DOE for fitting First-Order Model

- First order model with ‘k’ variables: $$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \epsilon$$
- Using the experimental data, one would find the regression coefficients β_i
- There is a unique class of experimental designs that can minimize the variance of β_i ->

Orthogonal First-Order Designs

- A first-order design is orthogonal if the off-diagonal elements of (X’X) matrix are ALL ZERO
- That is the <cross> products of the columns of the X matrix add to ZERO

$$\sum x_{1i} x_{2i} = 0$$

2^2

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

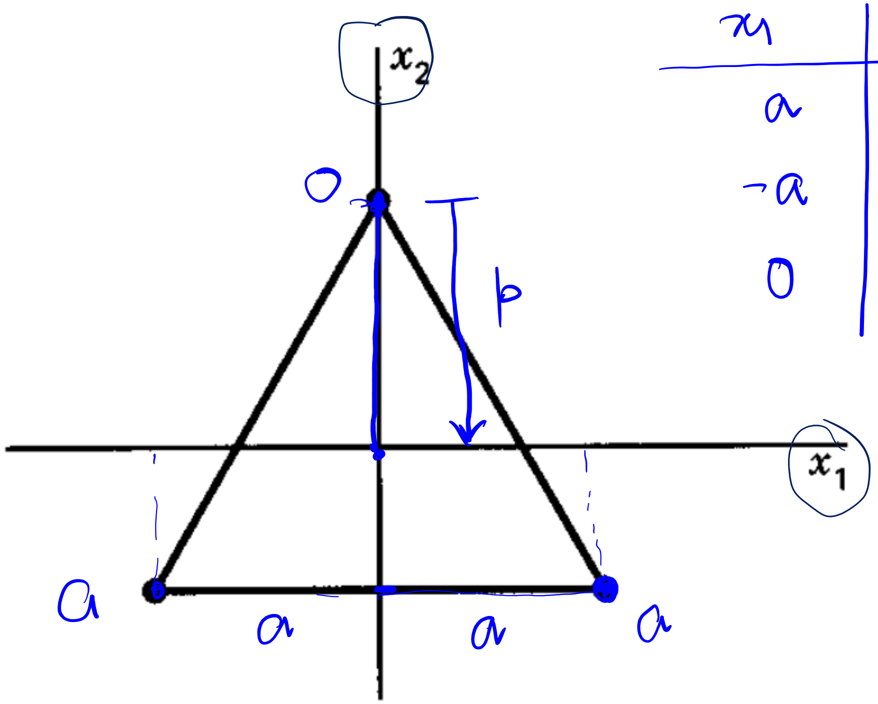
$$y_1 = \beta_0 - \beta_1 - \beta_2$$
$$y_2 = \beta_0 + \beta_1 - \beta_2$$
$$y_3 = \beta_0 - \beta_1 + \beta_2$$
$$y_4 = \beta_0 + \beta_1 + \beta_2$$

x_1	x_2	y
-1	-1	y_1
$+1$	-1	y_2
-1	$+1$	y_3
$+1$	$+1$	y_4

Orthogonal First-order Designs

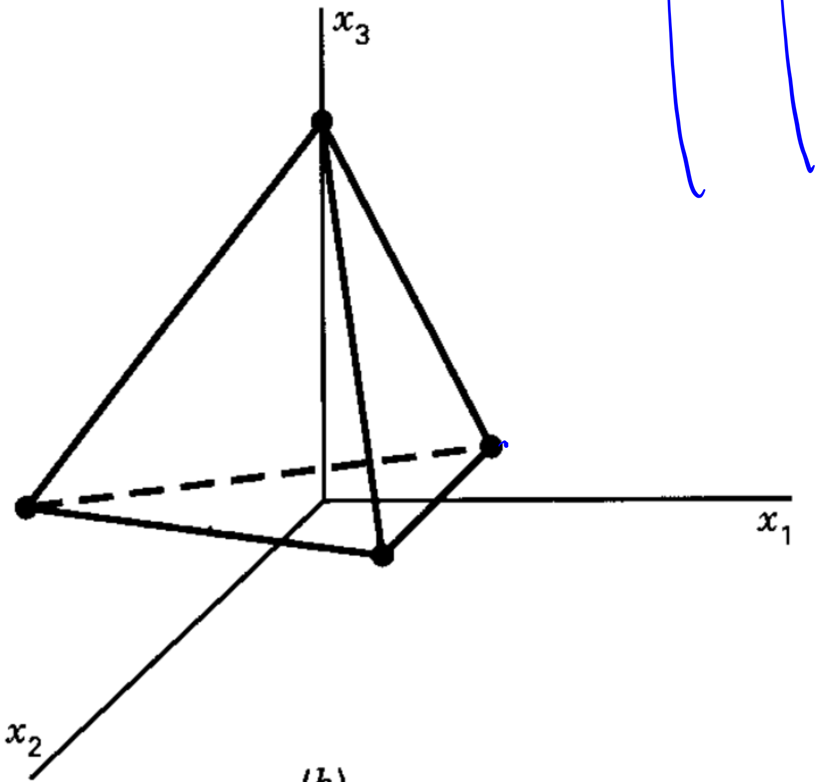
- Are 2^k factorial designs orthogonal?
- Yes – they are a part of orthogonal first-order designs
  - BUT, 2^k design does not afford an estimate of experimental error unless we do replication
  - A common method is to augment the 2^k design with several observations at the centre point
  - The addition of centre point doesn't influence the $\beta_1, \beta_2, \ldots$, BUT β_0 becomes a grand average of ALL the observations
  - Also, note how addition of centre point does not affect the orthogonality of the design

