ME 794

Statistical Design of Experiments

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Response Surface Methodology

Acknowledgement: Design and Analysis of Experiments by Montegamory. Some of the course material has been adopted from similar courses taught previously by Prof. Shiv Kapoor (UofI), and Prof. Suhas Joshi (IITB).

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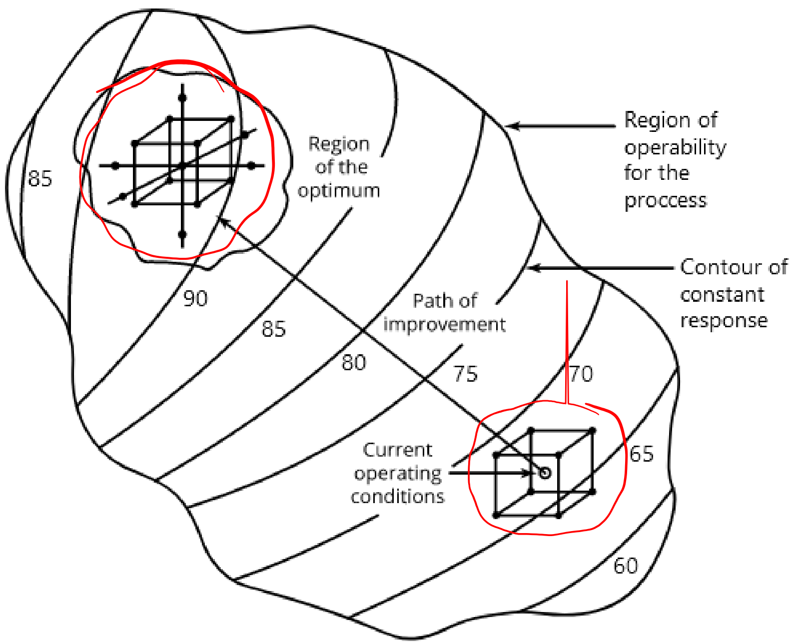
Goal of RSM

- 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

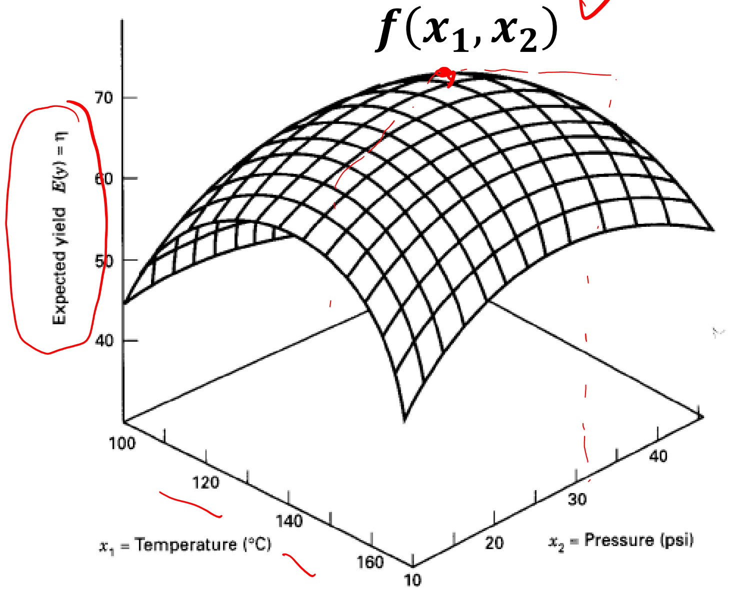
Suppose, yield (y) of a chemical process depends on temperature (x_1) and pressure (x_2). The chemical engineer would like to find out which levels of temperature and pressure give the maximum yield.

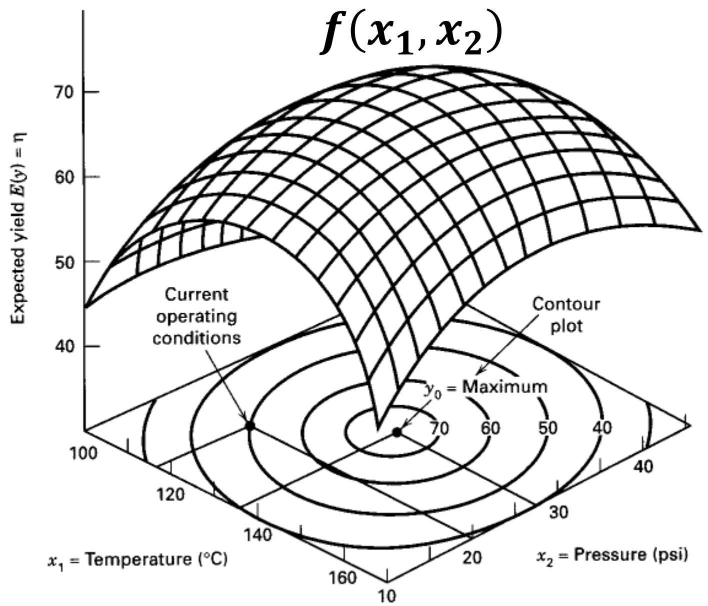
One may write, $$\boldsymbol{y = f(x_1, x_2) + \epsilon}$$

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

'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'**

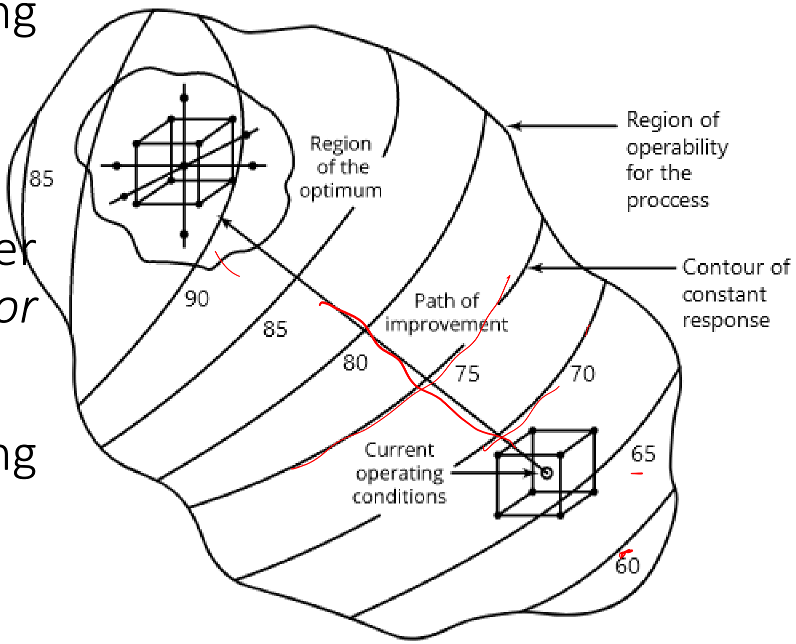
$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_k x_k + \epsilon$$

