ST-302
Design, Planning and Analysis of Experiments

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Topic 9: Response Surface Models

Experimental Design Objectives

Comparative objective: If you have one or several factors under investigation, but the primary goal of your experiment is to make a conclusion about one a-priori important factor, (in the presence of, and/or in spite of the existence of the other factors), and the question of interest is whether or not that factor is "significant", (i.e., whether or not there is a significant change in the response for different levels of that factor), then you have a comparative problem and you need a comparative design solution.

Introduction: RSM

- **Process optimization** is the procedure of finding the set of operating conditions for the process variables that result in the best process performance.

- **Response surface methodology** is an approach to optimization.

What is RSM?

Response surface methodology, or RSM , is a

- collection of mathematical and statistical techniques useful for modelling and analysis in applications where a response of interest is influenced by several variables and the objective is to **optimize** this response.

Need of designs for optimization

- One is always interested in gaining more and more information with

  - Minimum number of runs of the experiment

  - Minimum resources such as time, materials, manpower, machine utilization etc.

  - Level of complexity of statistical model should be minimum unless it is need of the situation.

  - Number of factors affecting the response at initial stage are too many and very few of them to be identified for optimization purpose.

What are response surface methods?

- Response surface methods are used to examine the relationship between a response variable and a set of experimental variables or factors.

- These methods are often employed after you have identified a "vital few" controllable factors and you want to find the factor settings that optimize the response.

- Designs of this type are usually chosen when you suspect curvature in the response surface.

What are response surface methods?

Response surface methods may be employed to

- find factor settings (operating conditions) that produce the "best" response

- find factor settings that satisfy operating or process specifications

- identify new operating conditions that produce demonstrated improvement in product quality over the quality achieved by current conditions

- model a relationship between the response and continuous and categorical factors

Objectives of RSM

- To determine the factor levels that will simultaneously satisfy a set of desired specifications

- To determine the optimum combination of factors that yield a desired response and describes the response near the optimum

- To determine how a specific response is affected by changes in the level of the factors over the specified levels of interest

Stages in RSM

- Perform screening experiments to identify the significant factors among several factors.

- Confirm whether you are within optimization region. If not perform one more screening experiment with modified factors/factor levels.

- For exact optimization select the appropriate designs. Possible choices may be,

  -Central composite design

  -Box Behnken design

Design Selection Guideline

Number of Factors	Comparative Objective	Screening Objective	Response Surface Objective
1	1-factor completely randomized design	–	–
2 - 4	Randomized block design	Full or fractional factorial	Central composite or Box-Behnken
5 or more	Randomized block design	Fractional factorial or Placket t-Burman	Screen first to reduce number of factors

Screening

- Aim – To identify significant factors among many factors (variables).

- A factor is 'significant' if its influence is greater than the 'noise' level (experimental error)

- Usual designs to carry out screening using reduced designs such as

   - factorial designs

   -Fractional factorial designs

   -Plackett-Burman designs

Experimental Design Objectives…

Screening objective: The primary purpose of the experiment is to select or screen out the few important main effects from the many less important ones. These screening designs are also termed main effects designs.

Designs for process parameter optimization

Response Surface Designs

- PBD, Fractional FD (Screening designs)

- 3-level factorial designs

- Box-Benkin designs (Designs for optimization)

- CCD (Designs for optimization)

Taguchi Designs

- Orthogonal arrays

Response Surface (method) objective

The experiment is designed to allow us to estimate interaction and even quadratic effects, and therefore give us an idea of the (local) shape of the response surface we are investigating. For this reason, they are termed response surface method (RSM) designs. RSM designs are used to:

- Find improved or optimal process settings
- Troubleshoot process problems and weak points
- Make a product or process more robust against external and non-controllable influences. "Robust" means relatively insensitive to these influences.

RSM Models

- If the response is well modeled by a <u>linear function</u> of the independent variables, then the approximating function is the **first-order model (linear model)**:

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

- If <u>curvature</u> is present in the system, then a model such as the **second-order model (quadratic model)** may be of use:

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i X_i + \sum_{i=1}^{k} \beta_{ii} X_i^2 + \sum_{\substack{i,j=1, \\ i<j}}^{k} \beta_{ij} X_i X_j + \varepsilon$$

RSM Models

- The **second-order model (quadratic model/polynomial model)** gives a better approximation of the true relationship over the entire space of the independent variables.

- The second-order RSM is fitted by using least square method.

- Designs which are used for fitting RSM are called Response Surface Designs.

Location of a stationary point

- Consider the following **second-order RSM**

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i X_i + \sum_{i=1}^{k} \beta_{ii} X_i^2 + \sum_{\substack{i,j=1, \\ i<j}}^{k} \beta_{ij} X_i X_j + \varepsilon$$

- When it is fitted then it can be written as

$$\hat{y} = \hat{\beta}_0 + \sum_{i=1}^{k} \hat{\beta}_i X_i + \sum_{i=1}^{k} \hat{\beta}_{ii} X_i^2 + \sum_{\substack{i,j=1, \\ i<j}}^{k} \hat{\beta}_{ij} X_i X_j$$

$$\hat{y} = \hat{\beta}_0 + \underline{X}' \underline{b} + \underline{X}' B \underline{X}$$

Location of a stationary point…

$$\hat{y} = \hat{\beta}_0 + \underline{X}'\underline{b} + \underline{X}'B\underline{X}$$

where $\underline{b} = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix}$ and $B = \begin{bmatrix} \hat{\beta}_{11} & \dfrac{\hat{\beta}_{12}}{2} & \cdots & \dfrac{\hat{\beta}_{1k}}{2} \\ \dfrac{\hat{\beta}_{12}}{2} & \hat{\beta}_{22} & \cdots & \dfrac{\hat{\beta}_{2k}}{2} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\hat{\beta}_{1k}}{2} & \dfrac{\hat{\beta}_{2k}}{2} & \cdots & \hat{\beta}_{kk} \end{bmatrix}$

Here $\underline{b}$ and B are known when we have the fitted model.

To obtain stationary point differentiate $\hat{y}$ with respect to $\underline{X}$ and equate to $\underline{0}$.

Location of a stationary point…

$$\hat{y} = \hat{\beta}_0 + \underline{X}'\underline{b} + \underline{X}'B\underline{X}$$

$$\frac{\mathrm{d}\hat{y}}{\mathrm{d}\underline{X}} = \underline{0}$$

$$\Rightarrow \underline{b} + 2B\underline{X} = \underline{0}$$

$$\Rightarrow 2B\underline{X} = -\underline{b}$$

$$\Rightarrow \underline{X} = -\frac{1}{2}B^{-1}\underline{b}$$

$$\Rightarrow \underline{X}_s = -\frac{1}{2}B^{-1}\underline{b}$$

Response at stationary point

$$\hat{y}_s = \hat{y}\big|_{\underline{X}=\underline{X}_s}$$

$$= \hat{\beta}_0 + \left(-\frac{1}{2}B^{-1}\underline{b}\right)' \underline{b} + \left(-\frac{1}{2}B^{-1}\underline{b}\right)' B \left(-\frac{1}{2}B^{-1}\underline{b}\right)$$

$$= \hat{\beta}_0 - \frac{1}{2}\underline{b}'B^{-1}\underline{b} + \frac{1}{4}\left(\underline{b}\right)' B^{-1}BB^{-1}\underline{b}$$

$$= \hat{\beta}_0 - \frac{1}{2}\underline{b}'B^{-1}\underline{b} + \frac{1}{4}\underline{b}'B^{-1}\underline{b}$$

$$= \hat{\beta}_0 - \frac{1}{4}\underline{b}'B^{-1}\underline{b} = \hat{\beta}_0 + \frac{1}{2}\underline{b}'\left(-\frac{1}{2}B^{-1}\underline{b}\right)$$

$$= \hat{\beta}_0 + \frac{1}{2}\underline{b}'\underline{X}_s$$

Nature of stationary point

- Suppose we wish to find the levels of variables $X_1, X_2, \ldots, X_k$ that optimize the predicted response. This point, if it exists, will be the point $\underline{x}_S$ such that

  $$\frac{d\hat{y}}{d\underline{x}_S} = \underline{0}.$$ That is the set of variables for which the partial derivatives with respect to each is zero.