Another orthogonal first-order design is the **simplex**. The simplex is a regularly sided figure with $k + 1$ vertices in k dimensions. Thus, for $k = 2$ the simplex design is an equilateral triangle and for $k = 3$ it is a regular tetrahedron. Simplex designs in two and three dimensions are shown in Figure 11-19.



(a)

x_1	x_2
a	$-\sqrt{3}/2\,a$
$-a$	$-\sqrt{3}/2\,a$
0	0



(b)

x_1	x_2	x_3

Central Composite Design

- CCD consists of 2^k factorial design with n_F runs, 2k axial or star runs, and n_c center runs

total runs = $n_F + 2k + n_c$

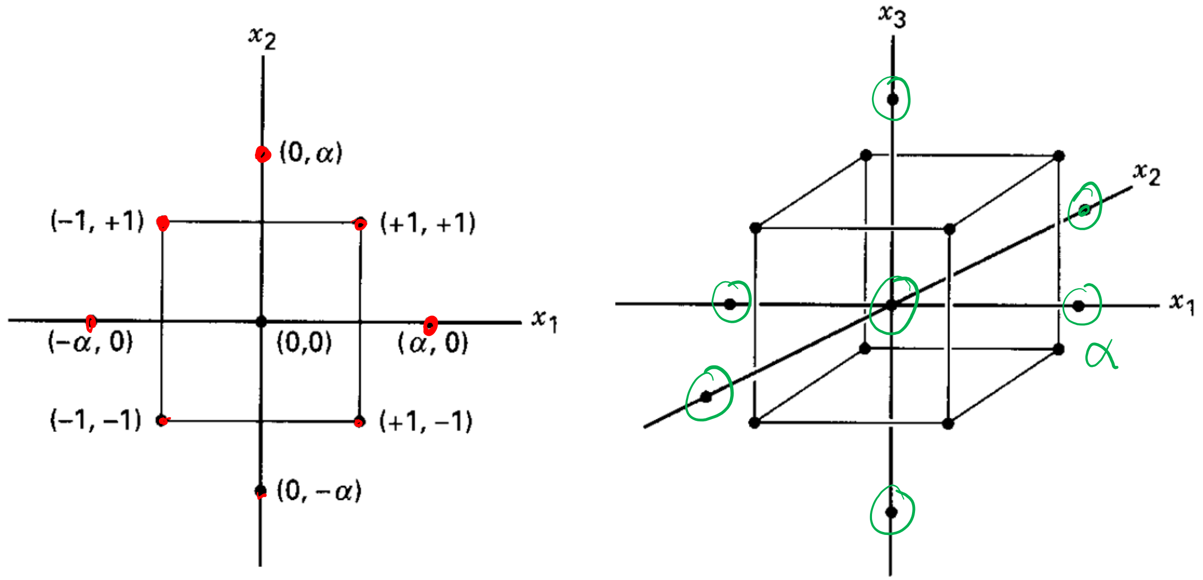


Figure 11-20 Central composite designs for $k = 2$ and $k = 3$.

how do you choose α

Central Composite Design

- CCD consists of 2^k factorial design with n_F runs, 2k axial or star runs, and n_c center runs

