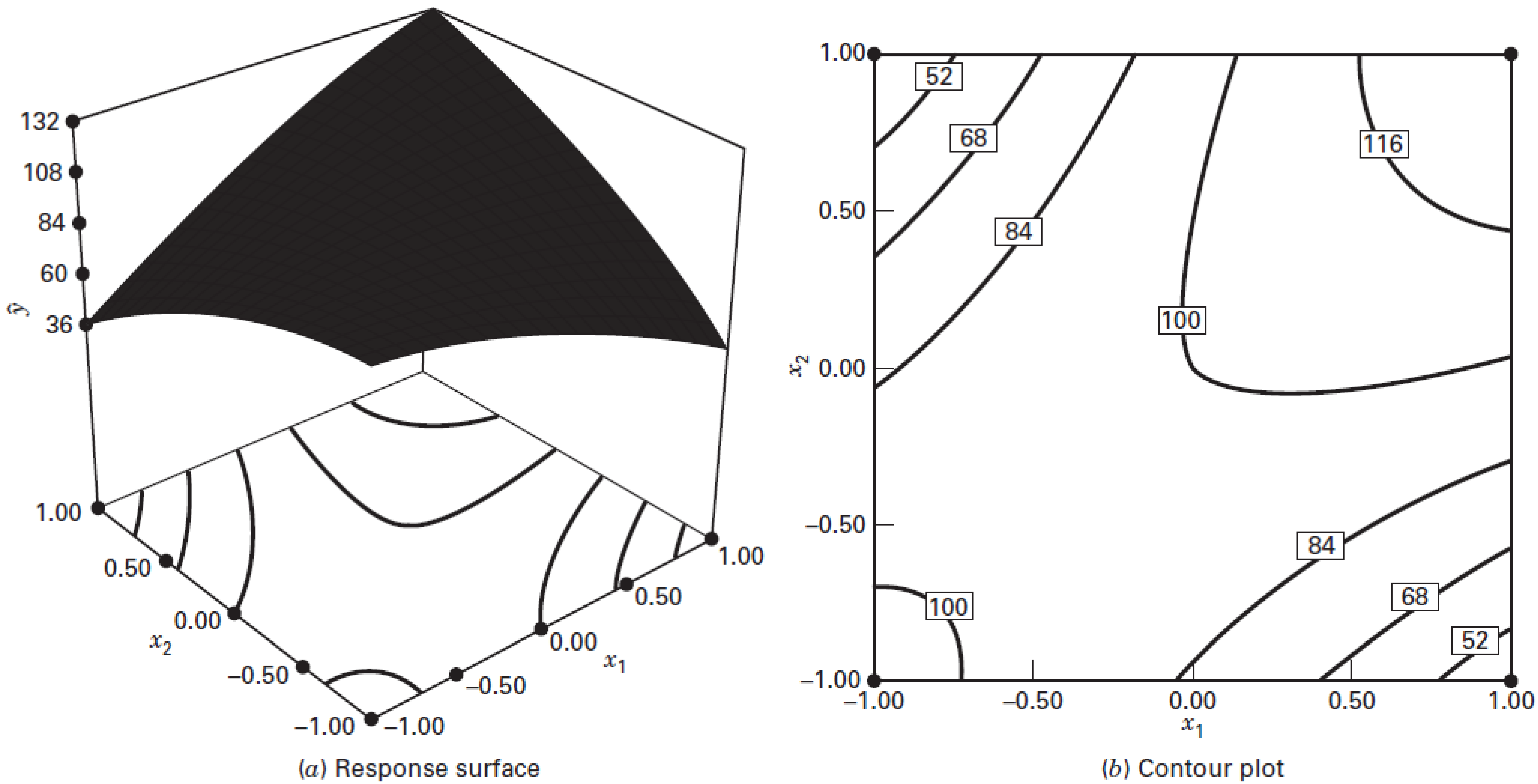
■ **FIGURE 11.6** Response surface and contour plot illustrating a surface with a maximum

Analysis of a Second-Order Response Surface



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

Analysis of a Second-Order Response Surface



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

Example for Second-Order Response Surface.

Response surface for certain manufacturing process was defined by the given equation($Z = 17x_1 + 27x_2 - x_1^2 - 0.9x_2^2$). Determine the approximate optimum operating point using the method of steepest ascent. The starting point of research should be X1=2 and X2=3 and step size C=4.

$Z = 17x_1 + 27x_2 - x_1^2 - 0.9x_2^2$

Step size = 4.0

$x_1 = 2; x_2 = 3$

$Z(2,3) = 17x_1 + 27x_2 - x_1^2 - 0.9x_2^2 = 17(2) + 27(3) - 2^2 \ - 0.9(3^2\ ) = 102.9$

$$Gradient\ of x_1 = G1.P. = \frac{\partial z}{\partial x_1} = 17 - 2x_1$$

$$Gradient\ of x_2 = G2.P. = \frac{\partial z}{\partial x_2} = 27 - 1.8x_2$$

Example.