- This point, say $\underline{x}_S$ is called the stationary point. The stationary point could represent

  (1) a point of maximum response,

  (2) a point of minimum response, or

  (3) a saddle point
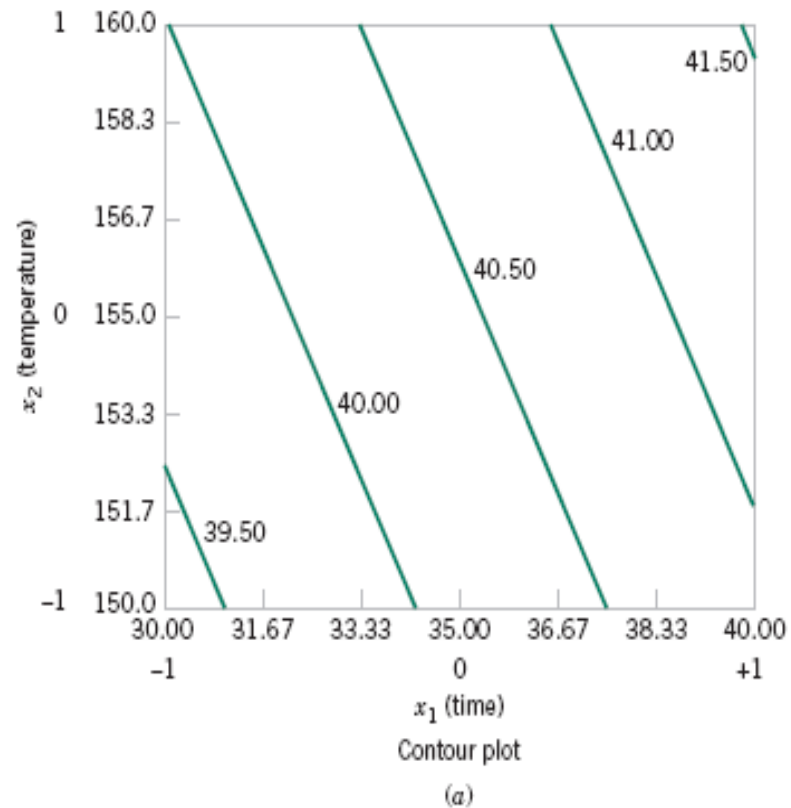
Example:

- Consider the following response surface model fitted for predicting response y for given predictor variables X_1 and X_2.
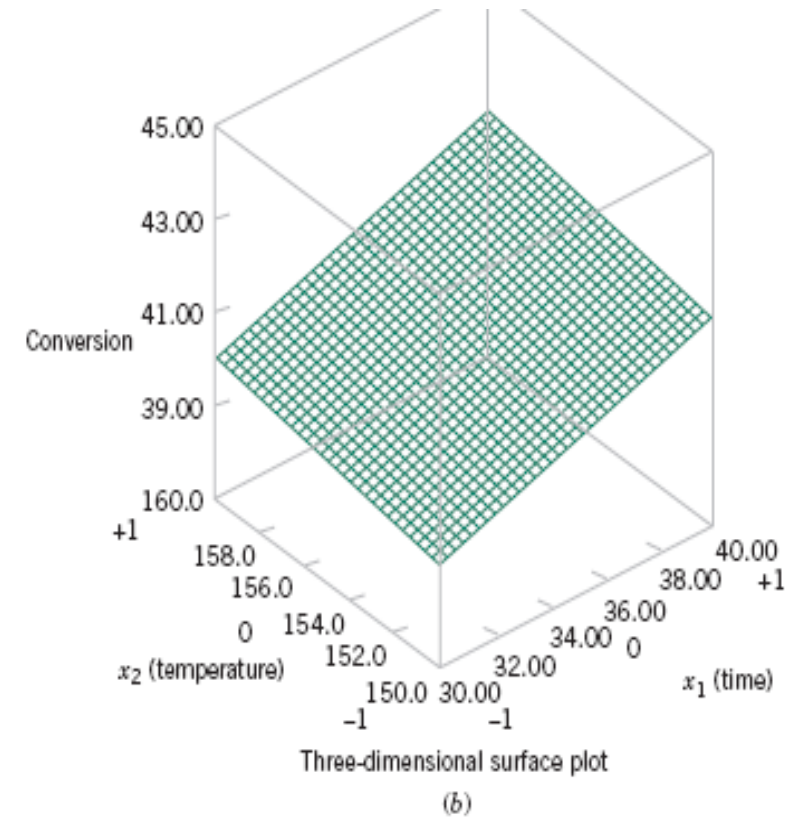
$$\hat{y} = 70 - 16x_1 + 11x_2 - 9x_1^2 - 6x_2^2 - 2x_1x_2$$

Obtain the stationary point and response at stationary point.
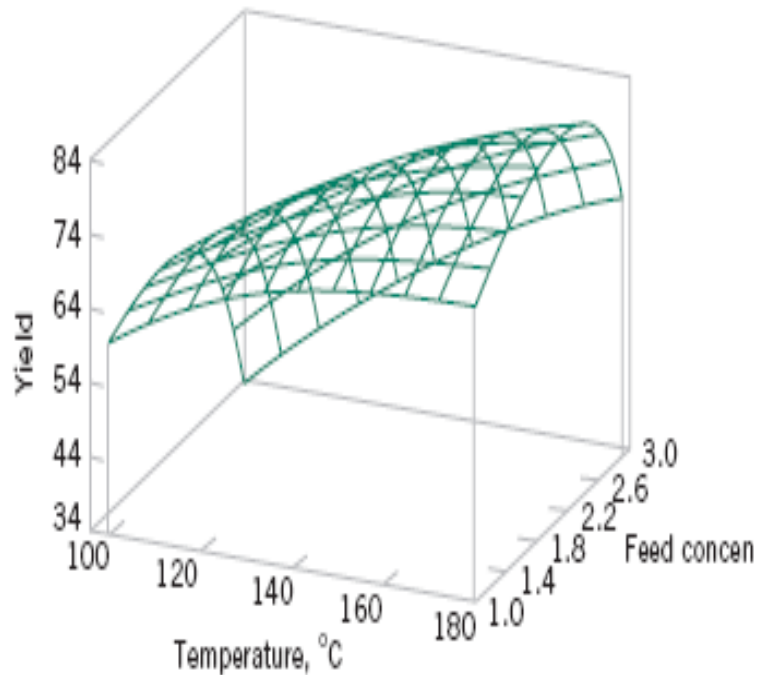
Example : Fitting first order RSM
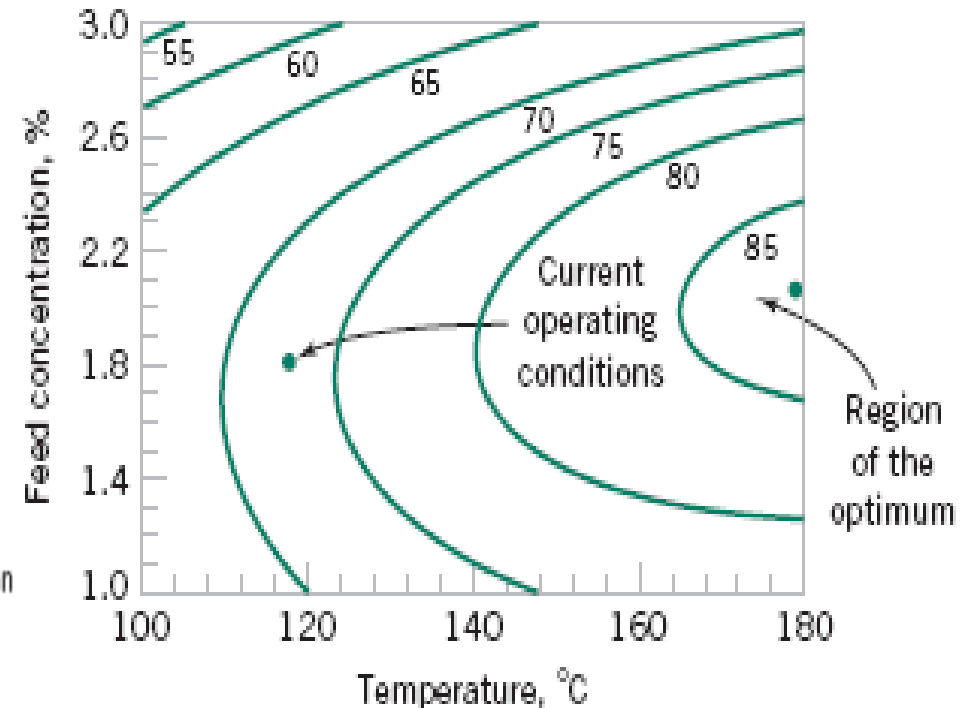

