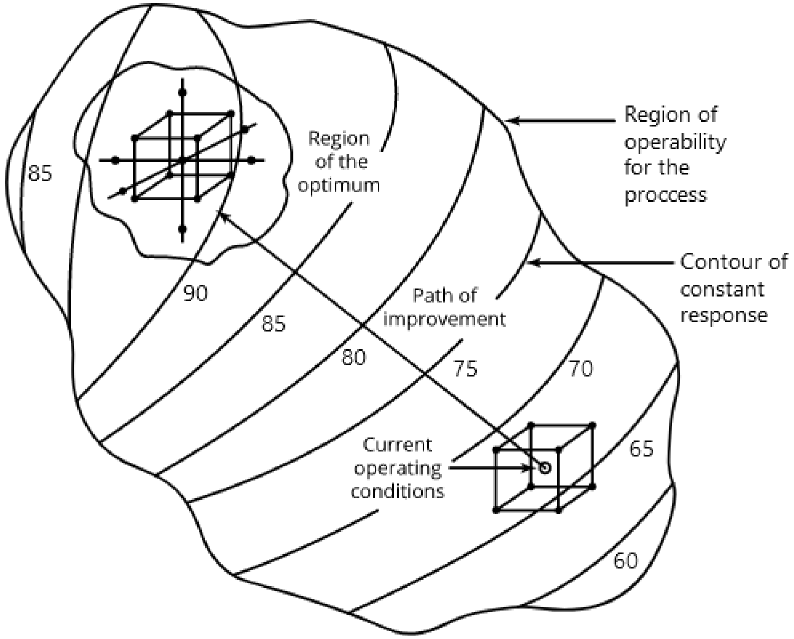
Why RSM?

- So far, the focus of the design of experiments was ***'factor screening'*** – which factors strongly affect the process, which factors are less important, how the factors interact ..
- After screening, we now shift our focus to ***optimization*** – which factor level combinations give us maximum (e.g. yield) or minimum (e.g. cost), or target result.
- *The objective of Response Surface Methods (RSM) is optimization, finding the best set of factor levels to achieve some goal.*



Example

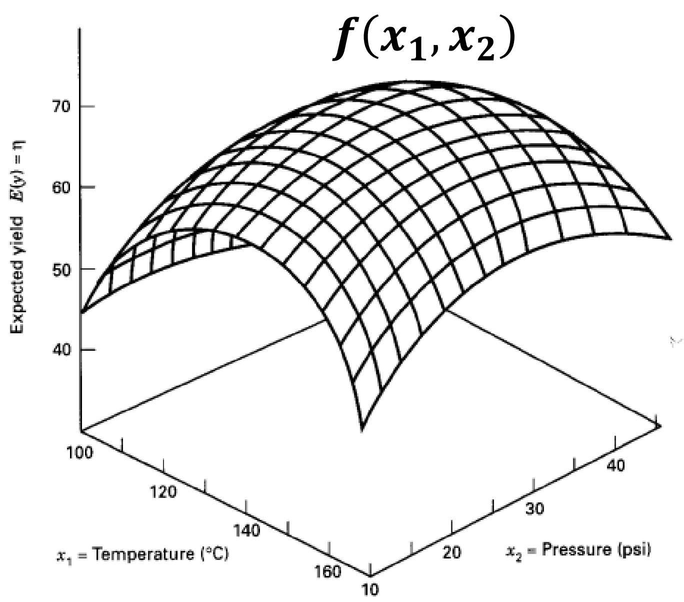
Suppose, yield (y) of a chemical process depends on temperature (x_1) and pressure (x_2). The chemical engineer would like to find out which levels of temperature and pressure give the maximum yield.

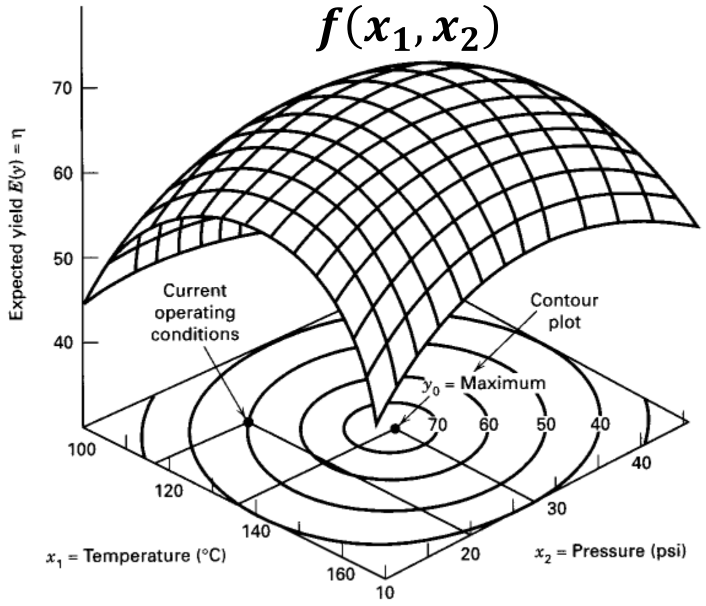
One may write, $$\boldsymbol{y = f(x_1, x_2) + \epsilon}$$