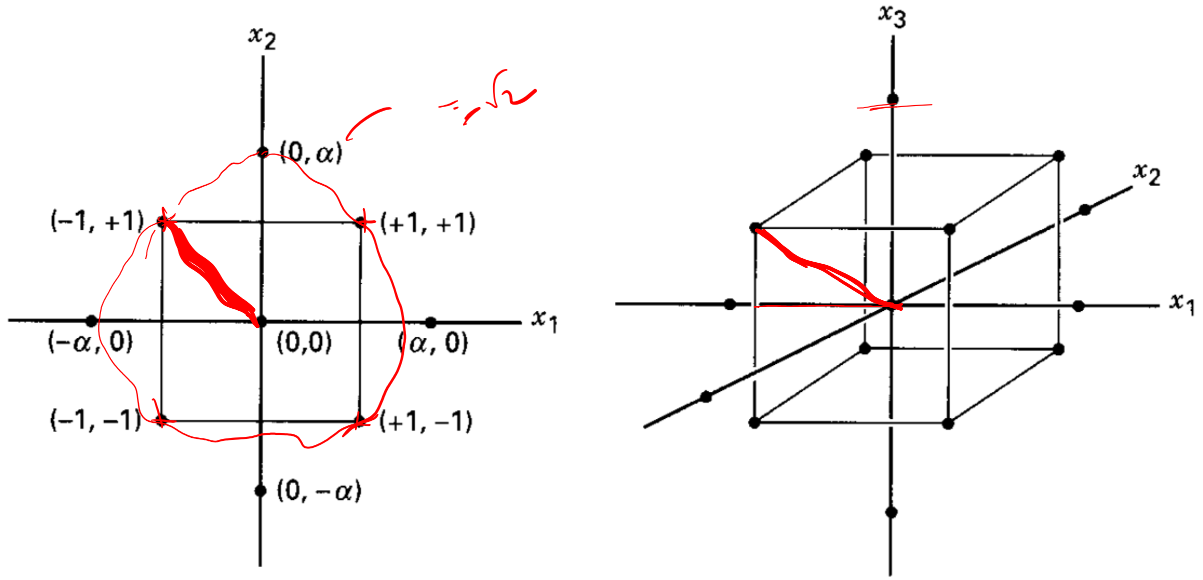


Figure 11-20 Central composite designs for $k = 2$ and $k = 3$.

Rotatibility

Rotatability

It is important for the second-order model to provide good predictions throughout the region of interest. One way to define ''good'' is to require that the model have a reasonably consistent and stable variance of the predicted response at points of interest **x**. Recall Equation 10-40 that the variance of the predicted response at some point **x** is

$E\left(\left(\hat{y}(x) - E(\hat{y}(x))\right)^2\right)$

$$V[\hat{y}(\mathbf{x})] = \sigma^2 \mathbf{x}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}$$

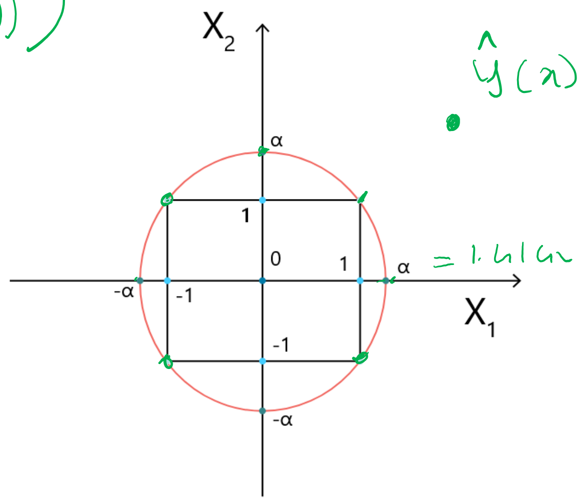
$\hat{y}(x)$

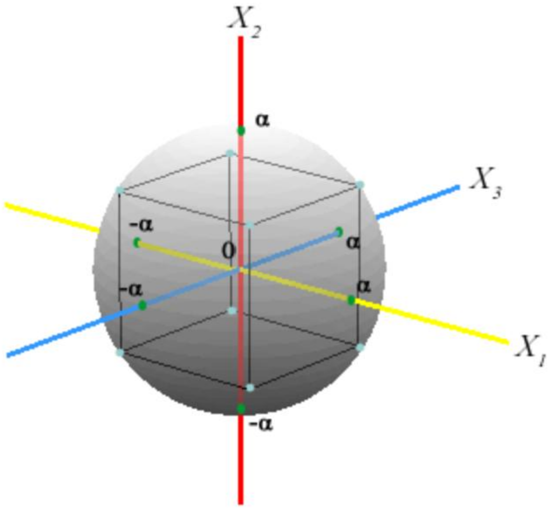
Box and Hunter (1957) suggested that a second-order response surface design should be **rotatable**. This means that the $V[\hat{y}(\mathbf{x})]$ is the same at all points **x** that are the same distance from the design center. That is, the variance of predicted response is constant on spheres.

Figure 11-21 (page 458) shows contours of constant $\sqrt{V[\hat{y}(\mathbf{x})]}$ for the second-order model fit using the CCD in Example 11-2. Notice that the contours of constant standard deviation of predicted response are concentric circles. A design with this property will leave the variance of $\hat{y}$ unchanged when the design is rotated about the center (0, 0, . . . , 0), hence, the name *rotatable* design.

Rotatability is a reasonable basis for the selection of a response surface design. Because the purpose of RSM is optimization and the location of the optimum is unknown prior to running the experiment, it makes sense to use a design that provides equal precision of estimation in all directions (it can be shown that any first-order orthogonal design is rotatable).

A central composite design is made rotatable by the choice of α. The value of α for rotatability depends on the number of points in the factorial portion of the design; in fact, $\alpha = (n_F)^{1/4}$ yields a rotatable central composite design where n_F is the number of points used in the factorial portion of the design.