A contour plot

A response surface plot

Example : Fitting second order RSM

A three-dimensional response surface showing the expected yield as a function of temperature and feed concentration.


A contour plot of yield

Contour Plot

- A contour plot is a graphical technique for representing a 3-dimensional surface by plotting constant z slices, called contours, on a 2-dimensional format. A contour plot displays a two-dimensional view in which points that have the same response value are connected to produce contour lines.

- That is given a value for z, lines are drawn for connecting all the (x, y) coordinates where that z value occurs.

- Contours are composed of all the (x, y) points which are at an equal distance from the X-Y plane (i.e. at an equal height)

- Contour plots of the response surface can be used to explore the effect of changing factor levels on the response

Contour Plot…

RSP (3D):
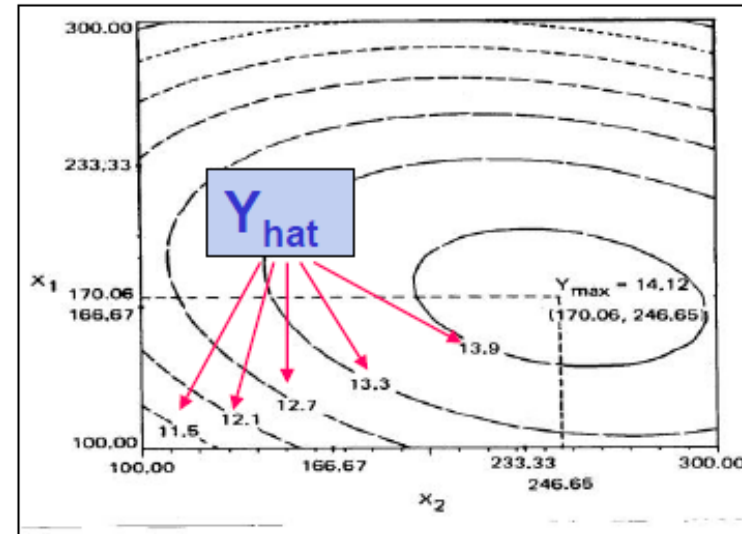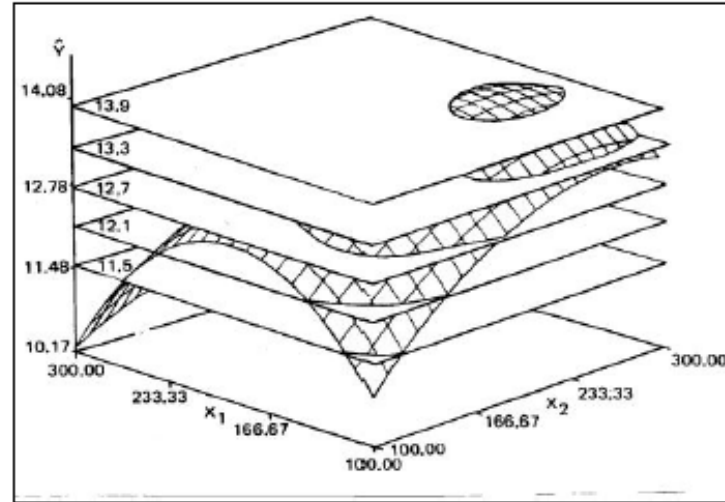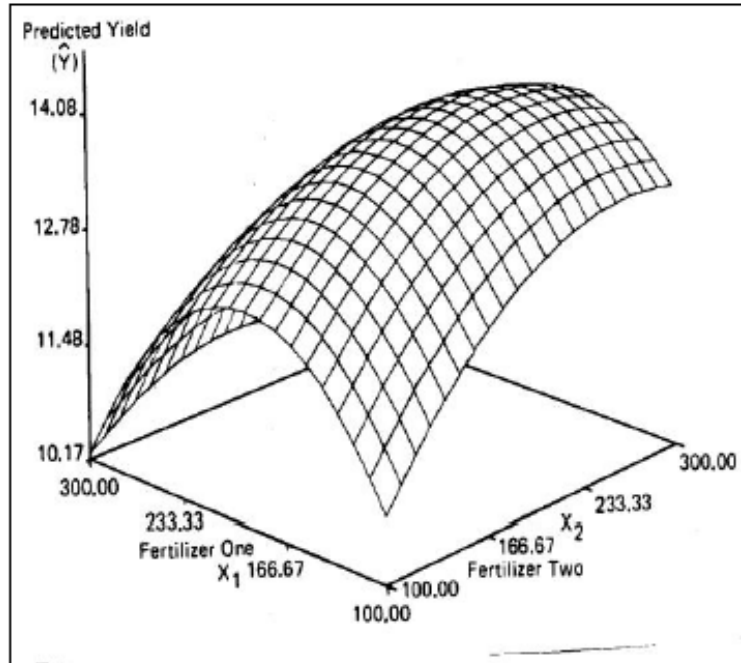
RSP and CP illustration surface with maximum