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 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 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 first order model.
- We then take the shortest and most efficient path towards the optimum
- As we near the optimum, there may be non-linearities, so we can employ higher order models



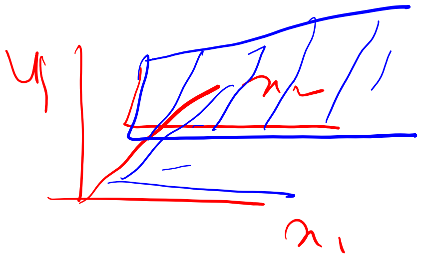
Method of Steepest Ascent

- 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 the path of steepest ascent, i.e., direction of the maximum increase i response.
- If minimization is desired, we follow the 'method steepest descent'
- If we use first order model, $\hat{y} = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i x_i$

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

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

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



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

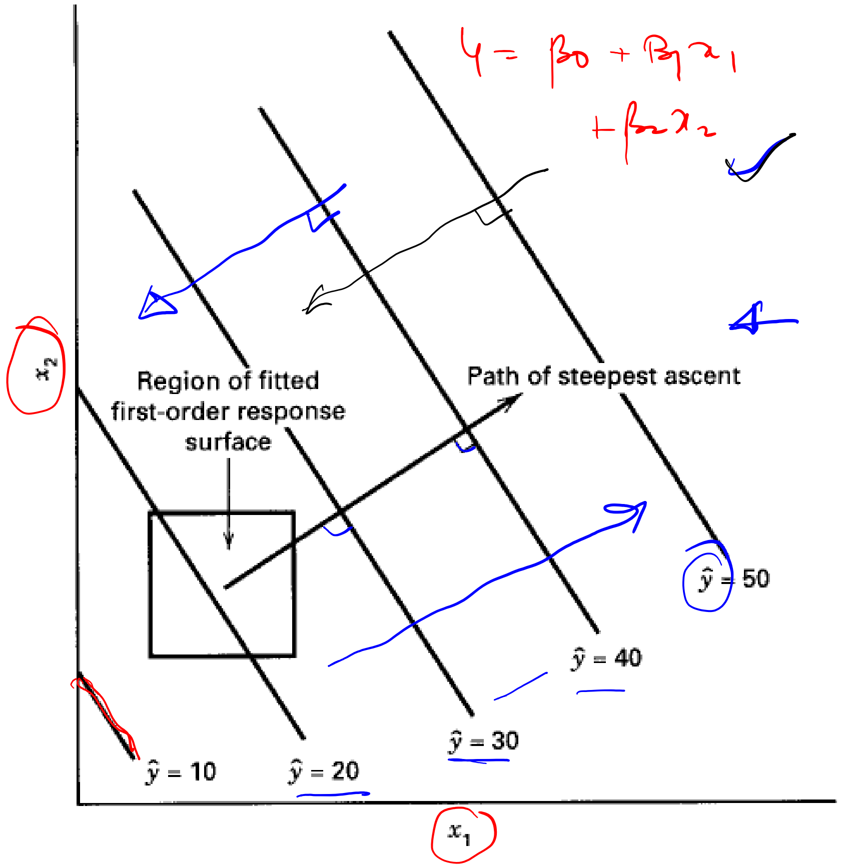
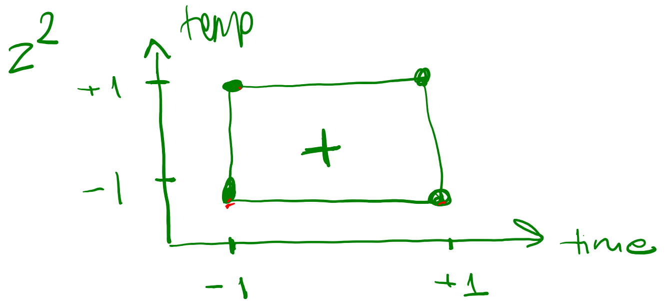


Figure 11-4 First-order response surface and path of steepest ascent.

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.



ξ_1 reaction time $\quad$ ξ_2 temperature

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

2^2 Factorial Analysis

Can we find which terms are important?

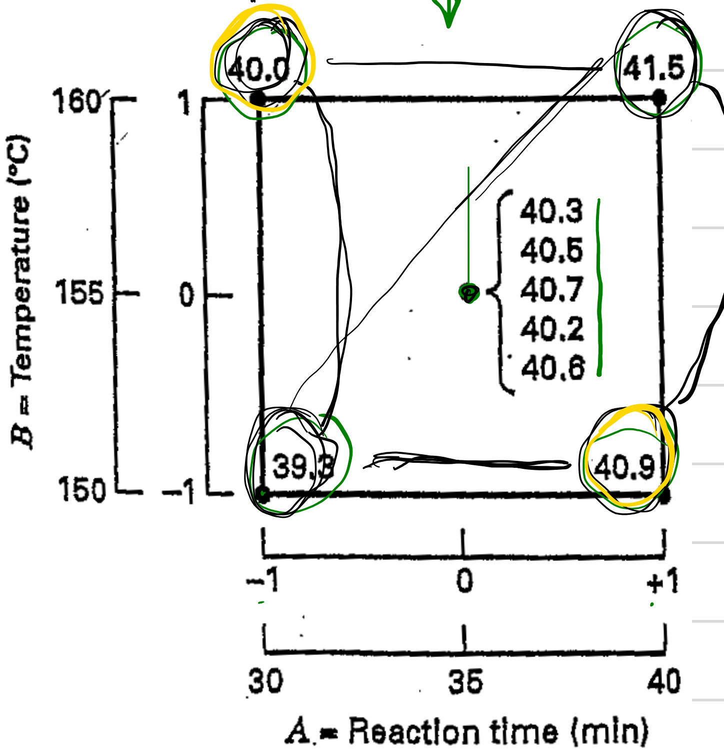
What will be the first-order model?

Will a first-order model be appropriate?

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

Obs

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



Natural Variables		Coded Variables		Response
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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)

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

$$\beta_0 = \left(\frac{39.3 + 40 + 40.9 + 41.5}{4}\right) = 40.425$$

$$\beta_1 = \frac{1}{2}(-39.3 - 40.0 + 40.9 + 41.5) = 1.55$$

$$\beta_2 = \frac{1}{2}(-39.3 + 40 - 40.9 + 41.5) = 0.65$$

$$\beta_{12} = -0.05$$

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

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

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	?		