Where $'\epsilon'$ is the error/noise observed in response ‘y’

The expected value of the response ‘y’ will be **E(y) =** $\boldsymbol{f(x_1, x_2)}$

One could show this graphically,





Sequential Process

Always Remember: 'RSM' is sequential procedure

- In most problems, *the exact relationship between the response variable and the independent variables is unknown*
- Therefore, the first step in RSM is to *find a suitable approximation* of the true functional relationship between response and independent variables.
- Typically, the approximations are in the *form of low-order polynomials* in some region of independent variables

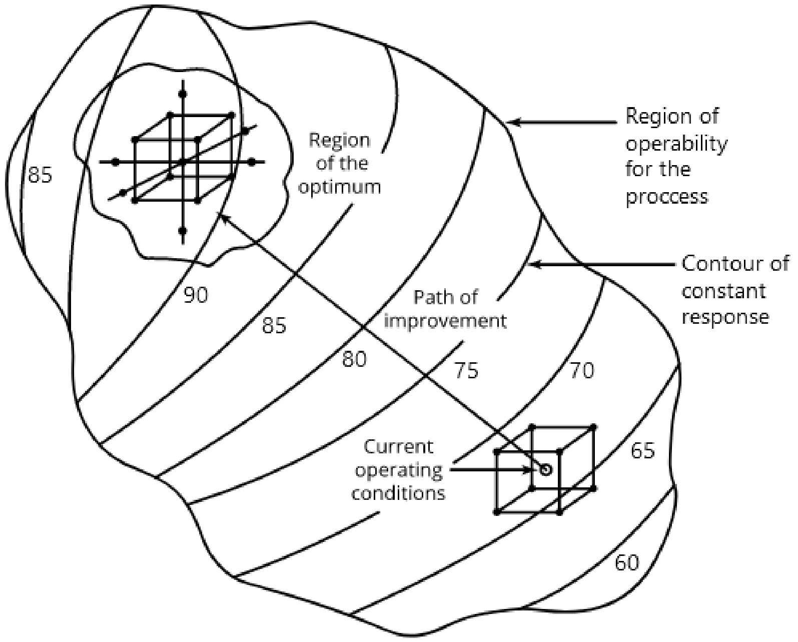
For example, if response (y) is well modeled by linear function of independent variables $(x_1, x_2, x_3, \dots, x_k)$, then we can write the approximate function as **'first order model'**

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

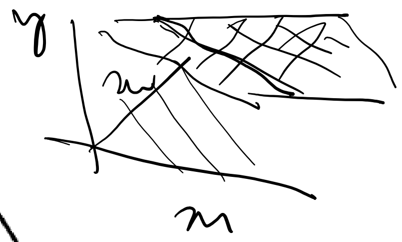
If there is curvature/non-linearity in the system, we must use polynomial of 2nd or higher degree,

For example, **second degree model** : $y = \beta_0 + \ \sum_{i=0}^{k} \beta_i x_i + \sum_{i=0}^{k} \beta_{ii} x_i^2 \ + \Sigma\Sigma\, \beta_{ij} x_i x_j + \epsilon$

- In real problems, it is unlikely that these polynomials will provide a reasonable approximation of the true functional relationship over the ENTIRE range of independent variables, but they work quite well for a relatively small region
- The coefficients in the RSM models (model parameters) are estimated using the least square method (least-square fitting)
- The response surface analysis is then performed on the fitted surface
- The model parameters can be obtained more effectively if proper experimental designs are used to collect the data (responses). *Designs for fitting the response surfaces are called response surface designs.*
- Often we start at a point that is far from optimum such as the existing operating conditions. If the region is linear, we use the first-order model.
- We then take the shortest and most efficient path towards the optimum
- As we near the optimum, there may be nonlinearities, so we can employ higher-order models



Method of Steepest Ascent



- If we want to find maximum response, then we will be 'climbing the hill', if we want to minimize the response, we will be 'descending into a valley'
- We then take the shortest and most efficient path towards the optimum
- 'Method of steepest ascent' is a procedure of moving sequentially along the path of steepest ascent, i.e., direction of the maximum increase in the response.
- If minimization is desired, we follow the 'method steepest descent'
- If we use first order model, $\hat{y} = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i$ ✓ $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2$

  Then, the contours of y will be a set of parallel lines

So the path of steepest ascent will be along a line perpendicular to the contours from center of the region