(a) Response surface
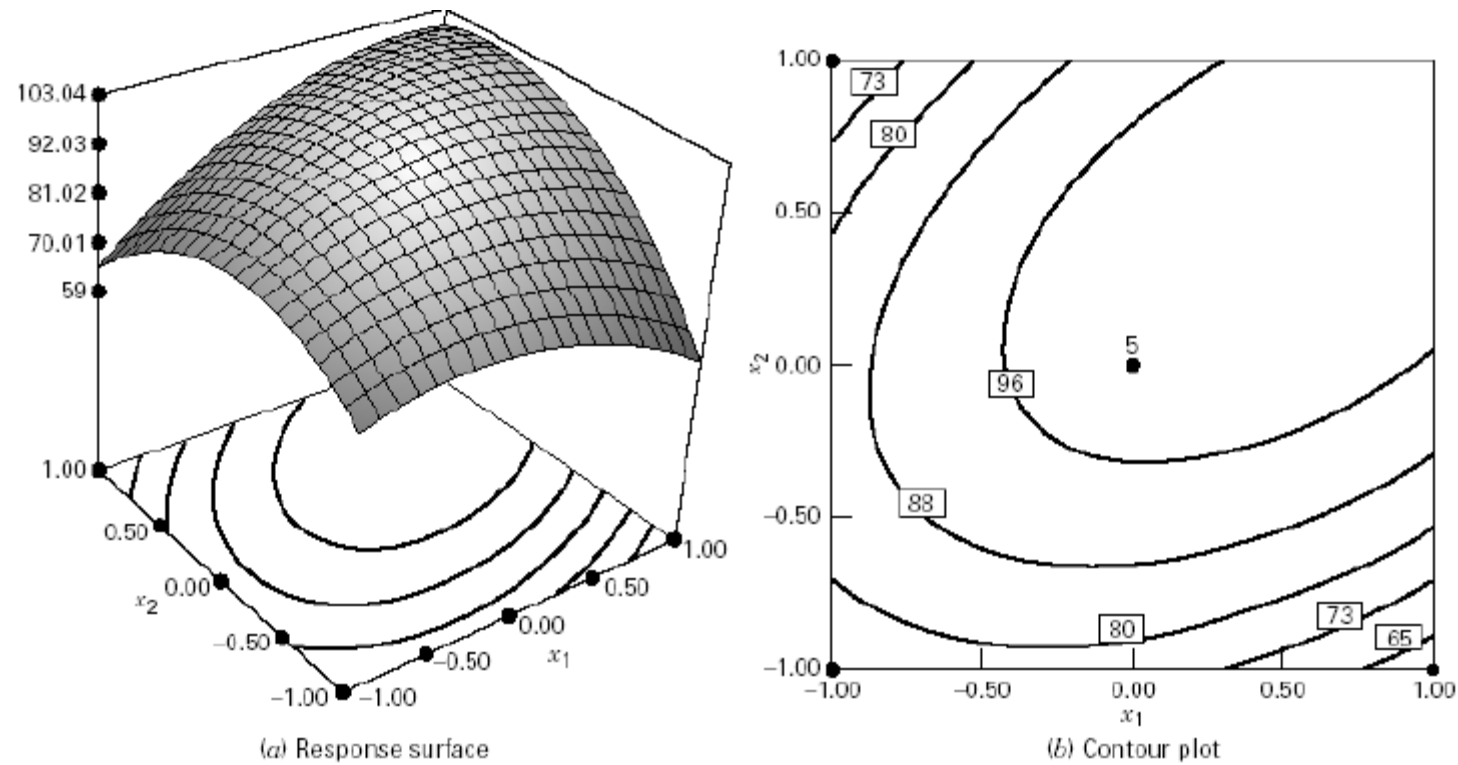
(b) Contour plot

RSP and CP illustration surface with minimum

(a) Response surface
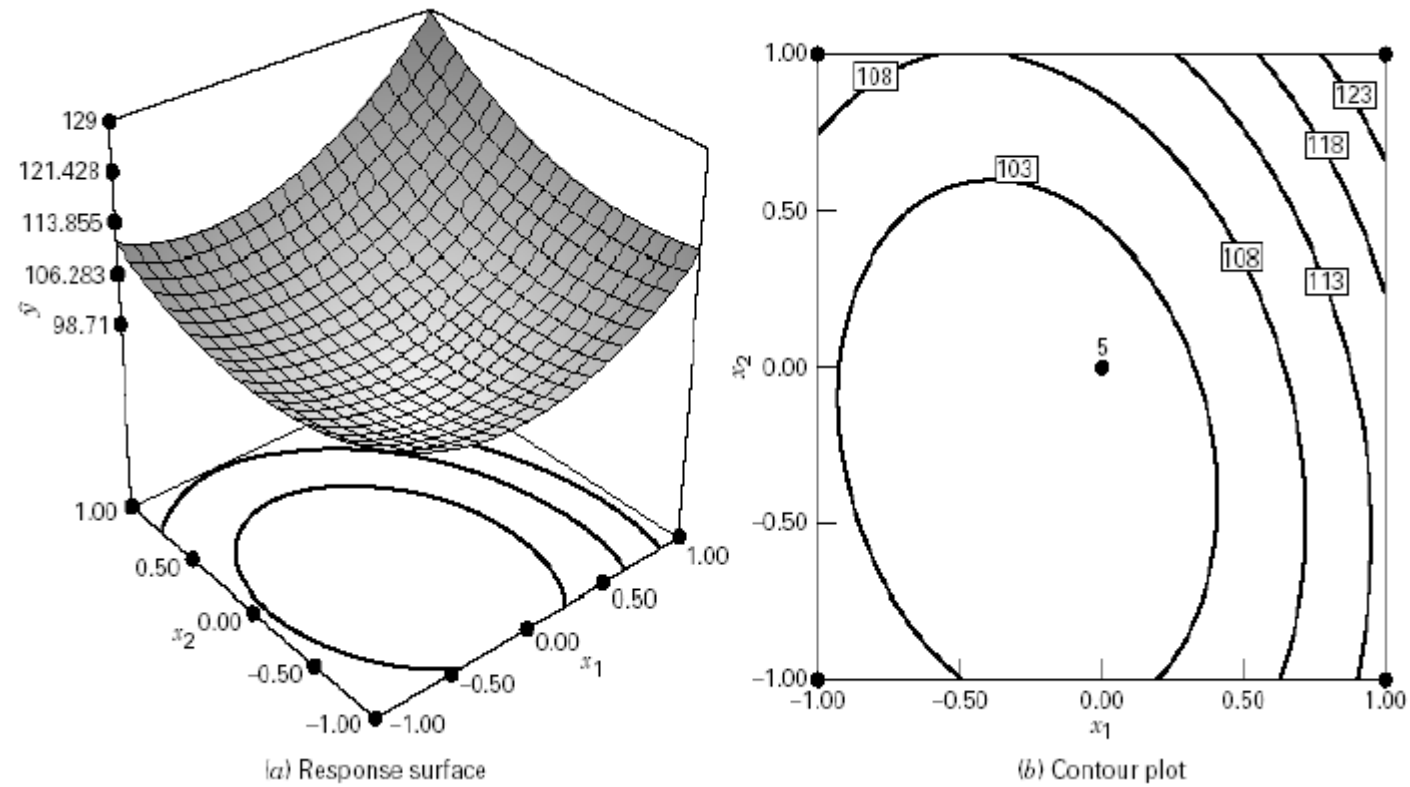
(b) Contour plot

RSP and CP illustration surface with saddle point or minimax
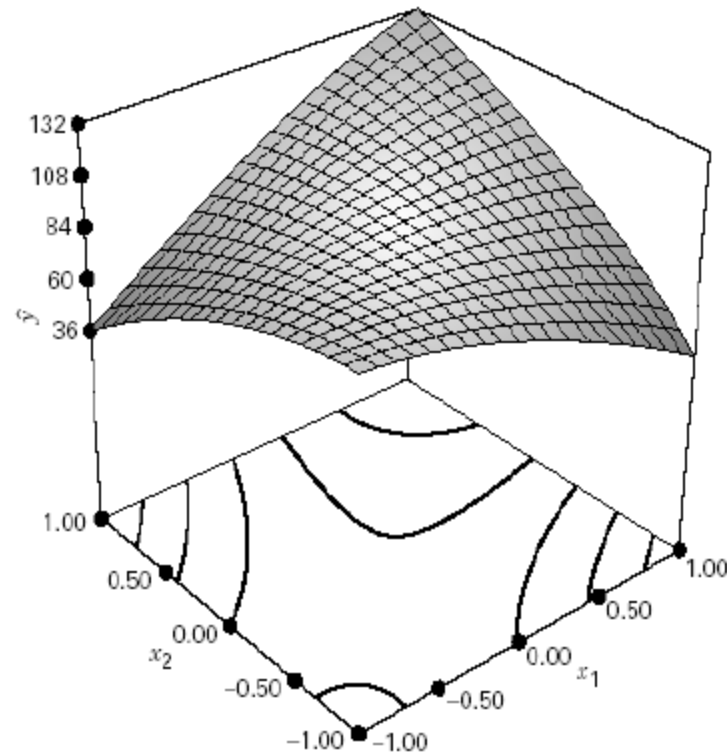
(a) Response surface
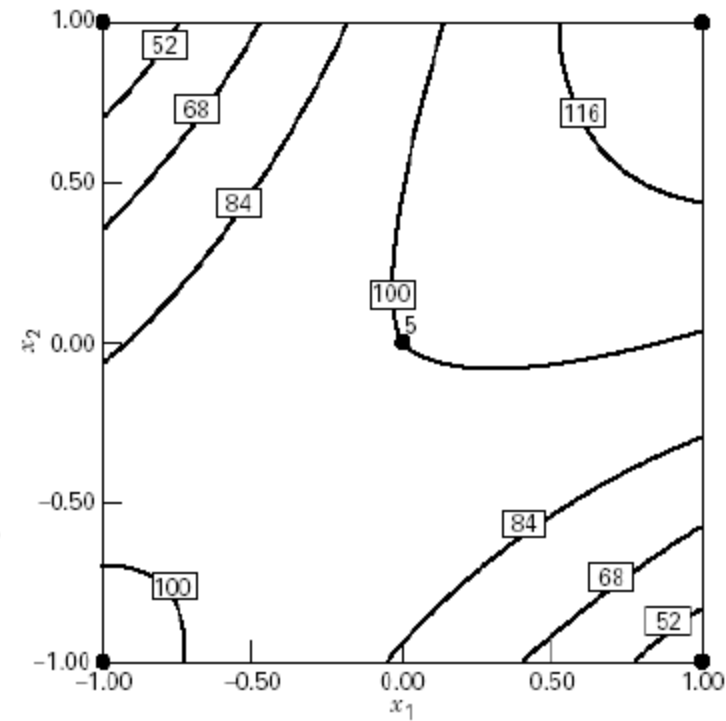
(b) Contour plot

Drawback of contour Plots

- When drawing the contour plots or response surfaces on the model chosen, one can only use 2 factors (one for each of the axes X and Y).

- If there are more than 2 factors then choose any two-factors at a time and set the remaining factors at one of their levels.

- This leads to contour plots for all pairs of variables when the other factors are set at a specified value.

Characterizing the RSM

- Once the stationary point is found then the response surface is characterized in the immediate vicinity of this point.

- The meaning of characterize is to determine whether the stationary point is a point of maximum or minimum response or a saddle point.

- The relative sensitivity of the response with respect to the variables $X_1, X_2, \ldots, X_k$ can be also studied.

- This can be done through a contour plot of the fitted model. But contour plots can be used only when there are two or three process variables.

- When there are more than two variables, it is recommended to use **canonical analysis**.

Steps in Canonical analysis

- Transform the model into a new coordinate system with the origin at the stationary point $\underline{x} = \underline{x}_s$ and then to rotate the axes of this system until they are parallel to the principal axes of the fitted response surface.

- This transformation of process variables X_i to canonical variables w_i is such that $(X_1, X_2, \ldots, X_k) \rightarrow (w_1, w_2, \ldots, w_k)$ is such that the transformed model is

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

  where λ_i are constant (in fact λ_i are just the eigen-values of B matrix in second order response surface model.

- The transformed model is called the ***canonical form of the model***.

Nature of response surface through Canonical analysis

- The nature of the response surface can be determined from the stationary point and the signs and magnitudes of λ_i's.

- First suppose that the stationary point is within the region of exploration for fitting the second-order model.

- If all $\lambda_i > 0 \Rightarrow \underline{x}_s$ is point of minimum response

- If all $\lambda_i < 0 \Rightarrow \underline{x}_s$ is point of maximum response

- If $\lambda_i's$ have different signs $\Rightarrow \underline{x}_s$ is a saddle point.

- Furthermore, the surface is steepest in the w_i direction for which is the greatest.

Central Composite Design (CCD): An Optimization Design

CCD: A Designs to fit RSM

- A **central composite design** is an experimental design, useful in response surface methodology, for building a second order (quadratic) model for the response variable without needing to use a complete three-level factorial experiment.