$Magnitude\ m_1 = \mathrm{Sqrt}\ ((\mathrm{G_1P})^2 + (\mathrm{G_2P})^2)$
$G_1P = 17 - 2x_1, where\ x_1 = 2$
$G_1P = 13$
$G_2P = 27 - 1.8x_2, where\ x_2 = 3$
$G_2P = 21.6$

Hence, $Magnitude\ m_1 = 25.2$

New, x1 and x2..i.e., $x_1' and x_2'$

$x_1' = x_1 + C\left(\frac{G_1P}{m}\right) = 4.063$
$x_2' = x_2 + C\left(\frac{G_2P}{m}\right) = 6.43$

Example.

$Then, Z(x_1', x_2') = \mathrm{Z}(4.063, 6.43) = 17x_1 + 27x_2 - x_1^2 - 0.9x_2^2$ = 188.981

$G_1P = \ 17 - 2x_1, where\ x_1 = 4.063$

$G_1P = 8.874$

$G_2P = 27 - 1.8x_1, where\ x_2 = 6.43$

$G_2P = 15.426$

$Magnitude\ m_1 = \mathrm{Sqrt}\ ((\mathrm{G_1P})^2 + (\mathrm{G_2P})^2) = 17.79$

New, x1 and x2..i.e., $x_1' and x_2'$

$$New\ x_1 = x_1 + C\left(\frac{G_1P}{m}\right) = 6.06$$

$$New\ x_2 = x_2 + C\left(\frac{G_2P}{m}\right) = 9.89$$

$Then, Z(x_1', x_2') = \mathrm{Z}(6.06, 9.89) = 17x_1 + 27x_2 - x_1^2 - 0.9x_2^2$ = 245.3

Example.

$Then, Z(x_1', x_2') = Z(6.06, 9.89) = 17x_1 + 27x_2 - x_1^2 - 0.9x_2^2$ = 245.3

$G_1P = \ 17 - 2x_1, where\ x_1 = 6.06$

$G_1P = 4.88$

$G_2P = 27 - 1.8x_1, where\ x_2 = 9.89$

$G_2P = 9.198$

$Magnitude\ m_1 = \mathrm{Sqrt}\ ((\mathrm{G_1P})^2 + (\mathrm{G_2P})^2) = 10.41$

New, x1 and x2..i.e., $x_1' and x_2'$

$New\ x_1 \ = x_1 \ + C\left(\frac{G_1P}{m}\right) = 7.935$

$New\ \ x_2 \ = x_2 \ + C\left(\frac{G_2P}{m}\right) = 13.42$

$Then, Z(x_1', x_2') = Z(7.935, 13.42) = 17x_1 + 27x_2 - x_1^2 - 0.9x_2^2$ = 272.19

Example.

$Then, Z(x_1', x_2') = \mathrm{Z}(7.935, 13.42) = 17x_1 + 27x_2 - x_1^2 - 0.9x_2^2$ = 272.19

$G_1P = \ 17 - 2x_1, where\ x_1 = 7.935$

$G_1P = 1.13$

$G_2P = 27 - 1.8x_1, where\ x_2 = 13.42$

$G_2P = 2.844$

$Magnitude\ m_1 = \mathrm{Sqrt}\ ((\mathrm{G_1P})^2 + (\mathrm{G_2P})^2) = 3.06$

New, x1 and x2..i.e., $x_1' and x_2'$

$$New\ x_1 \ = x_1 \ + C\left(\frac{G_1P}{m}\right) = 9.412$$

$$New\ \ x_2 \ = x_2 \ + C\left(\frac{G_2P}{m}\right) = 17.13$$

$Then, Z(x_1', x_2') = \mathrm{Z}(7.935, 13.42) = 17x_1 + 27x_2 - x_1^2 - 0.9x_2^2$ = 269.84

Example.