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

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

$$SS_{x_1x_2} = 2\left((40.45-40.425)^2 + (40.9-40.2425)^2\right)$$

$$= 0.0025$$

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

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

$$=$$

ANOVA

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

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

‘Climbing the hill’

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

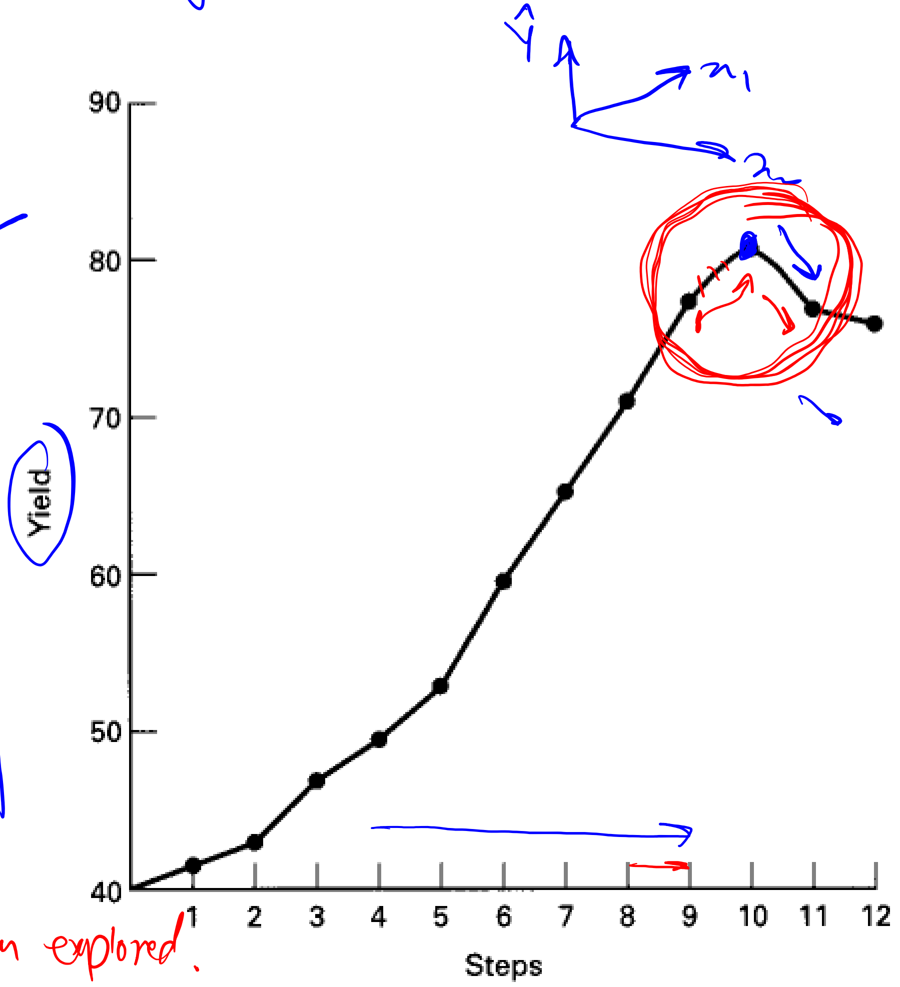
$$\hat{y} = 40.44 + 0.775x_1 + 0.325x_2$$

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 ξ_1	Natural Variables ξ_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
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

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

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 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

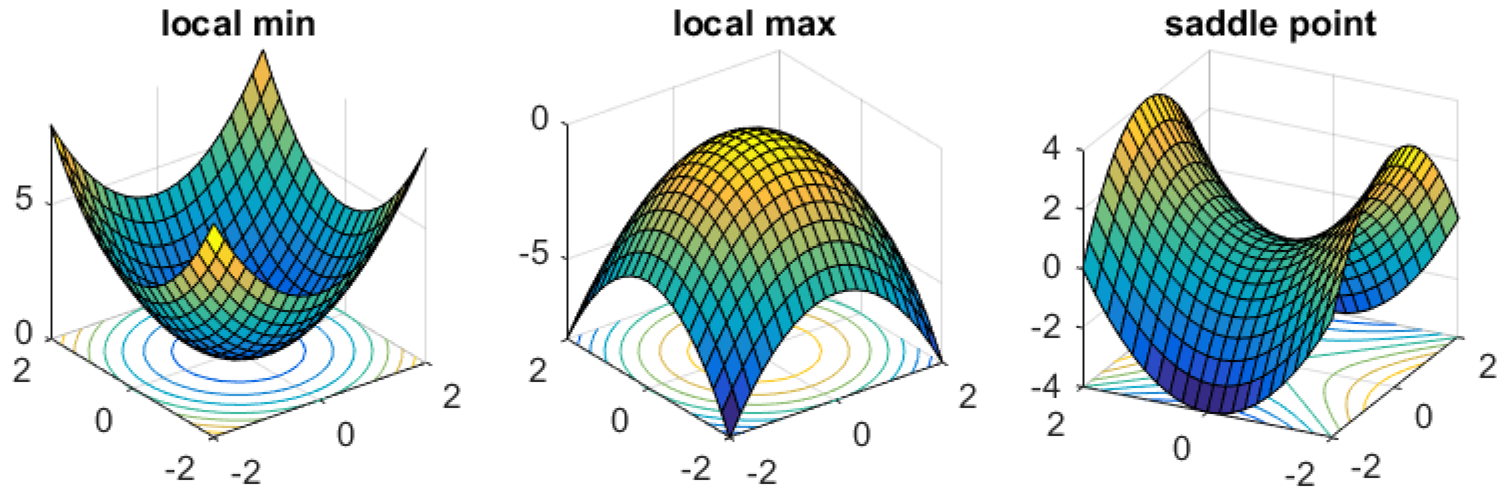
$$\Delta x_i = \frac{\hat{\beta}_i}{\hat{\beta}_j / \Delta x_j} \qquad i = 1, 2, \ldots, k; \qquad i \neq j$$

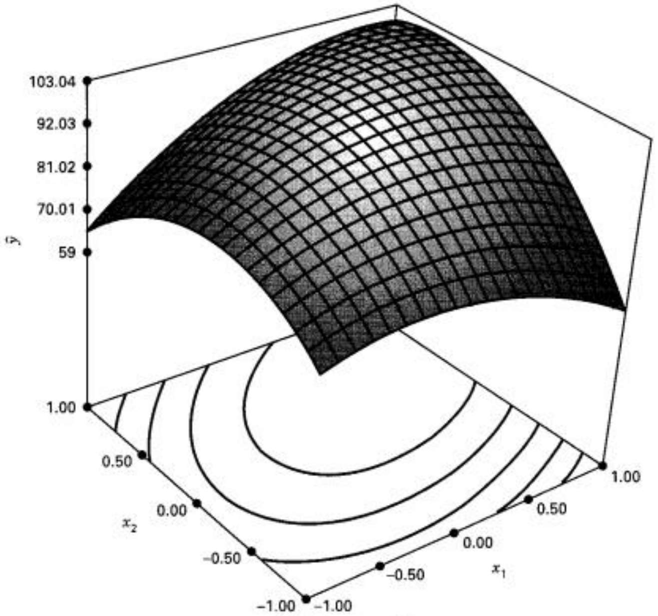
3. Convert the Δx_i from coded variables to the natural variables.