The actual step-size will be dependent on other practical considerations

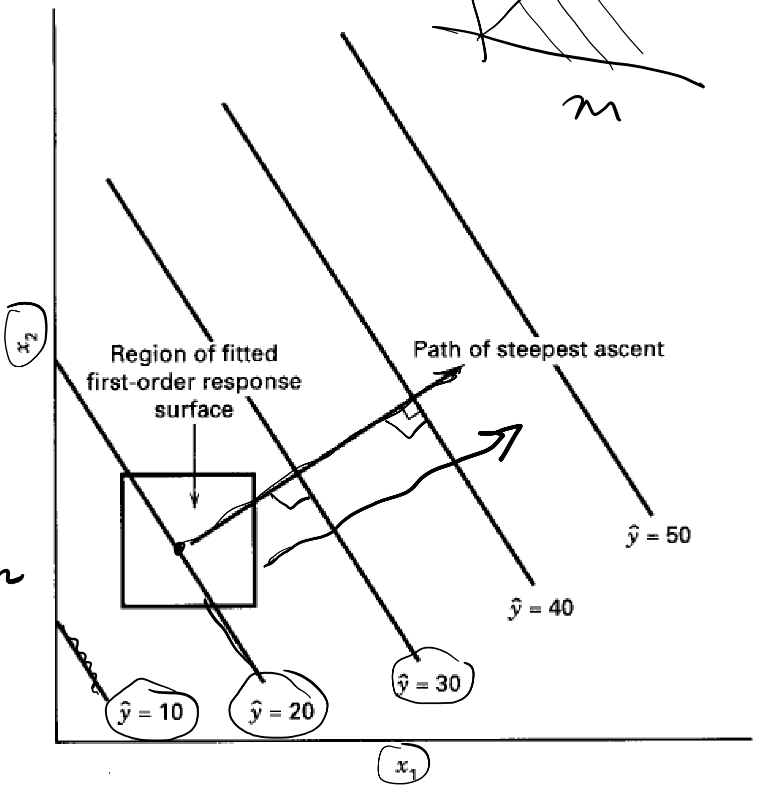


Figure 11-4 First-order response surface and path of steepest ascent.

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. Because it is unlikely that this region contains the optimum, she fits a first-order model and applies the method of steepest ascent.

Region of (30, 40) minutes of time, and (150, 160) F temperature was explored and responses were collected.

Note the experimental design is 2^2 factorial design augmented by five center points. 5 replications at the center point [35, 155] allow estimation of error as well as help us determine adequacy of linear (first-order) model

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

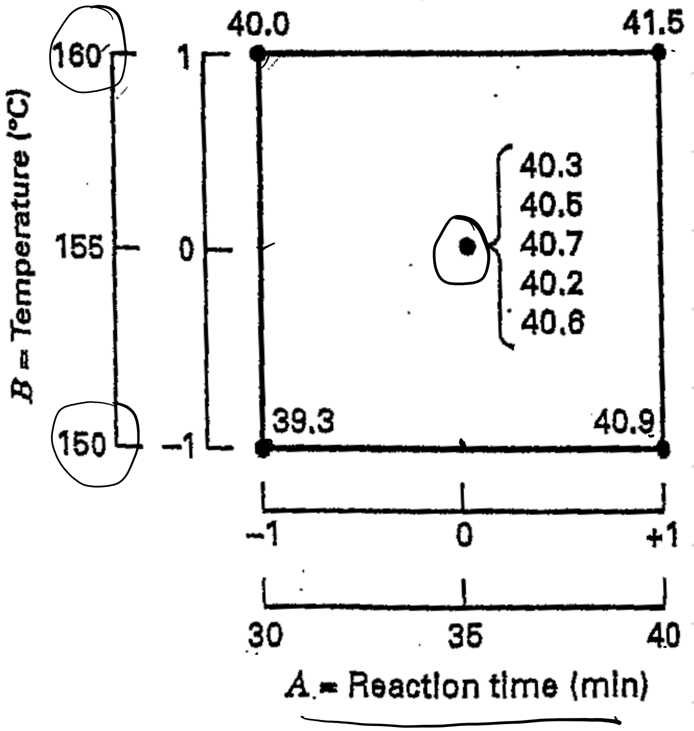
Time, Temp

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

Can we find which terms are important?

What will be the first-order model?

Will a first-order model be appropriate?



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

ANOVA

- ANOVA

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

?

can we reduce this to a 1-order model

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

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_1x_2	1	0.0025		0.06
mean	1			
ε	5-1	0.172		
and	1	?		

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

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

$$SS_{x_1x_2} = 2\left((40.45-40.425)^2 + (40.9-40.425)^2\right)$$

$$= 0.0025$$

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

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

$$=$$

Find $\underline{SS_{quad}} = \dfrac{n_F n_C (\bar{y}_F - \bar{y}_C)^2}{n_F + n_C} = \dfrac{4 \times 5 (40.425 - 40.46)^2}{9}$

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 β_{11} and β_{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