$Final\ points$:

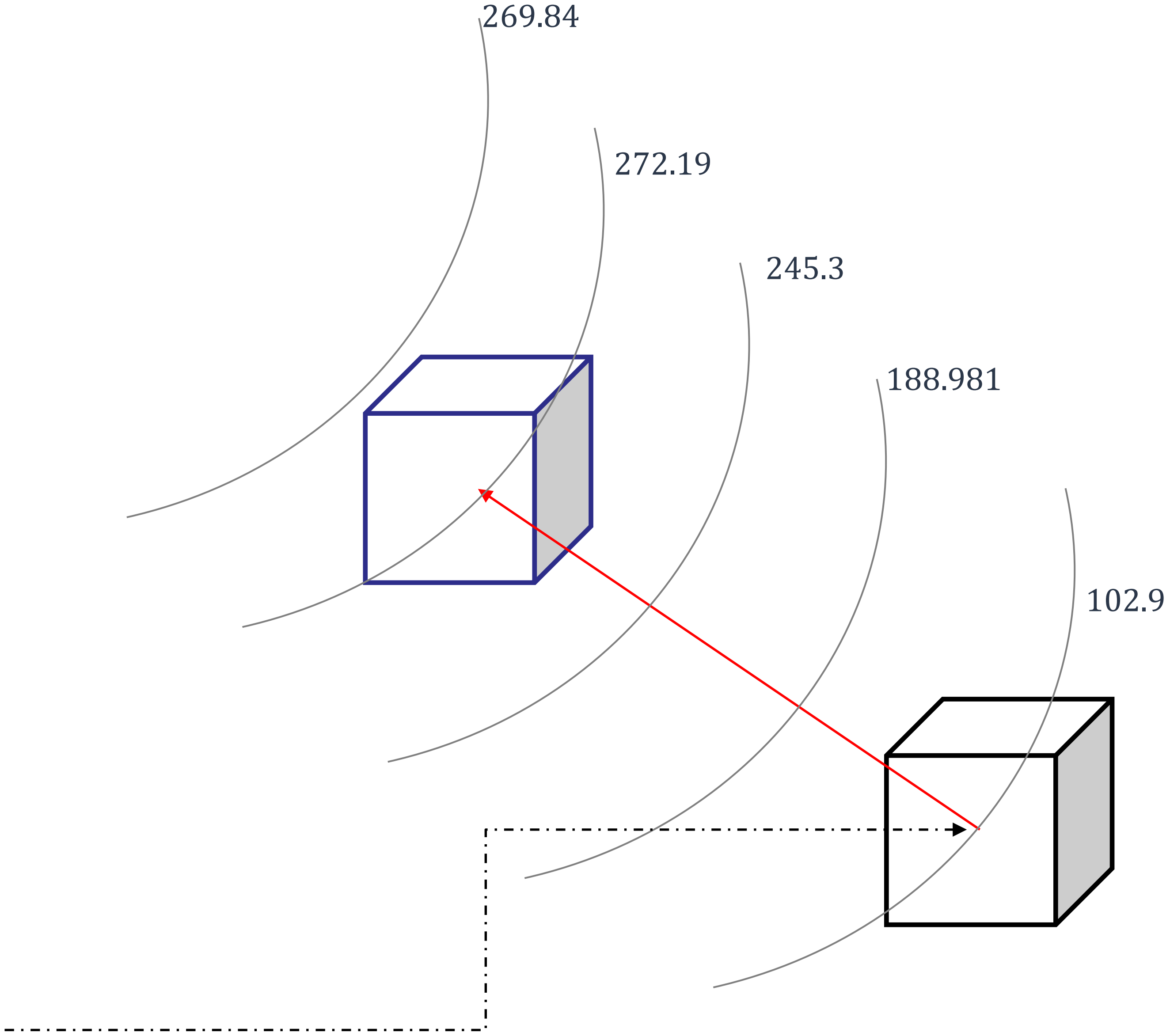
$Z(2,3) = 102.9$

$Z(4.063,6.43) = 188.981$

$Z(6.06,9.89) = 245.3$

$Z(7.935,13.42) = 272.19$

$Z(9.412,17.13) = 269.84$



Optimum region

Contours of constant response

Current operating condition

Features for selecting response surface design

Experimental Designs for Fitting Response Surfaces

When selecting a response surface design, some of the features of a desirable design are as follows:

1. Provides a reasonable distribution of data points (and hence information) throughout the region of interest
2. Allows model adequacy, including lack of fit, to be investigated
3. Allows experiments to be performed in blocks
4. Allows designs of higher order to be built up sequentially
5. Provides an internal estimate of error
6. Provides precise estimates of the model coefficients
7. Provides a good profile of the prediction variance throughout the experimental region
8. Provides reasonable robustness against outliers or missing values
9. Does not require a large number of runs
10. Does not require too many levels of the independent variables
11. Ensures simplicity of calculation of the model parameters

Design for fitting the Second-Order Model

There are two main types of response surface designs:

- **Central Composite designs (CCD)**
  - Central Composite designs can fit a full quadratic model. They are often used when the design plan calls for sequential experimentation because these designs can include information from a correctly planned factorial experiment.
- **Box-Behnken designs (BBD)**
  - Box-Behnken designs usually have fewer design points than central composite designs, thus, they are less expensive to run with the same number of factors. They can efficiently estimate the first- and second-order coefficients; however, they **can't include runs** from a factorial experiment. Box-Behnken designs **always have 3 levels per factor**, unlike central composite designs which can have up to 5. Also unlike central composite designs, Box-Behnken designs never include runs where all factors are at their extreme setting, such as all of the low settings.