Analysis of Second Order Response Surface

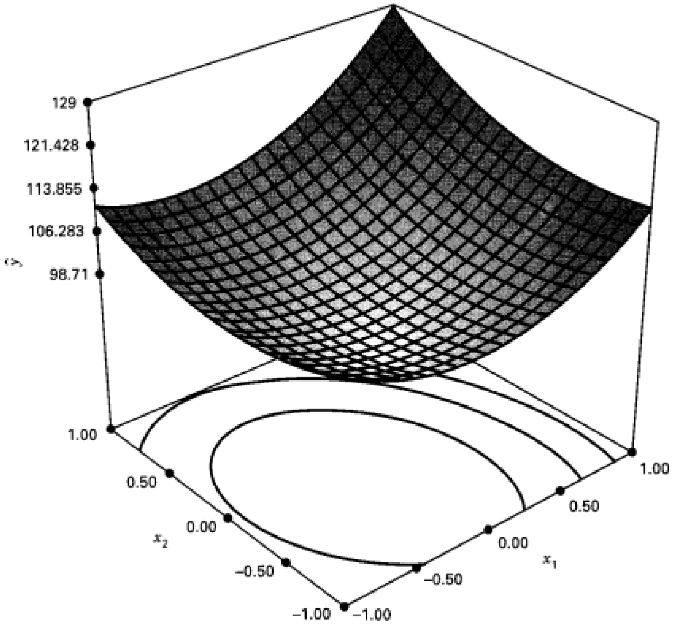
$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j}\sum \beta_{ij} x_i x_j + \epsilon$$

- 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



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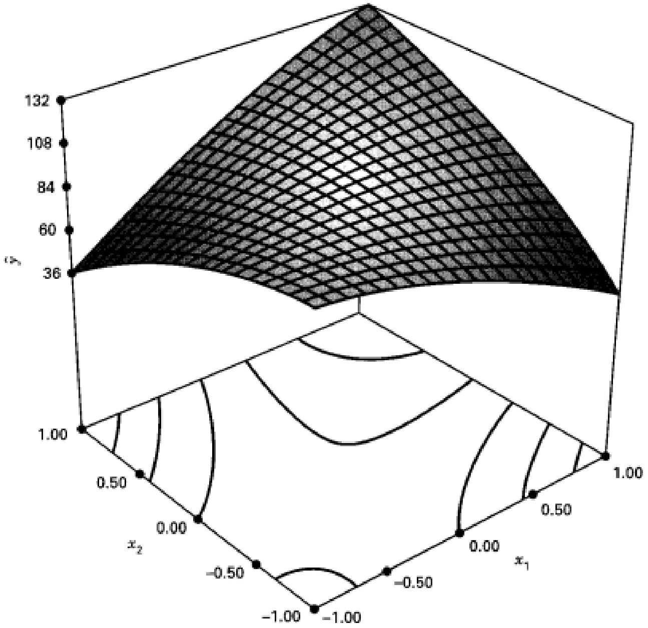

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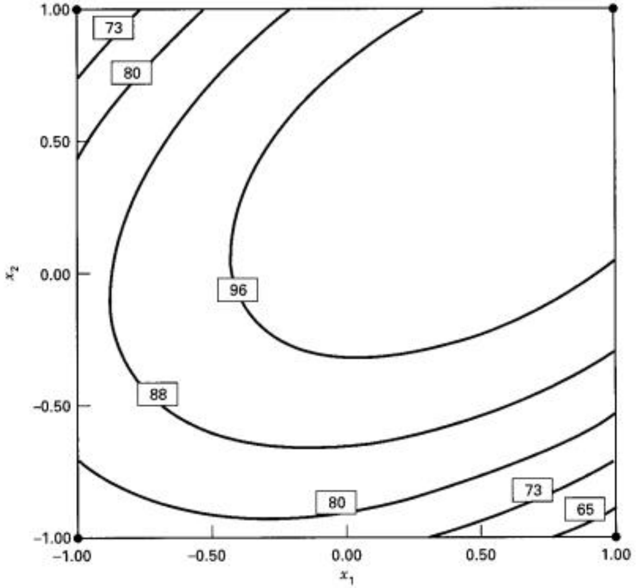
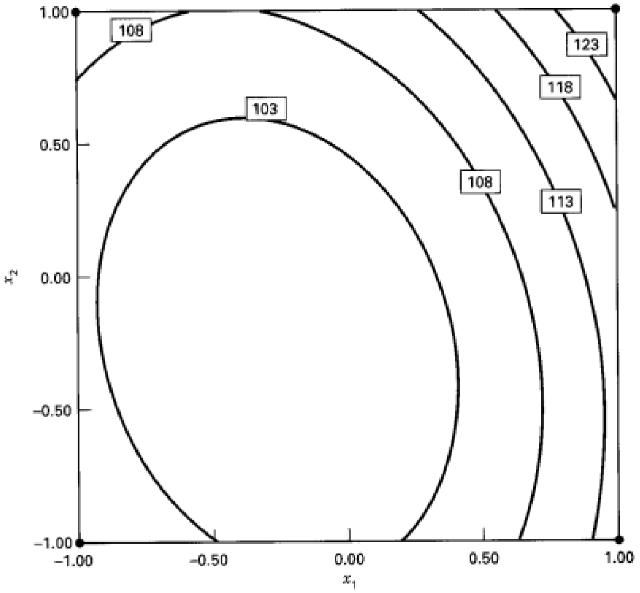


(b) Contour plot



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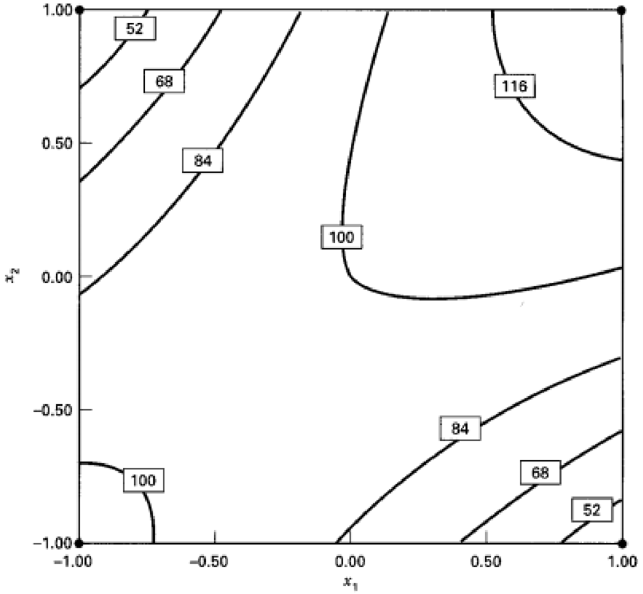