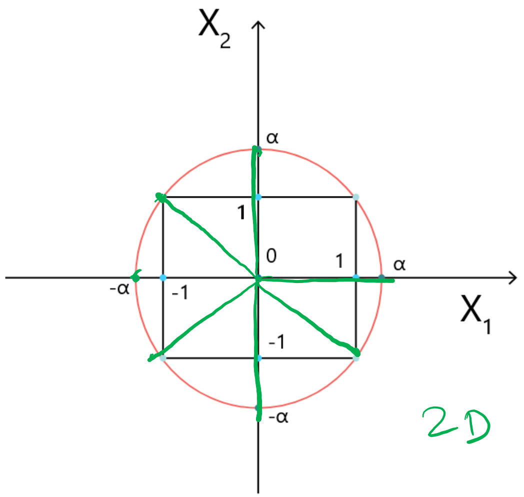
		k = 2	k = 3	k = 4	k = 5
Central Composite Designs	Factorial points 2^k	4	8	16	32
	Star points $2k$	4	6	8	10
	Center points n_c (varies)	5	5	6	6
	Total	13	19	30	48
3^k Designs		9	27	81	243
Choice of α	Spherical design ($\alpha = \sqrt{k}$)	1.4	1.73	2	2.24
	Rotatable design ($\alpha = (n_F)^{\frac{1}{4}}$)	1.4	1.68	2	2.38

n_F

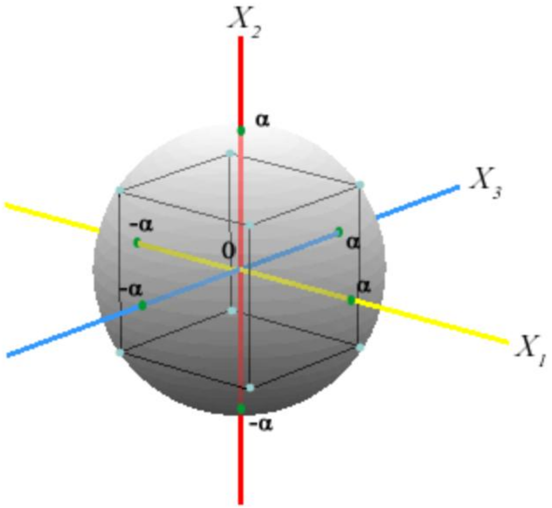
2^k

$+ 2k$ at

$+ n_c$



2D



3D

Center Runs in the CCD

The choice of α in the CCD is dictated primarily by the region of interest. When this region is a sphere, the design must include center runs to provide reasonably stable variance of predicted response. Generally, three to five center runs are recommended.

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

For example, if we have 2 variables $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \epsilon$

how many regression coeff $= 1 + k + {}^{k}C_2 + k$

$$= 1 + 2k + \frac{k(k-1)}{2} = \frac{k^2}{2} + \frac{3}{2}k + 1$$

$$= \frac{k^2 + 3k + 2}{2} = \frac{(k+1)(k+2)}{2}$$

$$= {}^{k+2}C_2$$

How to find 6 regression coeff.?

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \epsilon$$

$\beta_3 = \beta_{12}$, $x_3 = x_1 x_2$; $\beta_4 = \beta_{11}$, $x_4 = x_1^2$; β_{22}, x_2^2

	x_1	x_2	x_1x_2 (x_3)	x_1^2 (x_4)	x_2^2 (x_5)
1	1	1	1	1	1
1	1	-1	-1	1	1
1	-1	-1	1	1	1
1	-1	1	-1	1	1

X

$X_{n \times {}^{k+2}C_2}$

Box-Behnken Design

Table 11-8 A Three-Variable Box–Behnken Design

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

Table 11-8 shows a three-variable Box–Behnken design. The design is also shown geometrically in Figure 11-22. Notice that the Box–Behnken design is a spherical design, with all points lying on a sphere of radius $\sqrt{2}$. Also, the Box–Behnken design does not contain any points at the vertices of the cubic region created by the upper and lower limits for each variable. This could be advantageous when the points on the corners of the cube represent factor-level combinations that are prohibitively expensive or impossible to test because of physical process constraints.

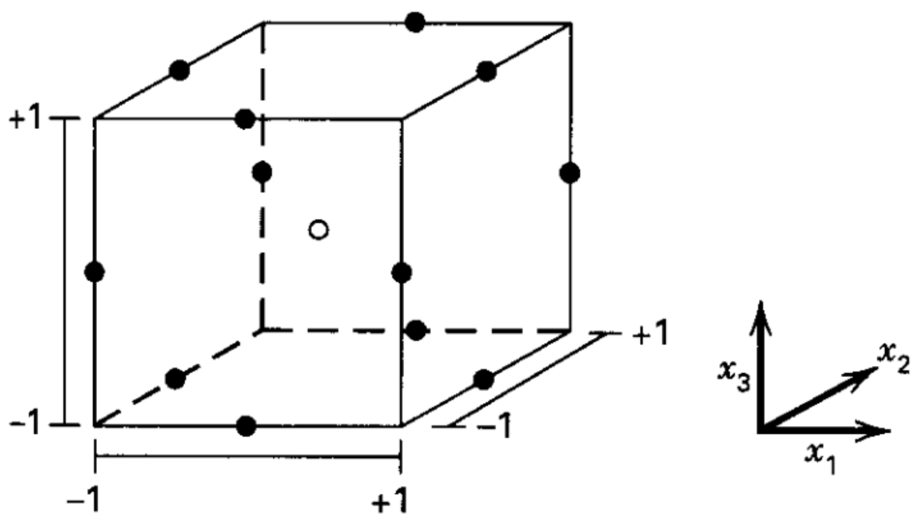


Figure 11-22 A Box–Behnken design for three factors.