Central Composite designs (CCD)

Central Composite designs (CCD)

- A central composite design is the most commonly used response surface designed experiment. **Central composite designs are a factorial or fractional factorial design with center points, augmented with a group of axial points (also called star points) that let you estimate curvature.** You can use a central composite design to:
  - Efficiently estimate first- and second-order terms.
  - Model a response variable with curvature by adding center and axial points to a previously-done factorial design.
- Central composite designs are especially useful in sequential experiments because you can often build on previous factorial experiments by adding axial and center points.

Central Composite designs (CCD)

Central Composite designs (CCD)

- For example, you would like to determine the best conditions for injection-molding a plastic part. You first run a factorial experiment and determine the significant factors: temperature (levels set at 190° and 210°) and pressure (levels set at 50MPa and 100MPa). If the factorial design detects curvature, you can use a response surface designed experiment to determine the optimal settings for each factor.

Central Composite designs (CCD)

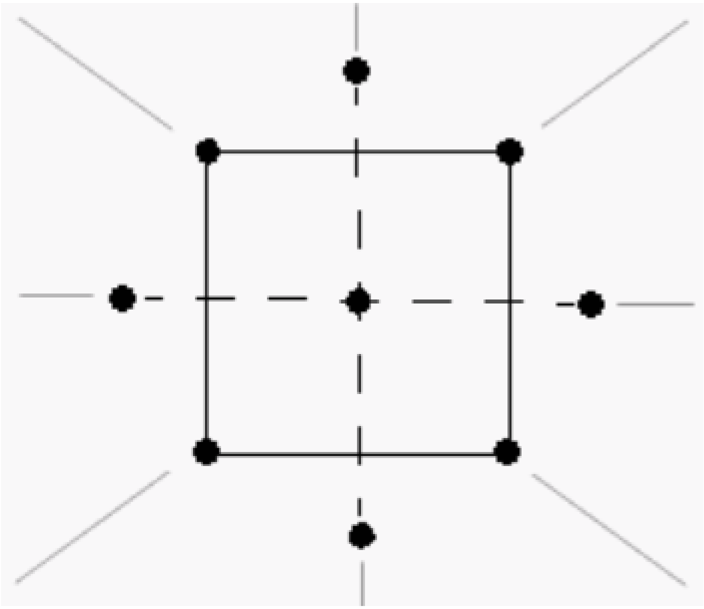
Central Composite designs (CCD)..continued

210°, 50MPa

214.1°, 75MPa (axial point)

210°, 100MPa

200°, 39.6MPa (axial point)



200°, 110.4MPa (axial point)

190°, 50MPa

185.9°, 75MPa (axial point)

190°, 100MPa

Central Composite designs (CCD)

Three parts:

1.

Factorial or reduced factorial design

Estimate of main effects and interactions

2.

At least one center point experiment

Possible to reveal curvature and estimate the experimental error

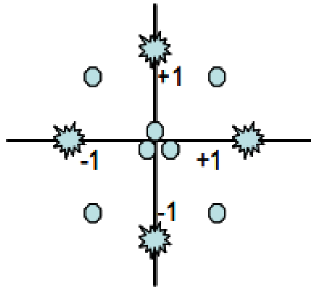
3.

Experiments $\pm\alpha$ on the variable axes

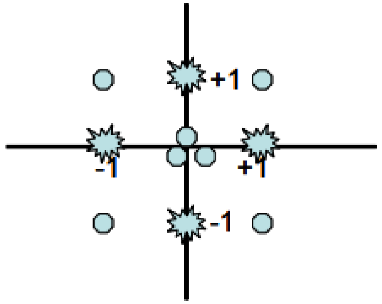
Possible to estimate quadratic terms

$$\alpha = \sqrt[4]{N_{FD}}$$

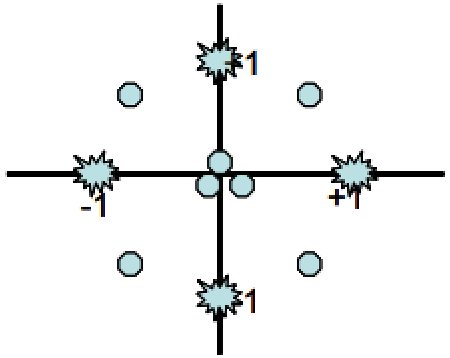
Central Composite designs (CCD)