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

Method of Steepest Ascent

- 'Climbing the $\hat{y} = 40.44 + 0.775x_1 + 0.325x_2$

β_{00} β_1 β_2

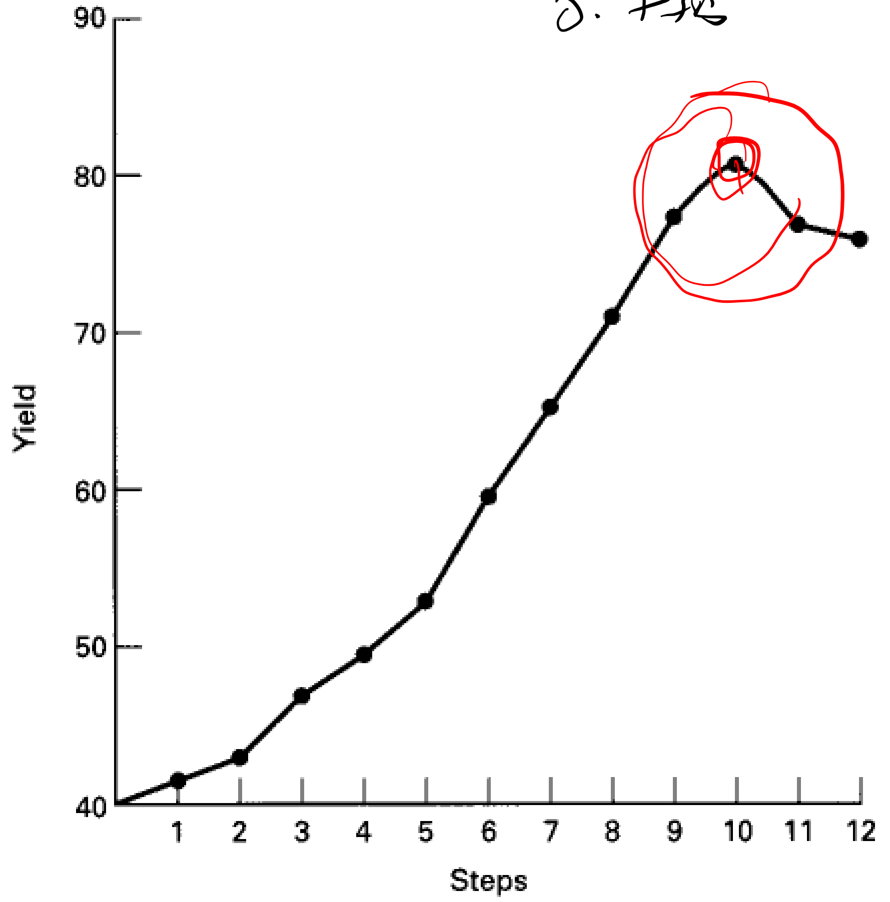
β_2/β_1

$\beta = (X^T X)^{-1} X^T Y$

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

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

Steps	Coded Variables x_1	Coded Variables x_2	Natural Variables ξ_1	Natural Variables ξ_2	Response y
Origin	0	0	35	155	40
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]

Table 11-4 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

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

$\beta_{11}x_1^2 + \beta_{22}x_2^2$

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.

Method of Steepest Ascent

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

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

β_2 / β_m

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 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

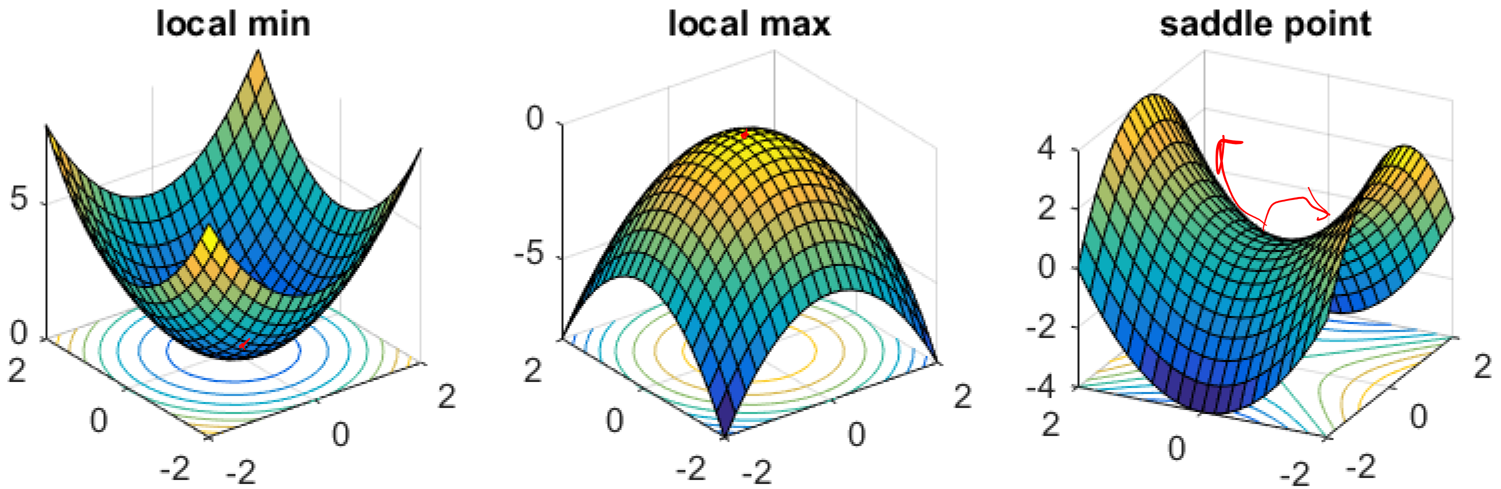
$$\Delta x_i = \frac{\hat{\beta}_i}{\hat{\beta}_j / \Delta x_j} \qquad i = 1, 2, \ldots, k; \qquad i \neq j$$