Taguchi Orthogonal Designs

L4 Array

Row Number	Col 1	Col 2	Col 3
1	1	1	1
2	1	2	2
3	2	1	2
4	2	2	1

L8 Array

Test No	Col1	Col2	Col3	Col4	Col5	Col6	Col7
1	1	1	1	1	1	1	1
2	1	1	1	2	2	2	2
3	1	2	2	1	1	2	2
4	1	2	2	2	2	1	1
5	2	1	2	1	2	1	2
6	2	1	2	2	1	2	1
7	2	2	1	1	2	2	1
8	2	2	1	2	1	1	2

L9 Array

Row No	Col 1	Col 2	Col 3	Col 4
1	1	1	1	1
2	1	2	2	2
3	1	3	3	3
4	2	1	2	3
5	2	2	3	1
6	2	3	1	2
7	3	1	3	2
8	3	2	1	3
9	3	3	2	1

DIY:

(a) What is the effects model for these designs?

(b) How would you perform ANOVA of these designs?

Taguchi Orthogonal Designs

L18 Array

Row Number	Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	Col 7	Col 8
1	1	1	1	1	1	1	1	1
2	1	1	2	2	2	2	2	2
3	1	1	3	3	3	3	3	3
4	1	2	1	1	2	2	3	3
5	1	2	2	2	3	3	1	1
6	1	2	3	3	1	1	2	2
7	1	3	1	2	1	3	2	3
8	1	3	2	3	2	1	3	1
9	1	3	3	1	3	2	1	2
10	2	1	1	3	3	2	2	1
11	2	1	2	1	1	3	3	2
12	2	1	3	2	2	1	1	3
13	2	2	1	2	3	1	3	2
14	2	2	2	3	1	2	1	3
15	2	2	3	1	2	3	2	1
16	2	3	1	3	2	3	1	2
17	2	3	2	1	3	1	2	3
18	2	3	3	2	1	2	3	1

DIY:

(a) What is the effects model for these designs?

(b) How would you perform ANOVA of these designs?

ME 794

Statistical Design of Experiments

Instructors: Prof. Suhas Joshi, Prof. Soham Mujumdar (sohammujumdar@iitb.ac.in)

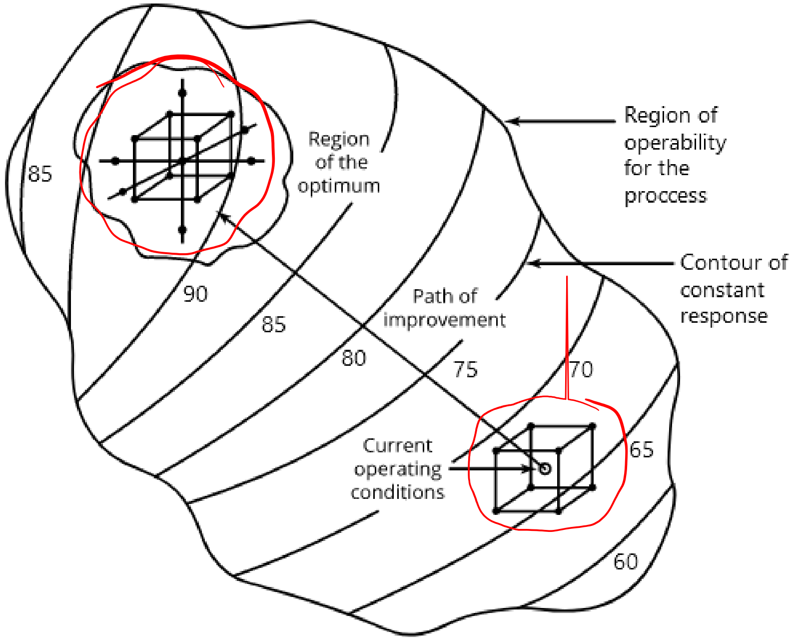
Response Surface Methodology

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).

Department of Mechanical Engineering
Indian Institute of Technology Bombay

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.