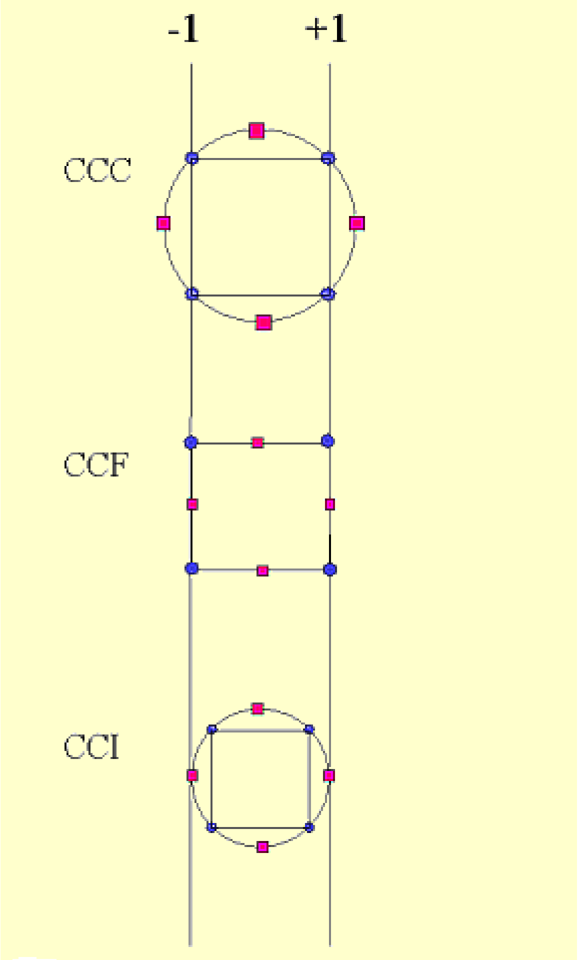
. CCC design for two factors.



. CCF design for two factors.



. CCI design for two factors



Comparison of the Three Types of

Central Composite Design (CCD) has three different design points: edge points as in two- level designs (±1), star points at ±α; |α 1≥| |that take care of quadratic effects and centre points,

Three variants exist:

1. Circumscribed (CCC)
2. Face centered (CCF)
3. Inscribed (CCI)

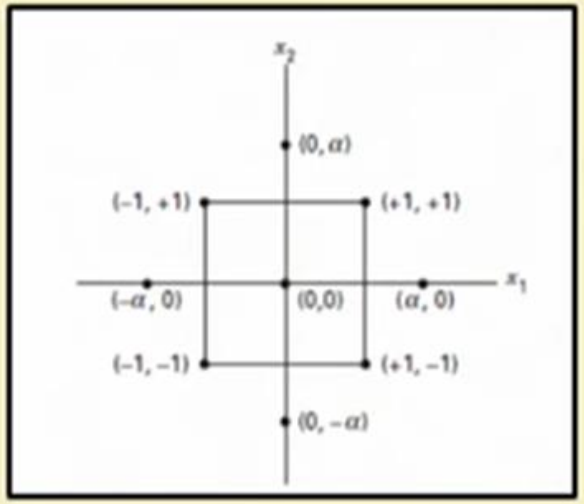
Central Composite designs (CCD)

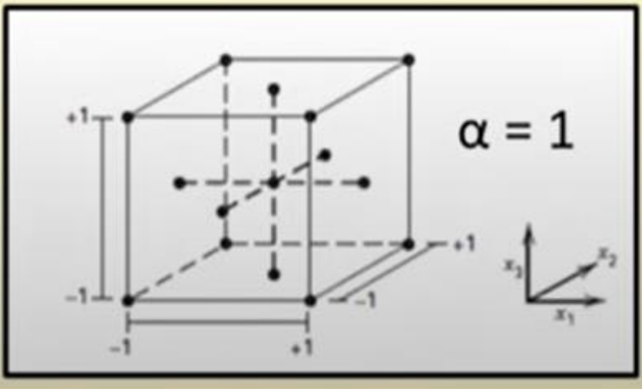
Design for fitting the second-order model