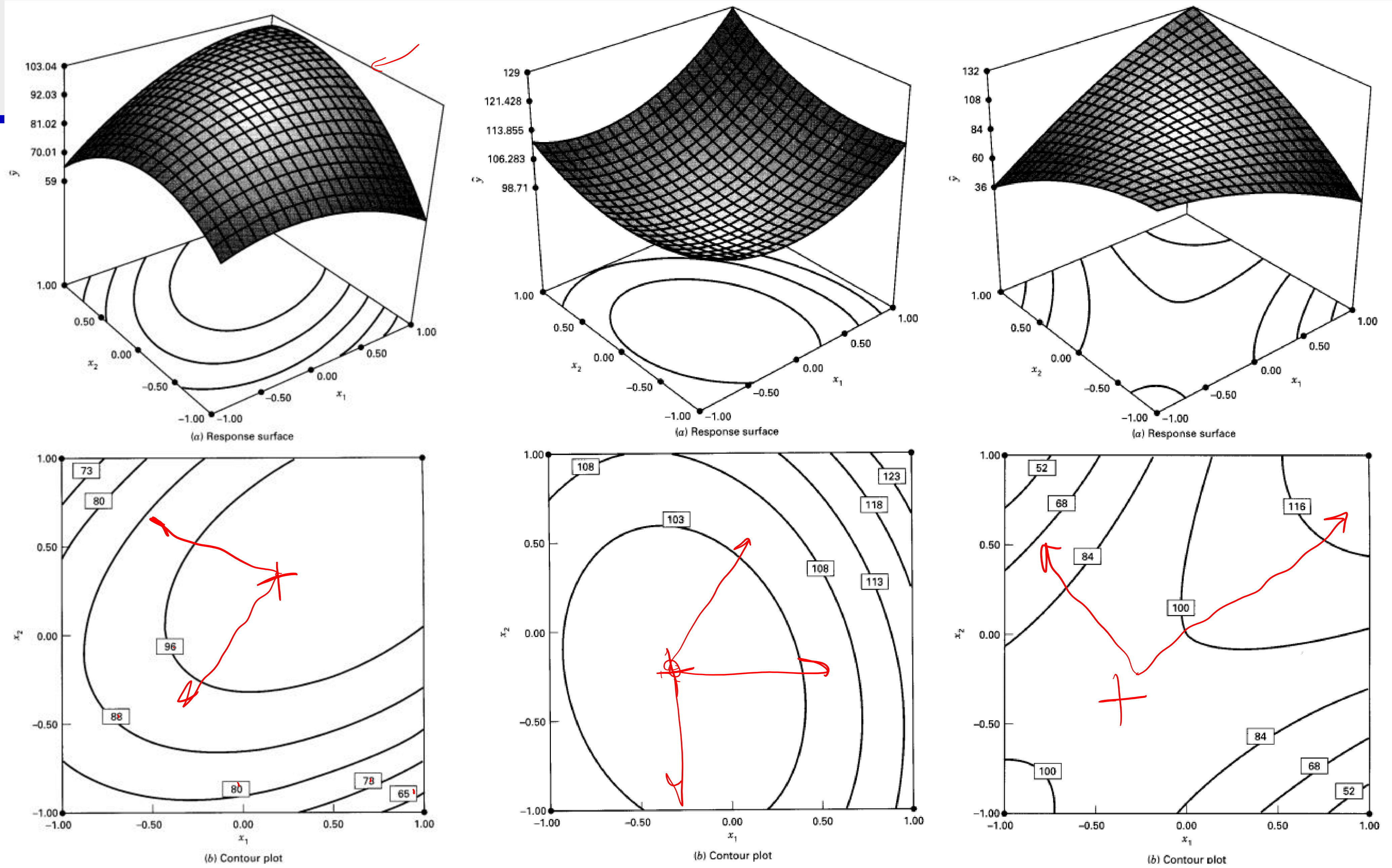
3. Convert the Δx_i from coded variables to the natural variables.