(b) Contour plot

Finding the Stationary Point

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

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

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

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

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

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

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 $\Rightarrow$

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

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

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

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

We know that, at stationary point

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

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

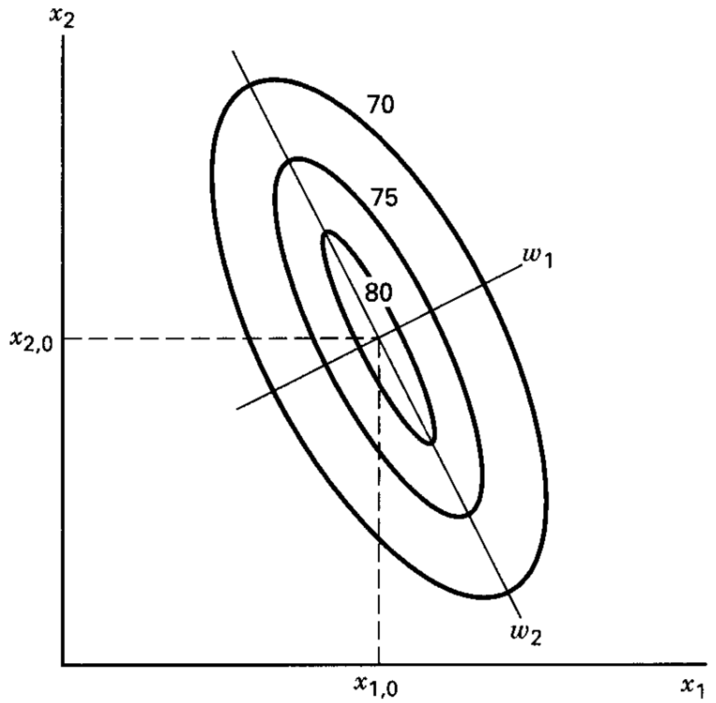
$x = x_s \rightarrow$ 11.5

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

Change of variable

$x_i \rightarrow w_i$

?

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

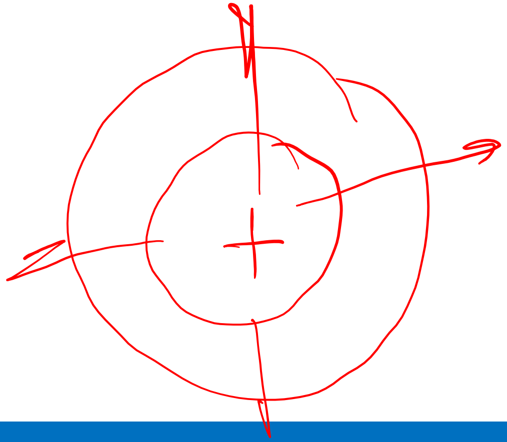
$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i<j}\sum \beta_{ij} x_i x_j \quad = \hat{\beta}_0 + \mathbf{x}'\mathbf{b} + \mathbf{x}'\mathbf{B}\mathbf{x} \qquad (1)$$

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)

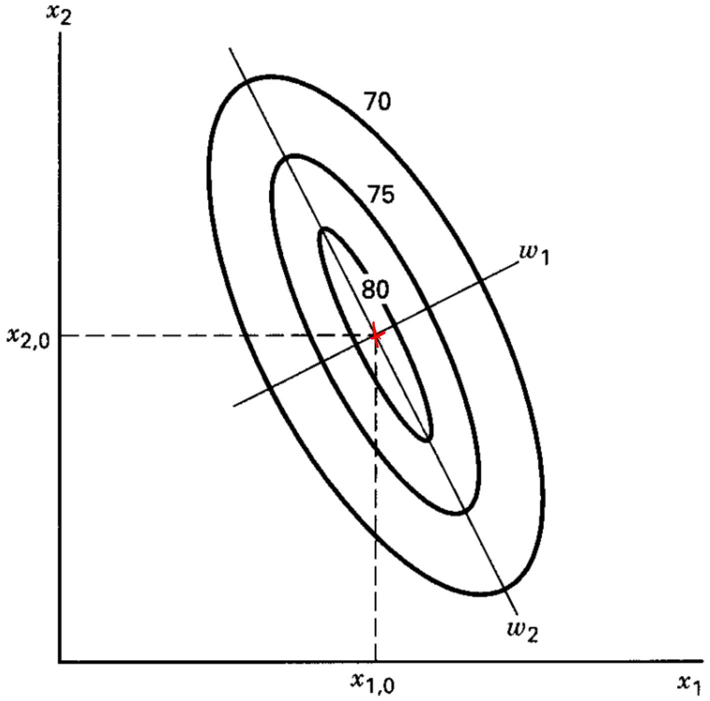
- Here, w_i are the new (transformed) independent variables, and λ_i are the constants
- This is called 'Canonical Form' of the model.
- λ_i are the eigen values of matrix **B**



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

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 (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

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

Example: Second Order Model

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

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?

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

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 * $time^2$
−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

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

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

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

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

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Final Equation in Terms of Actual Factors:

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−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

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

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

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 $\bar{x}_\lambda$

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

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

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

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

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

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

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

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

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

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

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

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

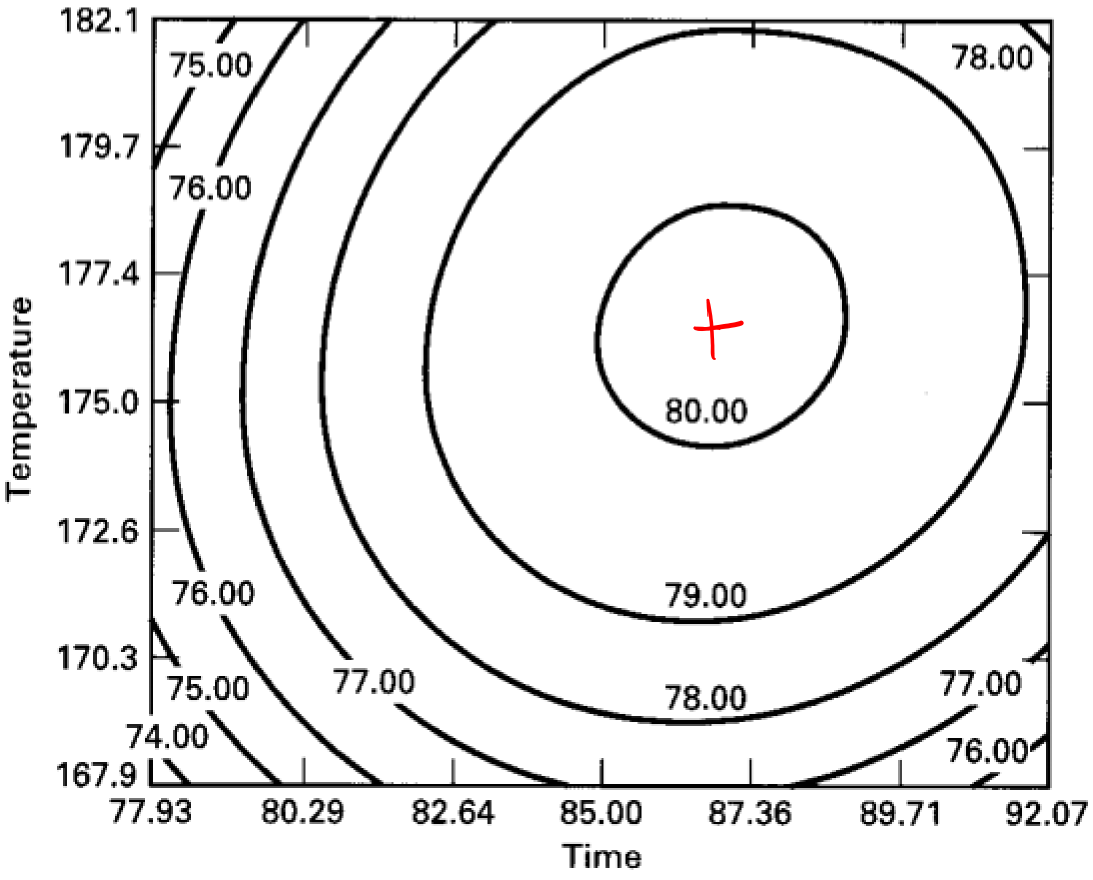
$$\hat{y} = \hat{y}_s + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \dots + \lambda_k w_k^2$$