- Central composite design or CCD
- Box-Behnken Design

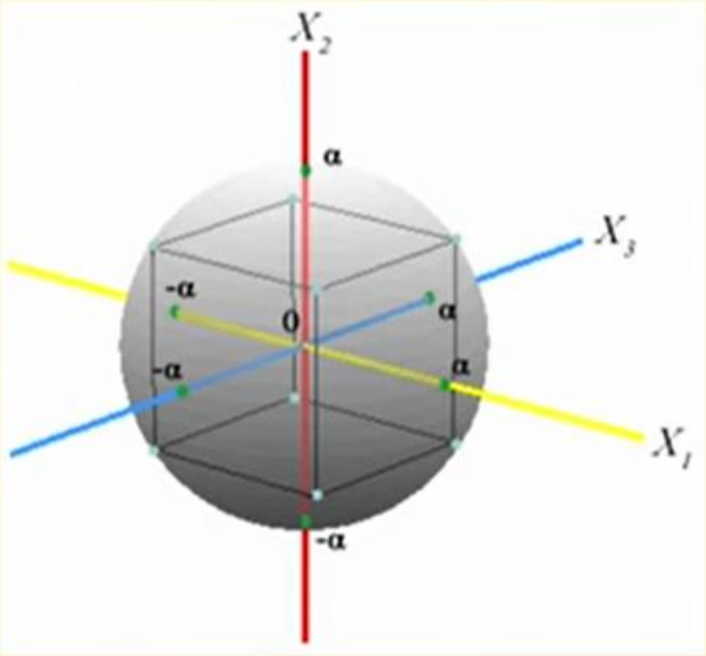
- **CCD** consists of a 2^k factorial (or 2^{k-p} with resolution V) with n_F factorial runs, $2k$ axial or star runs, and n_C center runs
- Choice of α
  - Spherical CCD: $\alpha = (k)^{1/2}$
  - Rotatable CCD: $\alpha = (n_F)^{1/4}$
  - Face-centered CCD: $\alpha = 1$

CCD for k=2





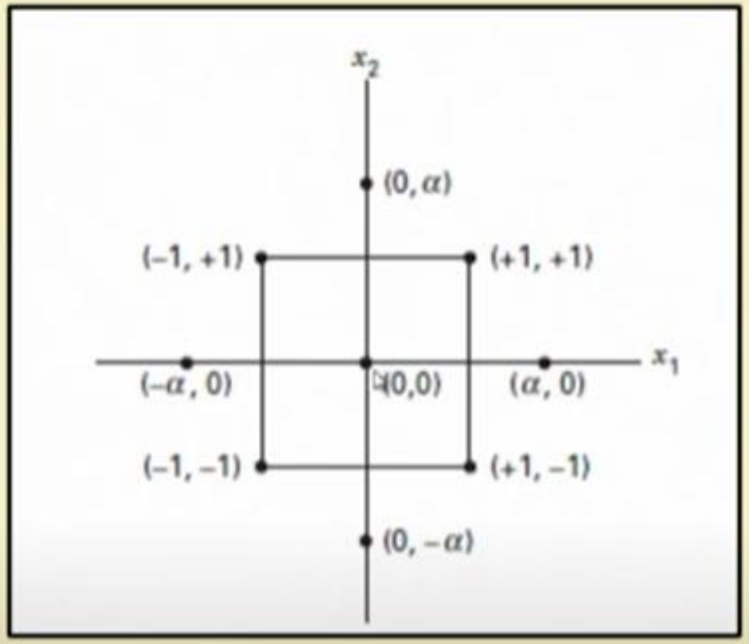
CCD for k=3



n_f = The number of factorial run

Central Composite designs (CCD)

CCD Example



Natural Variables		Coded Variables	
ξ_1	ξ_2	x_1	x_2
80	170	−1	−1
80	180	−1	1
90	170	1	−1
90	180	1	1
85	175	0	0
85	175	0	0
85	175	0	0
85	175	0	0
85	175	0	0
92.07	175	1.414	0
77.93	175	−1.414	0
85	182.07	0	1.414
85	167.93	0	−1.414

Central composite rotatable design for two variables

	x_1	x_2
Factorial points	-1	-1
(2^2)	1	-1
	-1	1
	1	1
Center points	0	0
	0	0
	.	.
	0	0
Axial points	-1.414	0
$\alpha=(4)^{1/4} \approx 1.414$	1.414	0
	0	-1.414
	0	1.414