- A Box-Wilson Central Composite Design, commonly called 'a central composite design,' is defined as a full factorial or fractional factorial design with center points that is augmented with a carefully chosen group of 'star points' that allow estimation of curvature.

CCD

- A CCD is composed of factorial points, axial points, and center points. Factorial points are the points from a 2^k design with levels coded as ±1 or the points in a 2^{k-f} fraction with resolution V or greater; center points are again n_c points at the origin.

Runs of CCD

A **central composite design** consists of following runs.

- **Full or fractional factorial runs:** The runs in which each factor is at level either +1 or -1. There are 2^k or 2^{k-f} runs.

- **Star or axial point runs:** The runs where one factor is set at non-zeros (α) level and rest of the factors are set at mid level (i.e. 0 level). Thus axial points have one design variable at $\pm\alpha$ and all other design variables at 0; there are $2k$ axial points.

- **Centre point runs:** All factors are set at zero-level. This experiment is replicated n_C times in CCD

Star points

- These are the points which are at an equal distance say α from centre point.

- When the runs are augumented with $\alpha = 1$ then the 2^k design is augmented to 3^k design. But with $\alpha > 1$ then range of factor variables is wider than that of $\alpha = 1$

- If the distance from the center of the design space to a factorial point is ± 1 unit for each factor, the distance from the center of the design space to a star point is more than 1 unit.

Star points…

- The precise value of α depends on certain properties desired for the design and on the number of factors involved.

Generation of CCD

- One of the reasons that CCD's are so popular is that you can start with a first-order design using a 2^k factorial runs and then augment it with axial points and perhaps more center points to get a second-order design.

- We can perform a lack of fit test for a first-order model fit to data from a first-order design.

- Thus Augment the first-order design by adding axial points and center points to get a CCD, which is a second-order design and can be used to fit a second-order model.

CCD with two factors

Central composite response surface designs are two{level full or fractional factorial designs that have a few extra observations added to allow estimation of second{order response surface models.
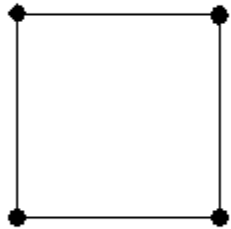
The points in the factorial portion of the design are coded to be -1 and $+1$.
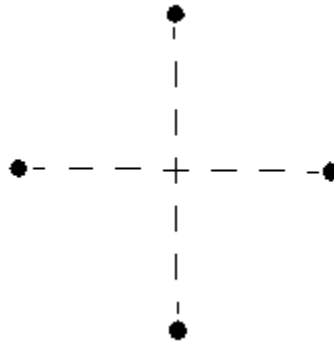
The points in the axial (star) portion of the design are at:$(+\alpha, 0)$, $(-\alpha, 0)$, $(0,+\alpha)$, $(0,-\alpha)$
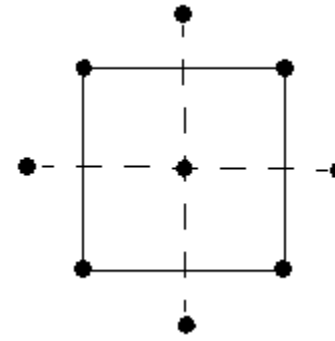
The factorial and axial portions along with the center point. The design center is at $(0,0)$.