Thus, canonical form of original eq.

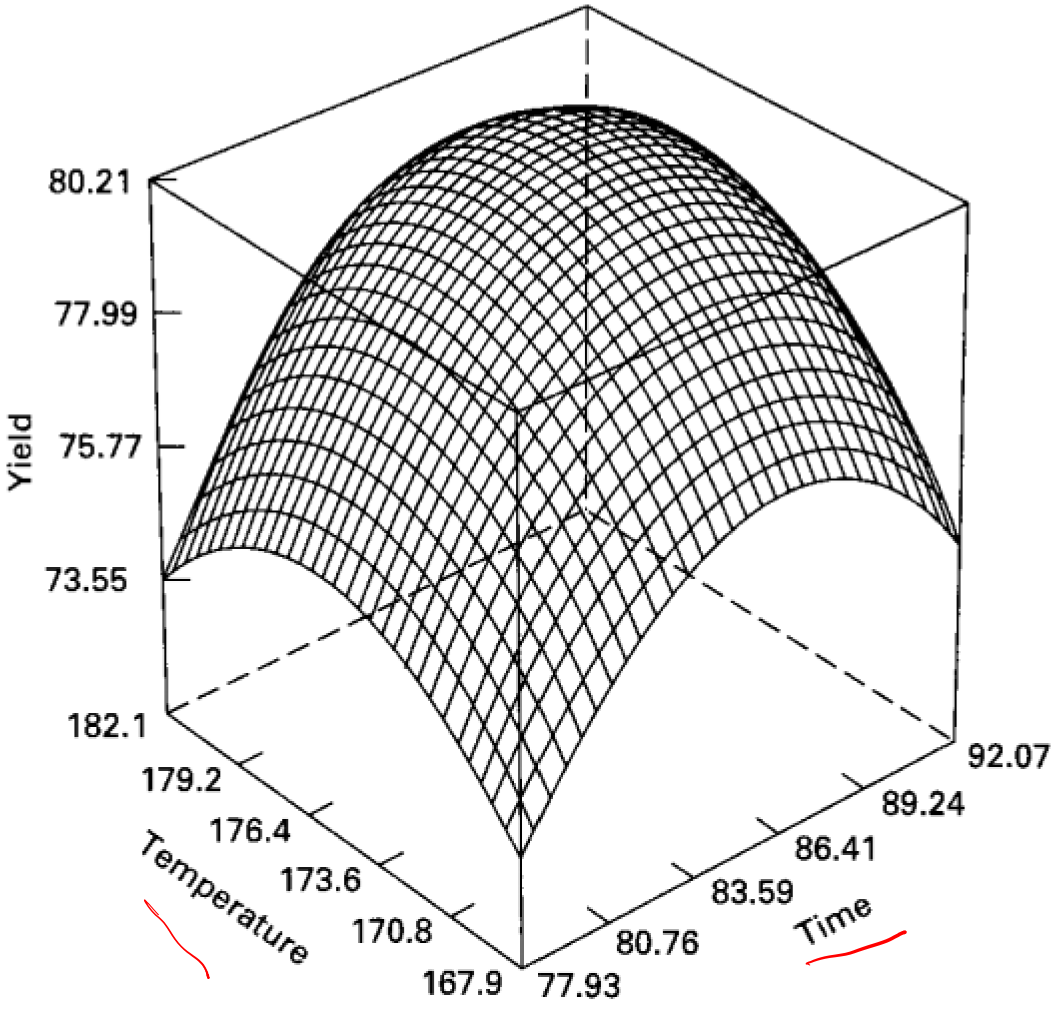
$$\boxed{\hat{y} = 80.21 - 0.9641\, w_1^2 - 1.4147\, w_2^2}$$

"maxima"

Example: Contour Plot



(a) The contour plot



(b) The response surface plot

Example: Change of Variables

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

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

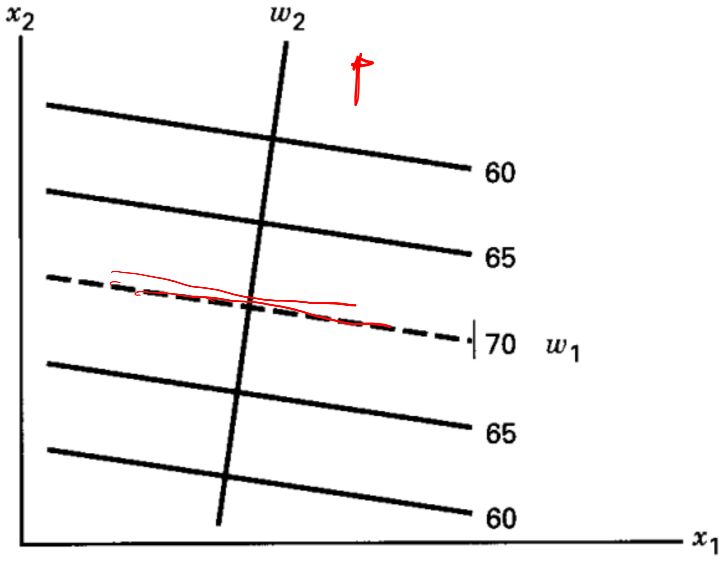


Figure 11-12 A contour plot of a stationary ridge system.