Number of experiments: $2^3 + 4 + 6 = \underline{18}$

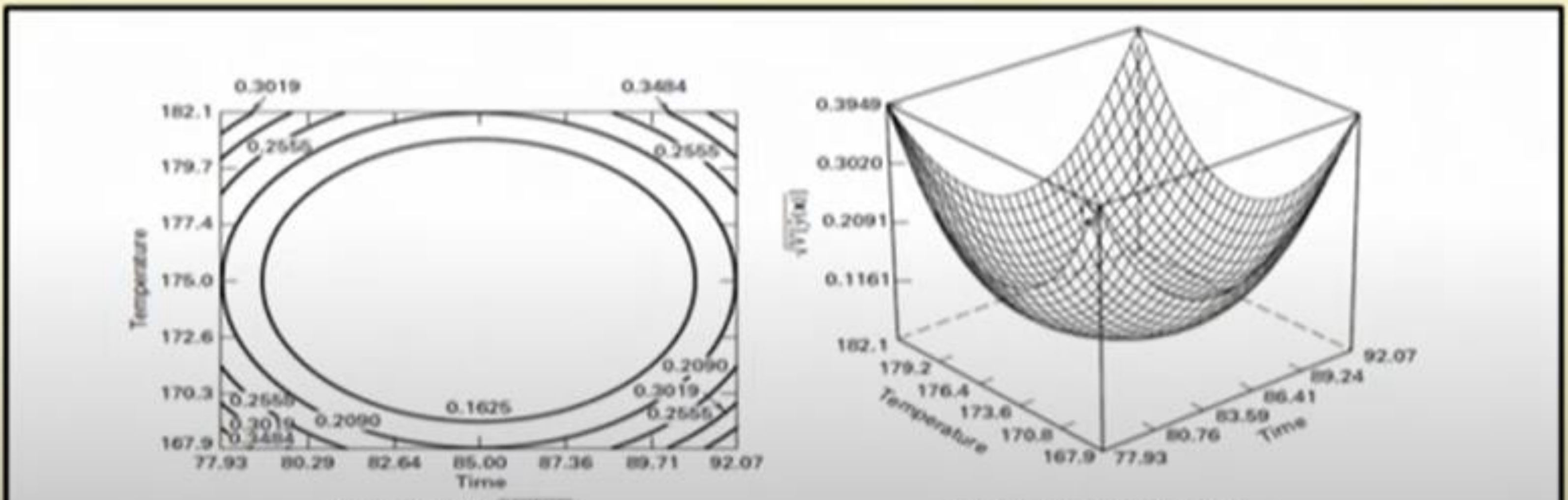
Central composite rotatable design for three variables

	x_1	x_2	x_3
Factorial points (2^3)	-1	-1	-1
	1	-1	-1
	-1	1	-1
	1	1	-1
	-1	-1	1
	1	-1	1
	-1	1	1
	1	1	1
Center points	0	0	0
	0	0	0
	.	.	.
	.	.	.
	0	0	0
Axial points $\alpha=(8)^{1/4} \approx 1.682$	-1.682	0	0
	1.682	0	0
	0	-1.682	0
	0	1.682	0
	0	0	-1.682
	0	0	1.682

Central Composite designs (CCD)

CCD (Contd.)

- **Rotatability**: An experimental design is said to be rotatable if the variance of the predicted response at any point is a function of the distance from the centre point alone
- The variance of the predicted response at some point x is $V[\hat{y}(x)] = \sigma^2 x'(X'X)^{-1}x$
- This variance is the same at all points x that are at the same distance from the design centre



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

(b) The response surface plot

Central Composite designs (CCD)

Number of runs required for CCD and its types, and 3^k design

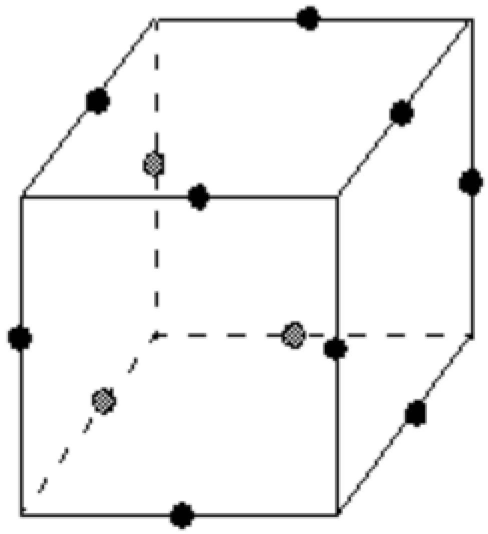
CCD (Contd.)

		K=2	K=3	K=4	K=5
CCD	Factorial points	4	8	16	32
	Axial points	4	6	8	10
	Centre points	5	5	6	6
	Total	13	19	30	48
3^k Designs		9	27	81	243
Choice of α	Spherical	1.4	1.73	2	2.24
	Rotatable	1.4	1.68	2	2.38

Box-Behnken designs (BBD)

Box-Behnken designs (BBD)

- Box-Behnken designs have treatment combinations that are at the midpoints of the edges of the experimental space and require at least three continuous factors. The following figure shows a three-factor Box-Behnken design. Points on the diagram represent the experimental runs that are done:



Box-Behnken designs (BBD)

Box-Behnken designs (BBD)