CCD with two factors with $\alpha > 1$
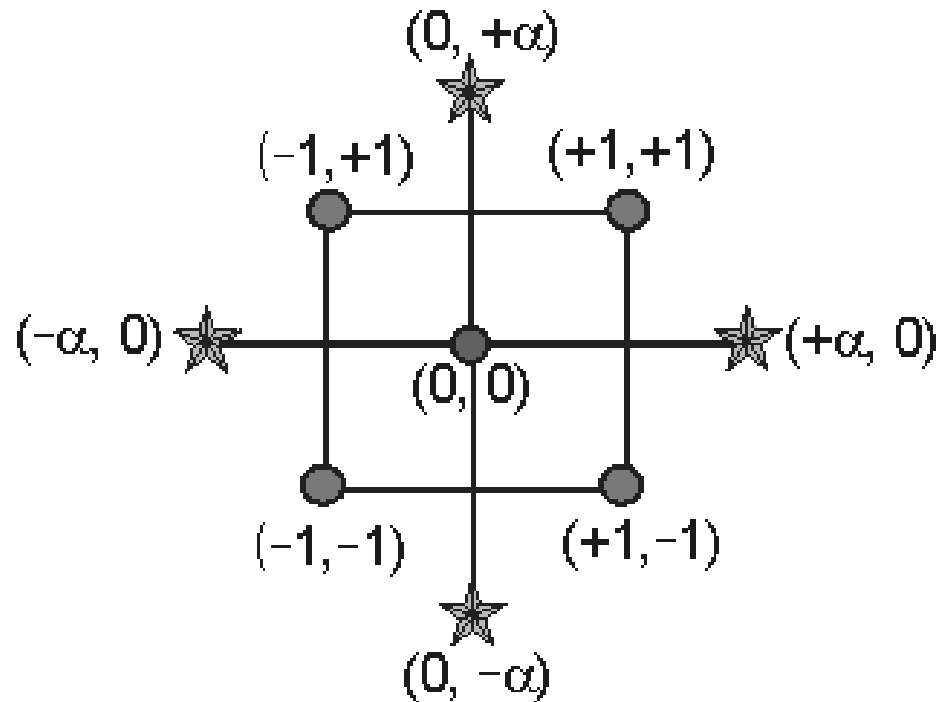
2-Factor CCD with factorial points, star/axial points and center points.

- Four corners of the square represent the factorial (± 1) design points
- Four star points represent the axial ($\pm \alpha$) design points
- Replicated center points

CCD with two factors with $\alpha = 1$
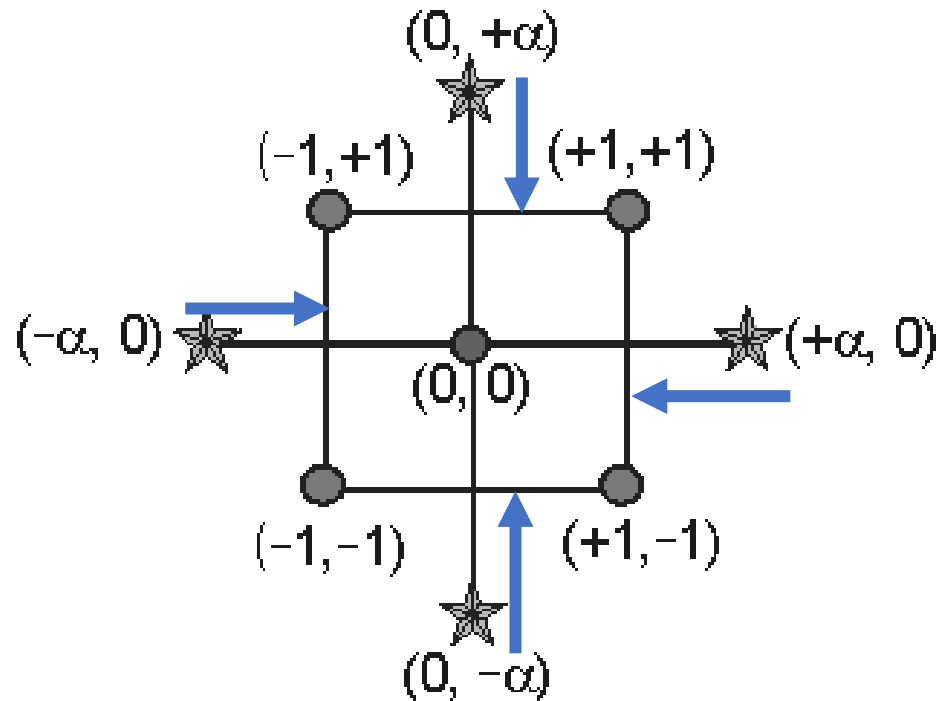
2-Factor CCD with factorial points, star/axial points and center points with $\alpha = 1$ reduces to 3^2 factorial design. The runs would be as follows.

$$(\pm 1, \pm 1) \qquad : 4 \text{ Factorial runs}$$

$$(0, \pm\alpha) = (0,1)$$

$$(\pm\alpha, 0) = (\pm 1, 0) \qquad : 4 \text{ star points}$$

$$(0,0) \qquad\qquad : n_c = 5 \text{ center points}$$

About run in a design

- Run is each experimental condition or factor level combination at which responses are measured.

- Typically, each run corresponds to a row in the layout and results in one or more response measurements, or observations.

- For example, we conduct a full factorial design with two factors, each with two levels., the experiment has four runs.

- Each run corresponds to a design point, and the entire set of runs is the design. Multiple executions of the same experimental conditions are considered separate runs and are called replicates.

Runs of CCD with k factors

- 2^k Factorial runs : $(\pm 1, \pm 1, \ldots, \pm 1)$

- $2k$ Star-point runs : $(\pm \alpha, 0, 0, \ldots, 0)$

$$(0, \pm \alpha, 0, \ldots, 0)$$

$$(0, 0, \pm \alpha, \ldots, 0)$$

$$(0, 0, 0, \ldots, \pm \alpha)$$

- n_c center point runs: $(0, 0, \ldots, 0)$

- Total runs if full factorial design is augmented$=2^k + 2k + n_c$

- Total runs if fractional factorial design is augmented$=2^{k-f} + 2k + n_c$

- n_c is usually chosen as 5 or 6.

Layout of CCD with two factors with and without blocks

Run	A	B
1	-1	-1
2	1	-1
3	-1	1
4	1	1
5	-1.414	0
6	1.414	0
7	0	-1.414
8	0	1.414
9	0	0
10	0	0
11	0	0
12	0	0
13	0	0

Run	A	B	Block
1	-1	-1	1
2	1	-1	1
3	-1	1	1
4	1	1	1
5	0	0	1
6	0	0	1
7	-1.414	0	2
8	1.414	0	2
9	0	-1.414	2
10	0	1.414	2
11	0	0	2
12	0	0	2
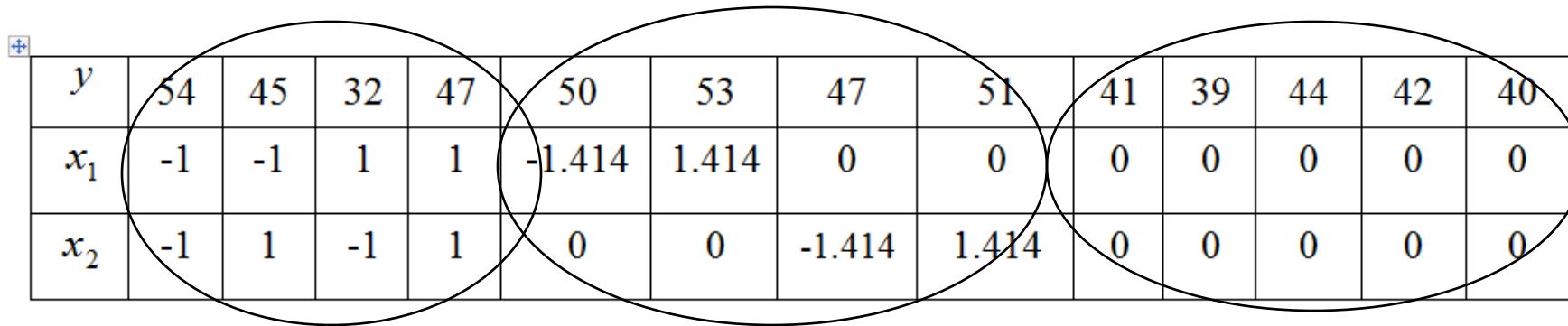
Layout of CCD with three factors with and without blocks