Analysis of Second-Order Response Surface

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

- 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 (a) Response surface (a) Response surface

(b) Contour plot (b) Contour plot (b) Contour plot

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

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

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

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

$x' = x^T$

$$\underset{1\times1}{\hat{y}} = \underset{1\times1}{\hat{\beta}_0} + \mathbf{x}'\mathbf{b} + \underset{1\times1}{\mathbf{x}'\mathbf{B}\mathbf{x}} \tag{11-5}$$

where

$$\underset{k\times1}{\mathbf{x}} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} \quad \underset{k\times1}{\mathbf{b}} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} \quad \text{and} \quad \underset{k\times k}{\mathbf{B}} = \begin{bmatrix} \hat{\beta}_{11}, & \hat{\beta}_{12}/2, & \ldots, & \hat{\beta}_{1k}/2 \\ & \hat{\beta}_{22}, & \ldots, & \hat{\beta}_{2k}/2 \\ & & \ddots & \\ \text{sym.} & & & \hat{\beta}_{kk} \end{bmatrix}$$

$\hat{y} = \hat{\beta}_0 + \underset{1\times2}{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T} \underset{2\times1}{\begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix}} + \underset{1\times2}{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^T} \underset{2\times2}{\begin{bmatrix} \beta_{11} & \beta_{12}/2 \\ \beta_{12}/2 & \beta_{22} \end{bmatrix}} \underset{2\times1}{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}}$

$= \hat{\beta}_0 + [x_1\ x_2]\begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + [x_1\ x_2]\left[\quad\right]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

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

We know that, at stationary point

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

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

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

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

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

y_s

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 →

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

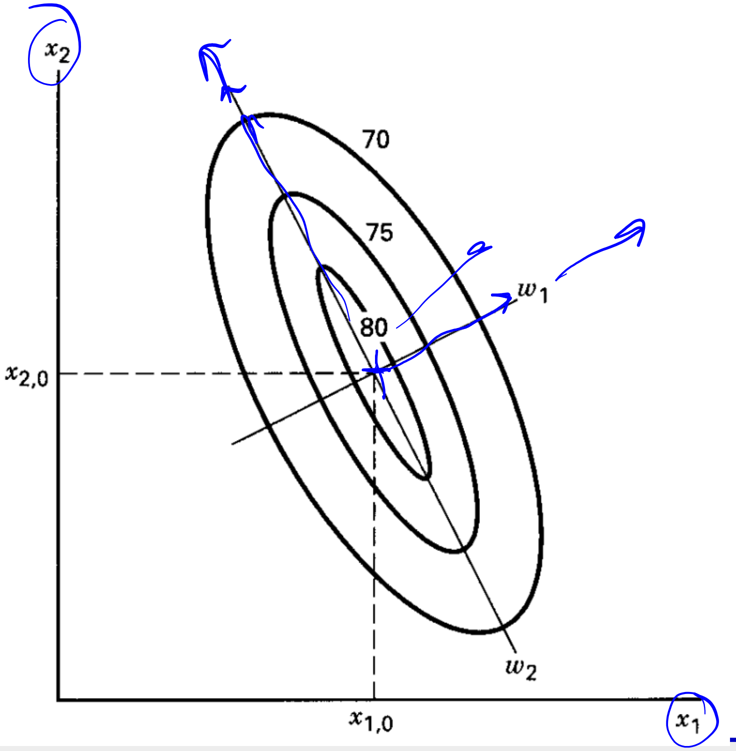
$x = x_s$

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 surfac



Canonical Form

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

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

$x_1 \rightarrow w_1$

$x_2 \rightarrow w_2$

takes the form of

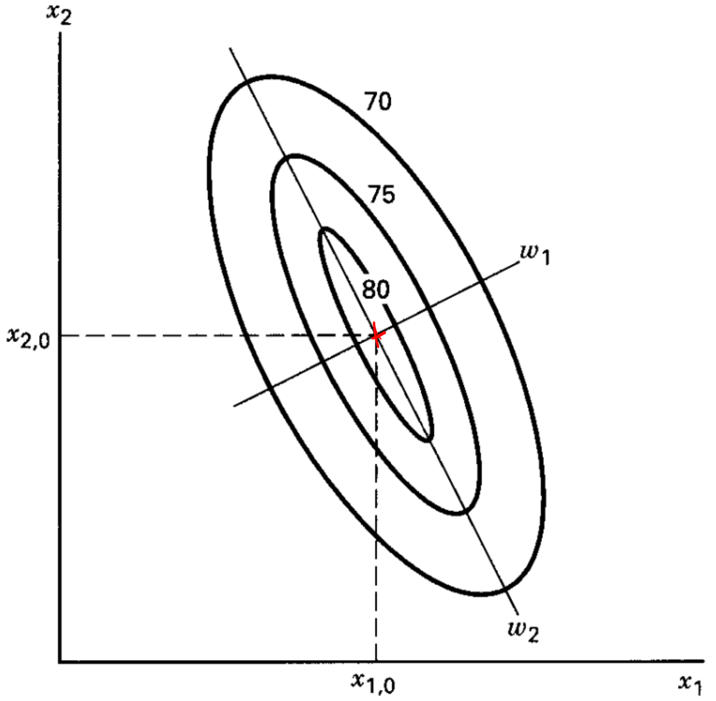
$$\hat{y} = \hat{y}_s + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \cdots + \lambda_k w_k^2$$

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

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

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 (λ_1 and λ_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

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

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?