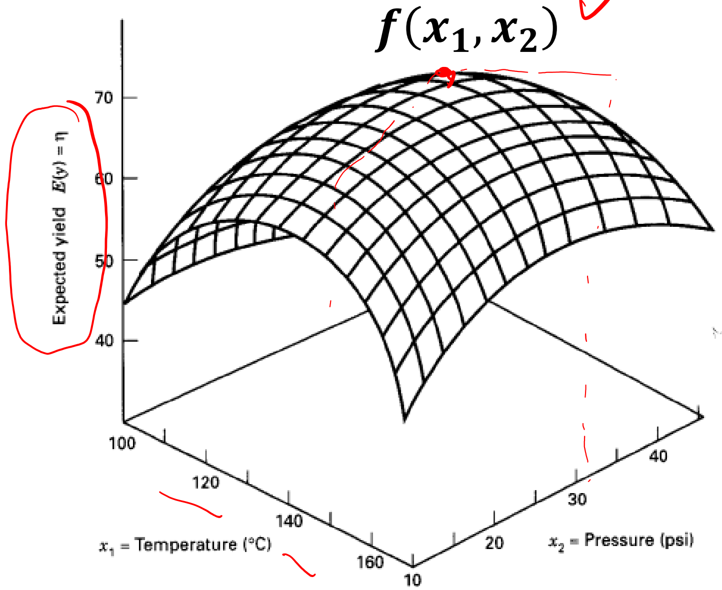
One may write, $\boldsymbol{y = f(x_1, x_2) + \epsilon}$

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

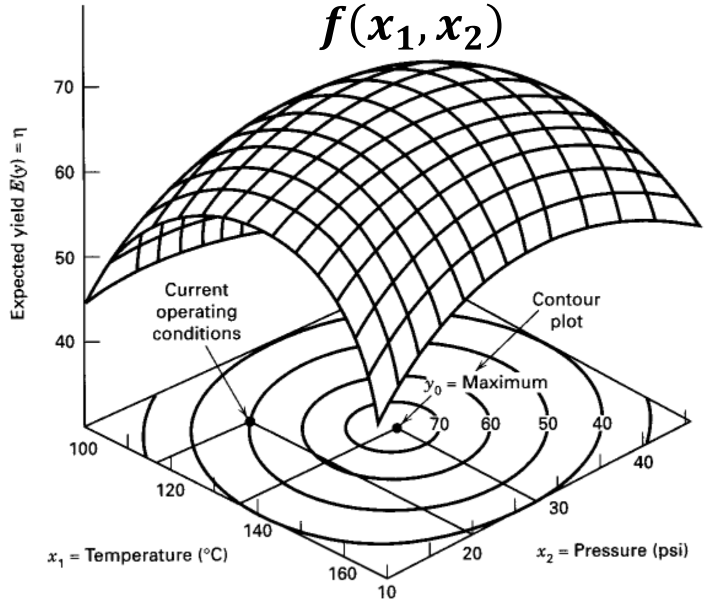
The expected value of the response 'y' will be **E(y) =** $\boldsymbol{f(x_1, x_2)}$

One could show this graphically,

$\boldsymbol{f(x_1, x_2)}$



$\boldsymbol{f(x_1, x_2)}$



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

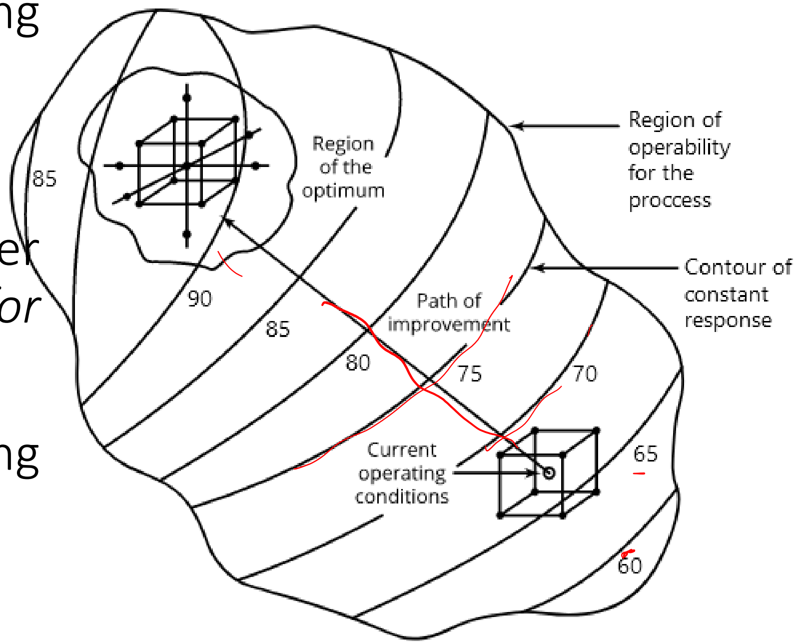
For example, if response (y) is well modeled by linear function of independent variables $(x_1, x_2, x_3, \ldots, x_k)$, then we can write the approximate function as 'first order model'