- 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'

Ridge System

- If the stationary point (x_s) is far outside the region of experimentation, and some λ_i are small, i.e., $\lambda_i \approx 0$
- Then the response surface could be a 'rising ridge' or 'falling ridge'
- In such type of systems, we can NOT draw conclusions about the true surface or the stationary point
- BECAUSE the stationary point is far outside the region where we fitted the model
- In this example, further exploration is needed in the w1 direction

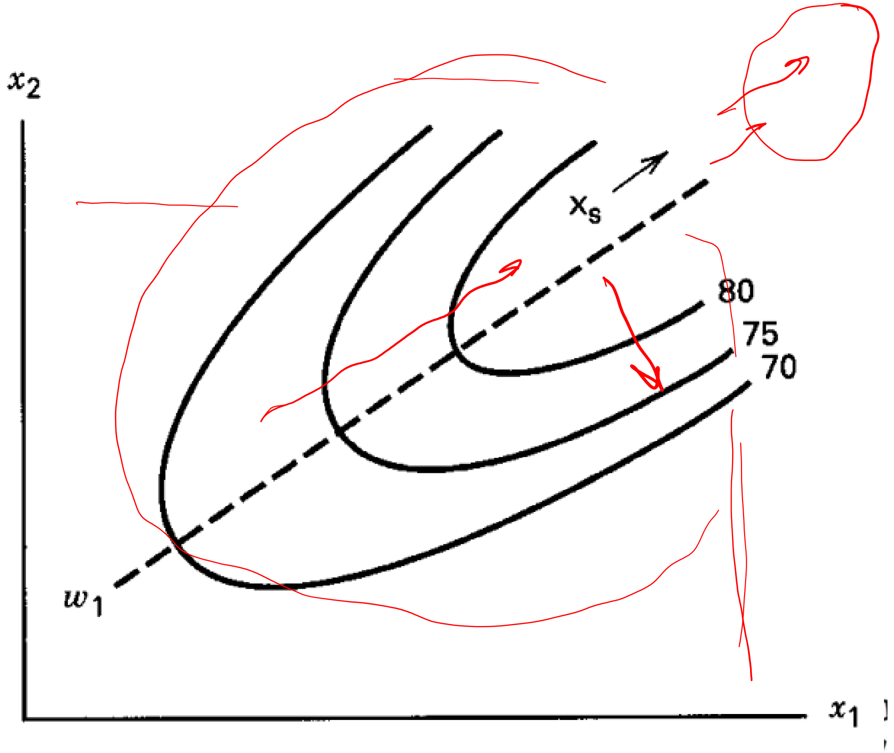


Figure 11-13 A contour plot of a rising ridge system.

Multiple Responses

- Consider the previous example

- Similar to yield, we can also obtain models for viscosity and molecular weight

We only found a response surface for ONE of the responses - Yield

Final Equation in Terms of Coded Factors:

yield =
+79.94
+0.99 * A
+0.52 * B
−1.38 * A²
−1.00 * B²
+0.25 * A * B

$$\hat{y}_2 = 70.00 - 0.16x_1 - 0.95x_2 - 0.69x_1^2 - 6.69x_2^2 - 1.25x_1x_2$$
$$\hat{y}_3 = 3386.2 + 205.1x_1 + 17.4x_2$$

In terms of the natural levels of time (ξ_1) and temperature (ξ_2), these models are

$$\hat{y}_2 = -9030.74 + 13.393\xi_1 + 97.708\xi_2 - 2.75 \times 10^{-2}\xi_1^2 - 0.26757\xi_2^2 - 5 \times 10^{-2}\xi_1\xi_2$$

and

$$\hat{y}_3 = -6308.8 + 41.025\xi_1 + 35.473\xi_2$$

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

How would you optimize multiple responses?

A relatively straightforward approach to optimizing several responses that works well when there are only a few process variables is to **overlay the contour plots** for each response. Figure 11-16 (page 451) shows an overlay plot for the three responses in Example 11-2, with contours for which y_1 (yield) ≥ 78.5, $62 \leq y_2$ (viscosity) ≤ 68, and y_3 (molecular weight Mn) ≤ 3400. If these boundaries represent important conditions that must be met by the process, then as the unshaded portion of Figure 11-16 shows, there are a number of combinations of time and temperature that will result in a satisfactory process. The experimenter can visually examine the contour plot to determine appropriate operating conditions. For example, it is likely that the experimenter would be most interested in the larger of the two feasible operating regions shown in Figure 11-16.

But what will you do if there are even more responses OR if there are more than two independent variables?

Graphical method won't work!

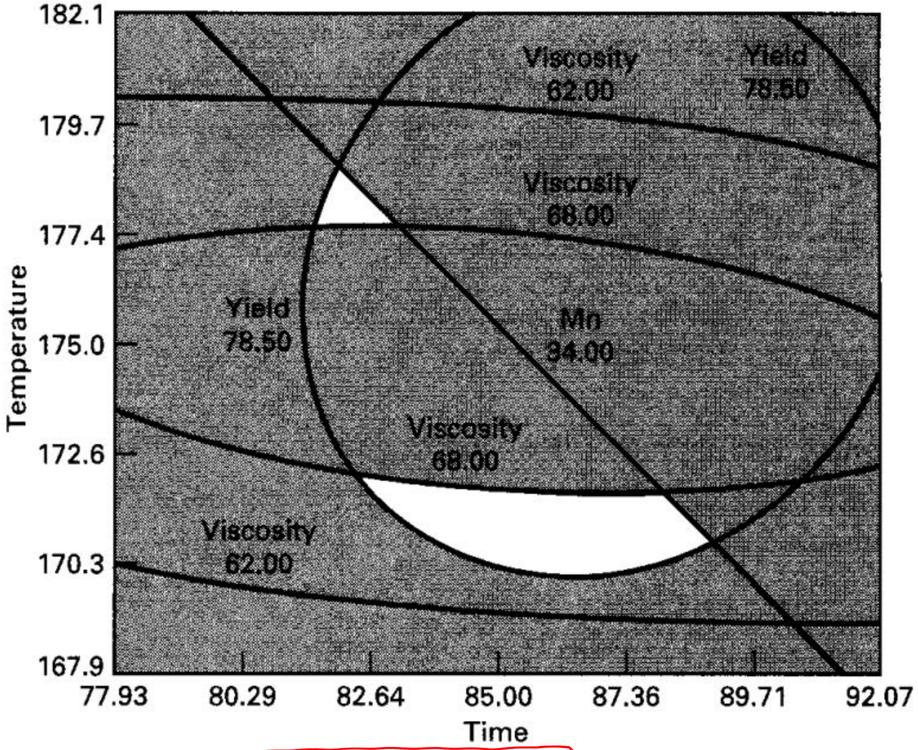


Figure 11-16 Region of the optimum found by overlaying yield, viscosity, and molecular weight response surfaces, Example 11-2.