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

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

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 * $time^2$
−0.040050 * $temp^2$
+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

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

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

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

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

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

Find Eigen values and Eigen vectors of B

$B = [\;]_{K\times K}$ if this is a transformation

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

$[\;]_{K\times K}[\;]_{K\times 1} = [\;]_{K\times 1}$

eigen vectors are those who do NOT change dir under B

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

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

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"

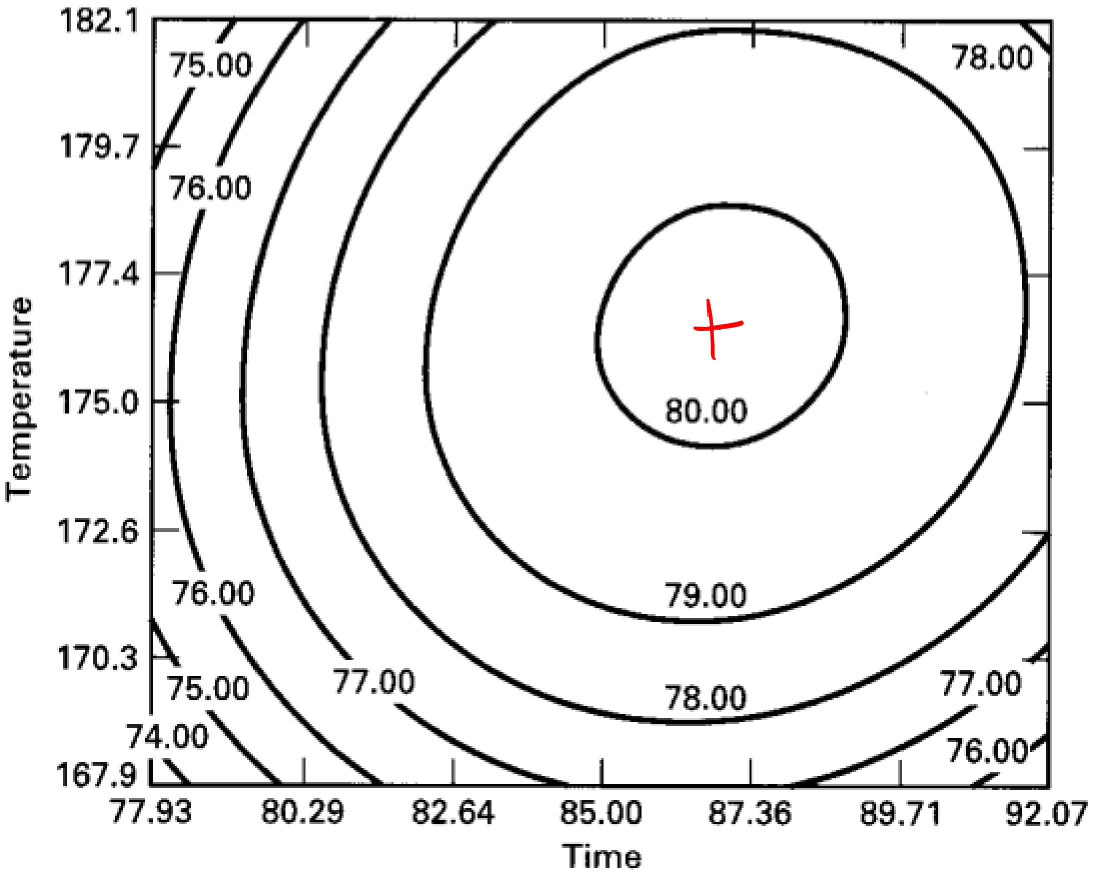
which reduces to

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

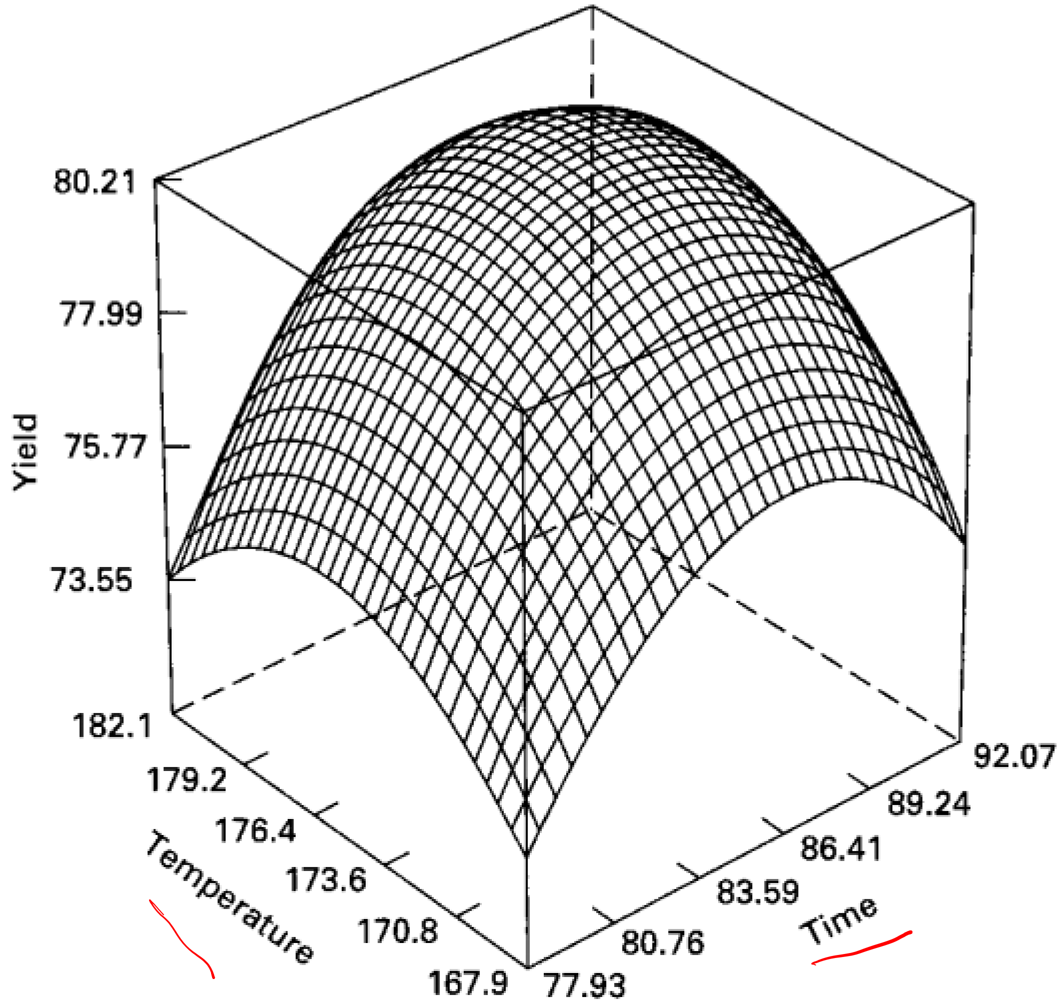
The roots of this quadratic equation are $\lambda_1 = -0.9641$ and $\lambda_2 = -1.4147$. Thus, the canonical form of the fitted model is

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