- A Box-Behnken design is a type of response surface design that does not contain an embedded factorial or fractional factorial design.
- For example, you would like to determine the best conditions for injection-molding a plastic part. The factors you can set are:
  - Temperature: 190° and 210°
  - Pressure: 50Mpa and 100Mpa
  - Injection speed: 10 mm/s and 50 mm/s
- For a Box-Behnken design, the design points fall at combinations of the high and low factor levels and their midpoints:
  - Temperature: 190°, 200°, and 210°
  - Pressure: 50Mpa, 75Mpa, and 100Mpa
  - Injection speed: 10 mm/s, 30 mm/s, and 50 mm/s

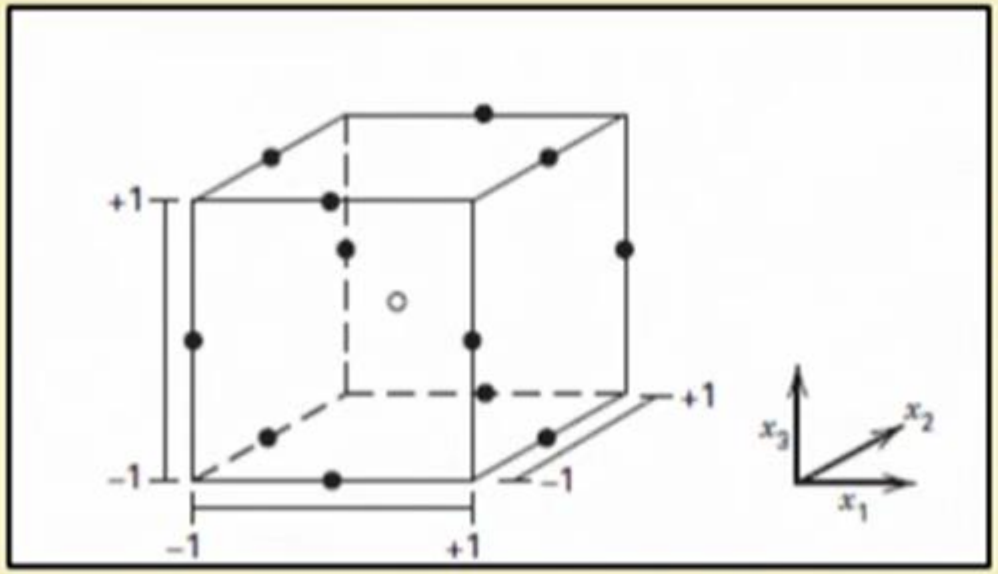
Box-Behnken designs (BBD)

The Box-Behnken Design (BBD)

- Box and Behnken (1960) designs are three-level factorial designs
- Formed by combining 2^k factorials with incomplete block designs.
- Is a spherical design, with all points lying on a sphere of radius $(2)^{1/2}$
- Does not contain any points at the vertices of the cubic
- Used to estimate 2nd degree polynomial
- No general rules for defining samples. So, tables are provided by the authors

Box-Behnken designs (BBD)

The Box-Behnken Design (BBD) – Example, k=3



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

Box-Behnken designs (BBD)

The Box-Behnken Designs (BBD) for Different k

Three factors:

$$\begin{bmatrix} \pm1 & \pm1 & 0 \\ \pm1 & 0 & \pm1 \\ 0 & \pm1 & \pm1 \\ 0 & 0 & 0 \end{bmatrix}$$

Four factors:

$$\begin{bmatrix} \pm1 & \pm1 & 0 & 0 \\ 0 & 0 & \pm1 & \pm1 \\ 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots \\ \pm1 & 0 & 0 & \pm1 \\ 0 & \pm1 & \pm1 & 0 \\ 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots \\ \pm1 & 0 & \pm1 & 0 \\ 0 & \pm1 & 0 & \pm1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Five factors:

$$\begin{bmatrix} \pm1 & \pm1 & 0 & 0 & 0 \\ 0 & 0 & \pm1 & \pm1 & 0 \\ 0 & \pm1 & 0 & 0 & \pm1 \\ \pm1 & 0 & \pm1 & 0 & 0 \\ 0 & 0 & 0 & \pm1 & \pm1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \pm1 & \pm1 & 0 & 0 \\ \pm1 & 0 & 0 & \pm1 & 0 \\ 0 & 0 & \pm1 & 0 & \pm1 \\ \pm1 & 0 & 0 & 0 & \pm1 \\ 0 & \pm1 & 0 & \pm1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Box-Behnken designs (BBD)

Comparison between CCD and BBD in terms of number of runs (N)

Number of factors	Box Behnken	Central Composite
2	-	13 (5 center points)
3	15	20 (6 center point runs)
4	27	30 (6 center point runs)
5	46	33 (fractional factorial) or 52 (full factorial)
6	54	54 (fractional factorial) or 91 (full factorial)

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