Run	A	B	C
1	-1	-1	-1
2	1	-1	-1
3	-1	1	-1
4	1	1	-1
5	-1	-1	1
6	1	-1	1
7	-1	1	1
8	1	1	1

Run	A	B	C
9	-1.633	0	0
10	1.633	0	0
11	0	-1.633	0
12	0	1.633	0
13	0	0	-1.633
14	0	0	1.633
15	0	0	0
16	0	0	0
17	0	0	0
18	0	0	0
19	0	0	0
20	0	0	0

An example of CCD with 2-factors

The following data was collected by a chemical engineer for the CCD with 2-factors temperature (x1) and pressure(x2). The response is filtration time (y).

y	54	45	32	47	50	53	47	51	41	39	44	42	40
x_1	-1	-1	1	1	-1.414	1.414	0	0	0	0	0	0	0
x_2	-1	1	-1	1	0	0	-1.414	1.414	0	0	0	0	0

Factorial runs   Star point runs   centre point runs

Graphical representation of Runs of CCD with 2 and 3 factors

Star point runs

Factorial runs

centre point runs

CCD with 2 factors

Paramter 3

Paramter 2

Paramter 1

a_1

b_1

■ Cube points

● Axial points

● Center point
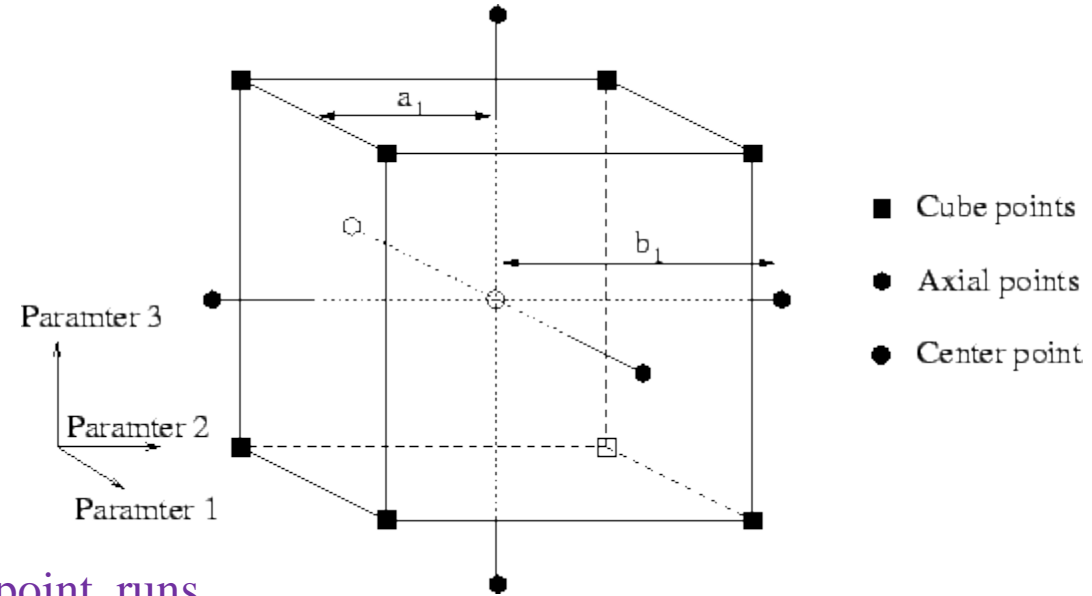
CCD with 3 factors

Role of different points in CCD

The effects that can be estimated depend on the point type:
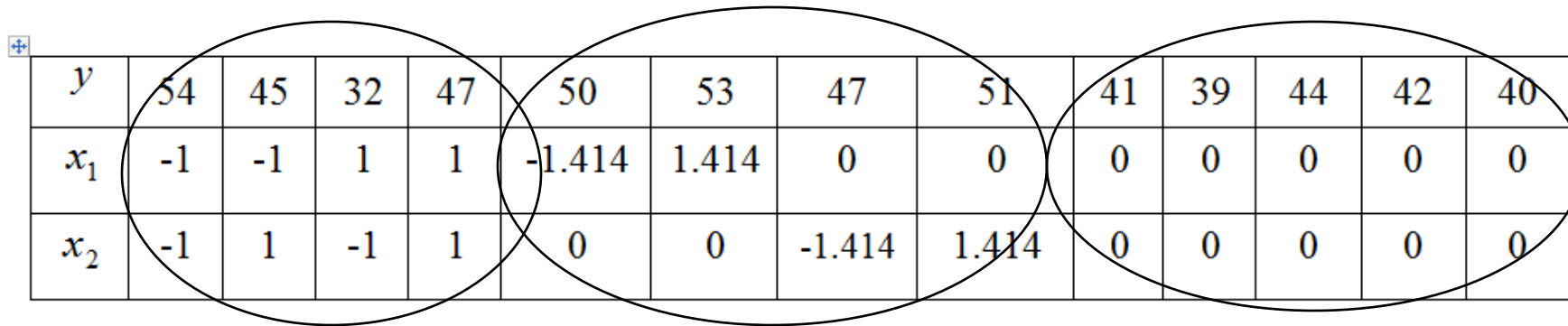
- Cube points - allow for the estimation of linear and interaction effects, but not curvature. (These points are comparable to a the corner points of a 2^K factorial design.)

- Center points - add center points to check for curvature, but not individual quadratic terms. (The point in the middle of the cube represents the center points for both the cube and the axial blocks.)

- Axial points - add axial points, in addition to center points, to estimate quadratic terms. (The points joined by dotted lines indicate points outside or on the surface of the cube.)

Role of star points in CCD

- A central composite design always contains twice as many star points as there are factors in the design.

- The star points represent new extreme values (low and high) for each factor in the design.

An example of CCD with 2-factors

The following data was collected by a chemical engineer for the CCD with 2-factors temperature (x1) and pressure(x2). The response is filtration time (y).
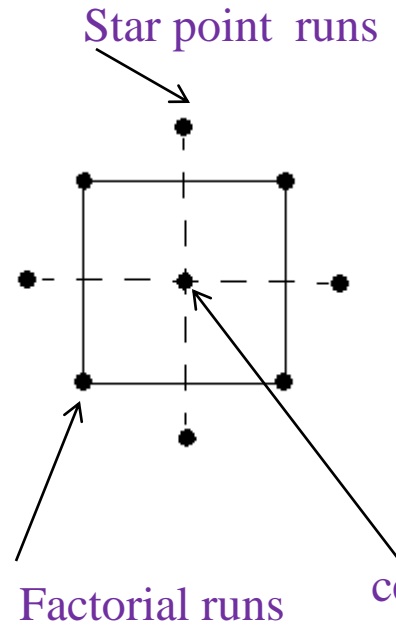
y	54	45	32	47	50	53	47	51	41	39	44	42	40
x_1	-1	-1	1	1	-1.414	1.414	0	0	0	0	0	0	0
x_2	-1	1	-1	1	0	0	-1.414	1.414	0	0	0	0	0