- Example: Contour Plot



(a) The contour plot



(b) The response surface plot

The stationary point we found was $x_{1,s} = 0.389$ and $x_{2,s} = 0.306$

In terms of original time and temperature units, $\xi_1 = 86.95 \simeq 87$ minutes of reaction time and $\xi_2 = 176.53 \simeq 176.5°F$.

What would you do if for some reason (e.g. cost) we cannot operate at this point?

- We can back away slightly from this optimum point and see if any other point in vicinity can work
- Where to go?

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

at x_s

$w_1 = w_2 = 0$

you would move first in dir where $|\lambda_i|$ is smallest

Ridge Systems

- Consider 2nd order model with canonical form $\hat{y} = \hat{y}_s + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \cdots + \lambda_k w_k^2$
- Suppose the stationary point (x_s) is in the region of experimentation, and some λ_i are small, i.e., $\lambda_i \approx 0$
- Then, the response variable y is very insensitive to variables with small λ

Is small

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

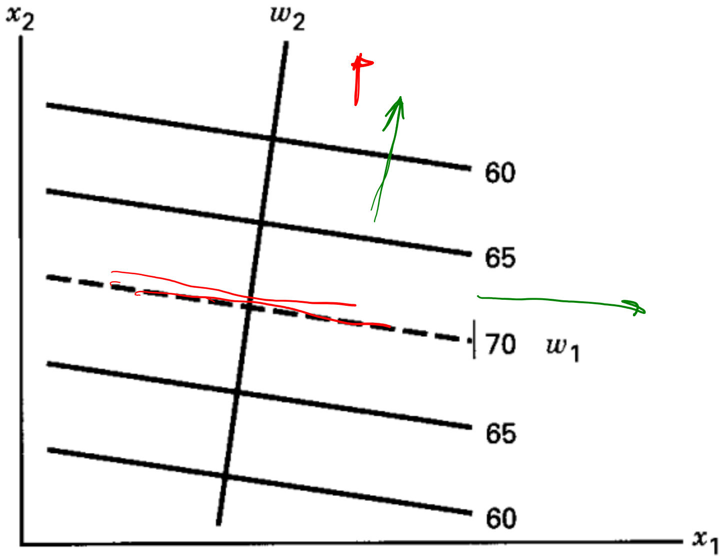


Figure 11-12 A contour plot of a stationary ridge system.

- Because of small λ_1, the optimum can be taken anywhere along the line of y = 70
- This type of response surface is called 'stationary ridge system'