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

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

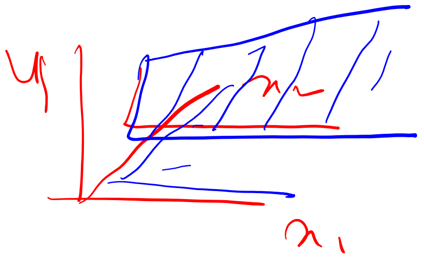
For example, second degree model : $y = \beta_0 + \sum_{i=0}^{k} \beta_i x_i + \sum_{i=0}^{k} \beta_{ii} x_i^2 + \Sigma\Sigma\, \beta_{ij} x_i x_j + \epsilon$

- 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’



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

- 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

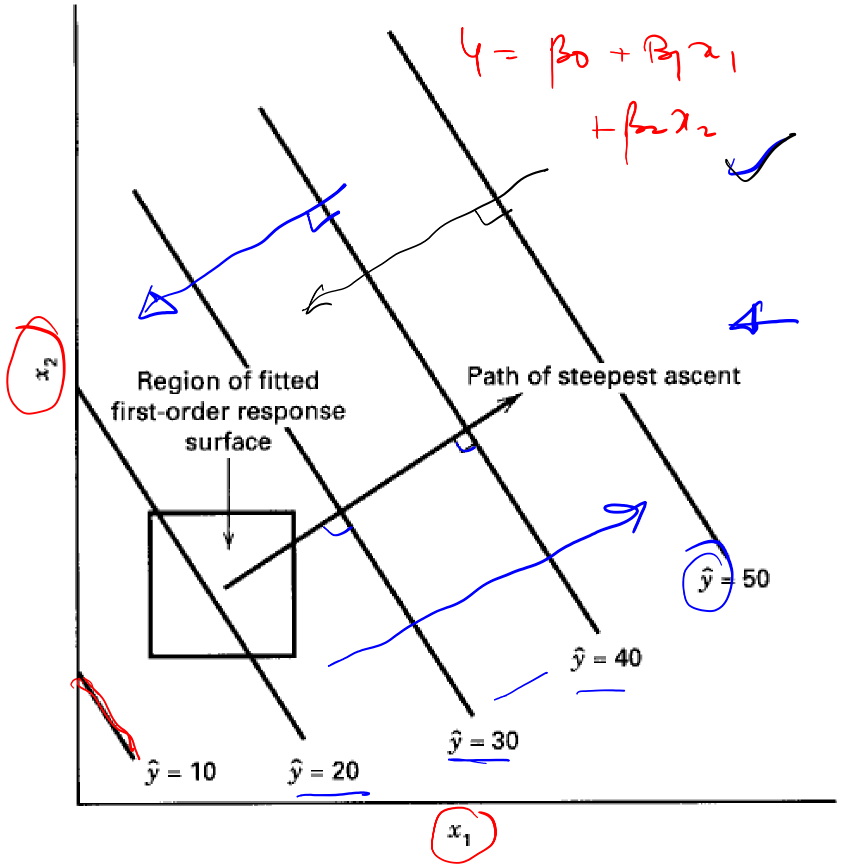
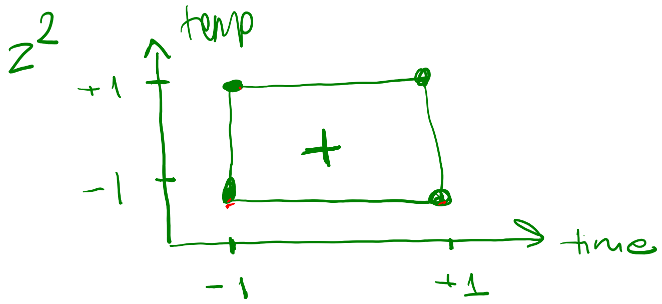


Figure 11-4 First-order response surface and path of steepest ascent.

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 $\quad\quad$ 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

2^2

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

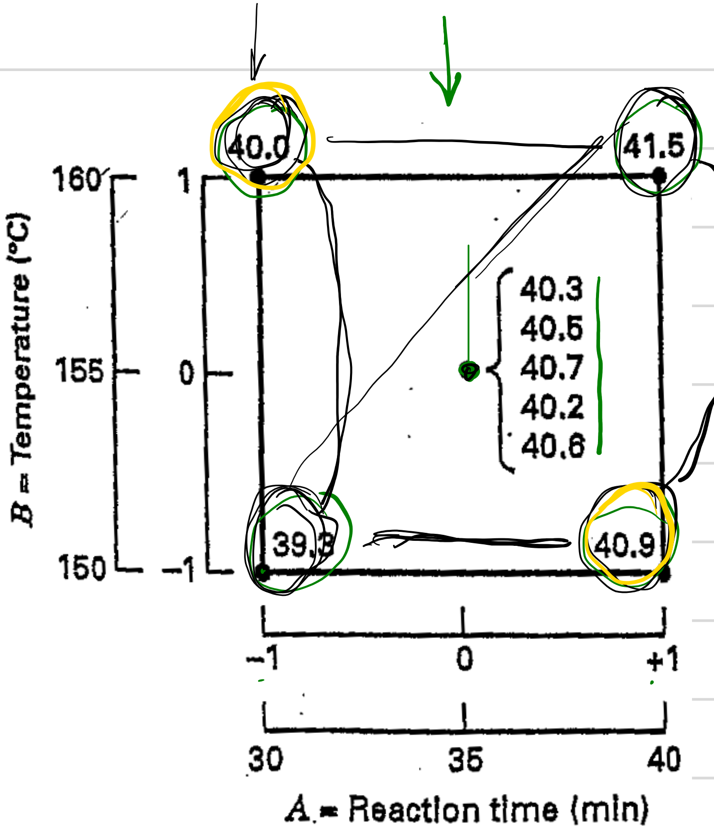
Can we find which terms are important?