Constrained Optimization

- Popular approach is to formulate the problem as constrained optimization problem
- For example,

$$\begin{gathered}\text{Max } y_1 \\ \text{subject to} \\ 62 \leqslant y_2 \leqslant 68 \\ y_3 \leqslant 3400\end{gathered}$$

- Then one can use numerical techniques to solve such a problem ('non-linear programming methods')

The two solutions found are

$$\text{time} = 83.5 \qquad \text{temp} = 177.1 \qquad \hat{y}_1 = 79.5$$

$$\text{time} = 86.6 \qquad \text{temp} = 172.25 \qquad \hat{y}_1 = 79.5$$

Desirability Functions

Another useful approach to optimization of multiple responses is to use the simultaneous optimization technique popularized by Derringer and Suich (1980). Their procedure makes use of **desirability functions**. The general approach is to first convert each response y_i into an individual desirability function d_i that varies over the range

$$0 \leqslant d_i \leqslant 1$$

where if the response y_i is at its goal or target, then $d_i = 1$, and if the response is outside an acceptable region, $d_i = 0$. Then the design variables are chosen to maximize the overall desirability

$$D = (d_1 \cdot d_2 \cdot \cdots \cdot d_m)^{1/m}$$

where there are m responses.

yield | visc | mol. wt

y_1 | y_2 | y_3

$y_1 = 80$

$d_1 = 1$

$y_1 \ngtr 70\%$

$y_1 \leq 70$

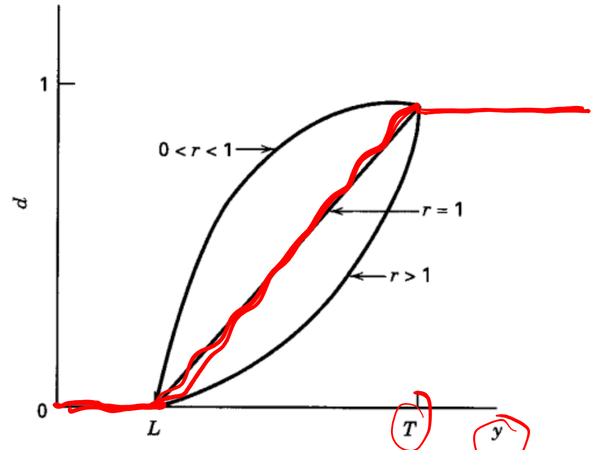
$d_1 = 0$

d_1

Desirability Functions

If the objective or target T for the response y is a maximum value,

$$d = \begin{cases} 0 & y < L \\ \left(\dfrac{y-L}{T-L}\right)^r & L \leqslant y \leqslant T \\ 1, & y > T \end{cases}$$

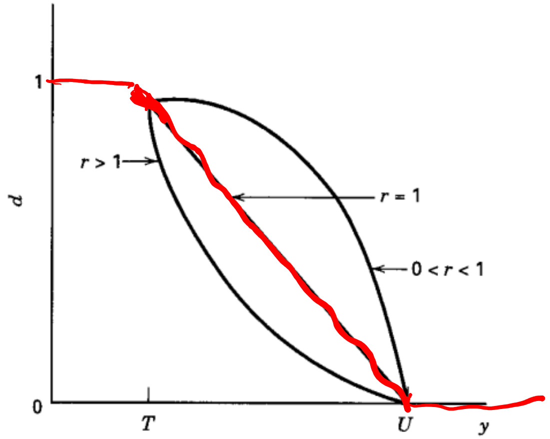


(a) Objective (target) is to maximize y

$y_1 \rightarrow d_1$

If the target for the response is a minimum value,

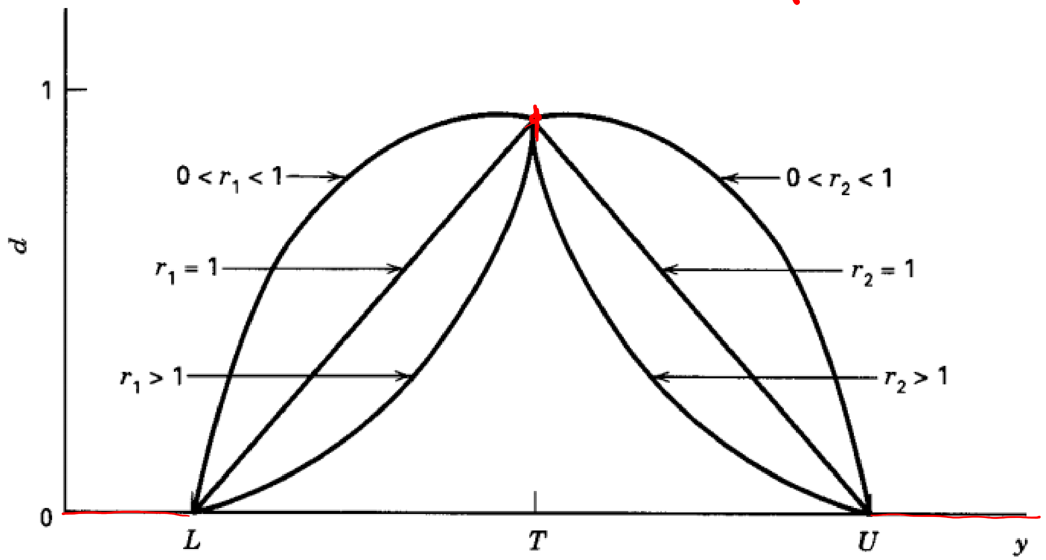
$$d = \begin{cases} 1 & y < T \\ \left(\dfrac{U-y}{U-T}\right)^r & T \leqslant y \leqslant U \\ 0 & y > U \end{cases}$$



(b) Objective (target) is to minimize y

The two-sided desirability function shown in Figure 11-17(c) assumes that the target is located between the lower (L) and upper (U) limits, and is defined as

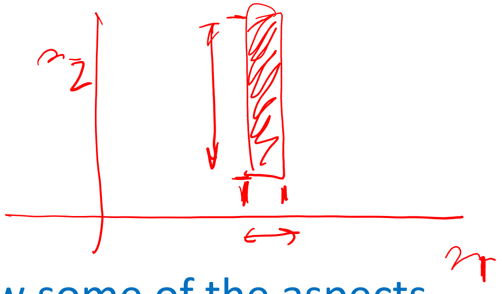
$$d = \begin{cases} 0 & y < L \\ \left(\dfrac{y-L}{T-L}\right)^{r_1} & L \leqslant y \leqslant T \\ \left(\dfrac{U-y}{U-T}\right)^{r_2} & T \leqslant y \leqslant U \\ 0 & y > U \end{cases} \qquad (11\text{-}13)$$



(c) Objective is for y to be as close as posible to the target

Design of Experiments for Fitting Response Surfaces

- Fitting and analysing a response surface can be made very effective by *proper choice of experimental design* to collect the data
- What is a 'good experimental design'?



Note how some of the aspects are conflicting -> We need to apply our judgement

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