What will be the first-order model?

Will a first-order model be appropriate?

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

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



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

First let's find out (DIY)

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

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

$= 40.425$

$\beta_1 = 1/2(-39.3-40.0+40.9+41.5)$

$= 1.55$

$\beta_2 = 1/2(-39.3+40-40.9+41.5)$

$= 0.65$

$\beta_{12} = -0.05$

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

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

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
$x_1 x_2$	1 ✓	0.0025		0.06
mean	1			
ε	5-1 ✓	0.172		
and	1	?		

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

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

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

$$= 0.0025$$

✓

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

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

$$=$$

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

Another check of the adequacy of the straight-line model is obtained by applying the check for pure quadratic curvature effect described in Section 6-6. Recall that this consists of comparing the average response at the four points in the factorial portion of the design, say $\bar{y}_F = 40.425$, with the average response at the design center, say $\bar{y}_C = 40.46$. If there is quadratic curvature in the true response function, then $\bar{y}_F - \bar{y}_C$ is a measure of this curvature. If 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'

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

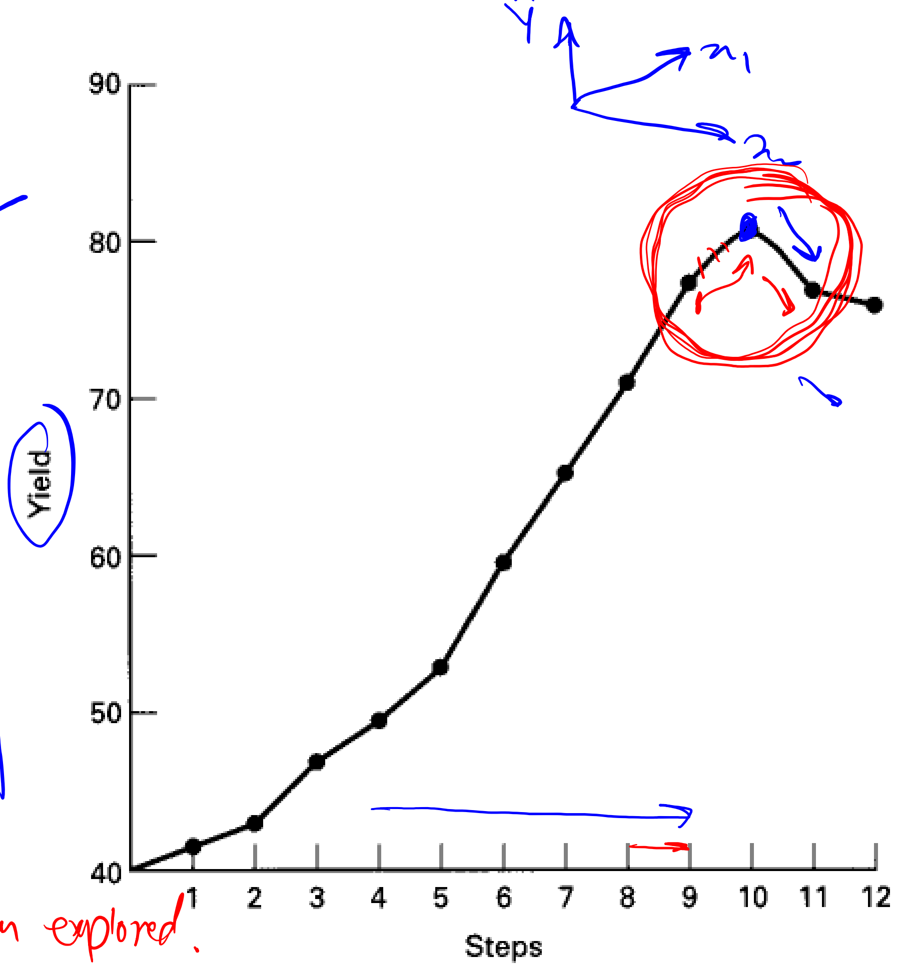
$$\hat{y} = 40.44 + 0.775x_1 + 0.325x_2$$

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

	Coded Variables		Natural Variables		Response
Steps	x_1	x_2	ξ_1	ξ_2	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]

these are outside the region you explored.