Factorial runs   Star point runs   centre point runs

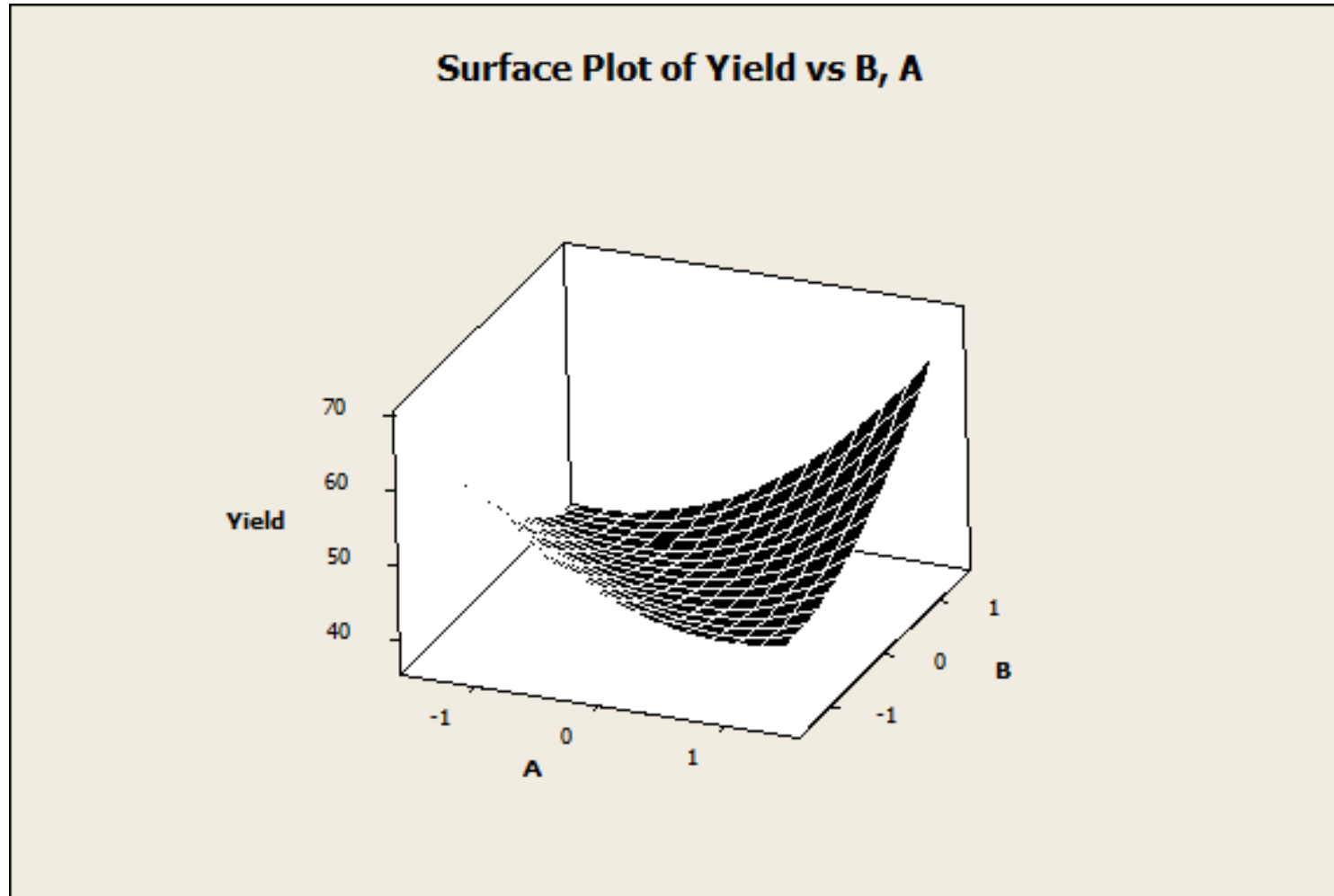# Analysis of CCD with 2-factors

The analysis was done using coded units.

Analysis of Variance for Yield

Source	DF	Seq SS	Adj SS	Adj MS	F	P
Regression	5	306.40	306.40	61.281	2.62	0.121
Linear	2	38.83	38.83	19.415	0.83	0.475
A	1	13.11	13.11	13.114	0.56	0.478
B	1	25.72	25.72	25.716	1.10	0.329
Square	2	123.58	123.58	61.788	2.64	0.140
A*A	1	81.39	95.88	95.879	4.10	0.082
B*B	1	42.18	42.18	42.184	1.80	0.221
Interaction	1	144.00	144.00	144.000	6.16	0.042
A*B	1	144.00	144.00	144.000	6.16	0.042
Residual Error	7	163.60	163.60	23.371		
Lack-of-Fit	3	148.80	148.80	49.598	13.40	0.015
Pure Error	4	14.80	14.80	3.700		
Total	12	470.00				

Estimated Regression Coefficients for Yield using data in uncoded units

Term	Coef
Constant	41.2000
A	1.28033
B	-1.79289
A*A	3.71250
B*B	2.46250
A*B	6.00000

Analysis of CCD with 2-factors

Surface Plot of Yield vs B, A

Analysis of CCD with 2-factors

Contour Plot of Yield vs B, A
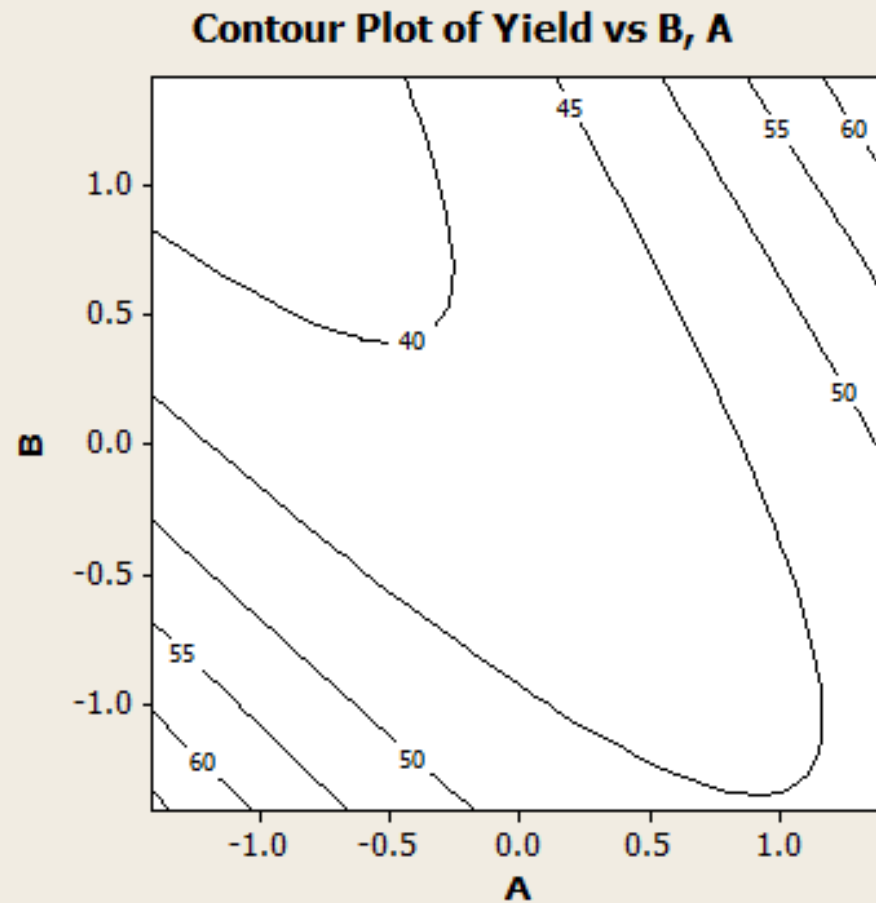
An example of CCD with 3-factors

A CCD with 3 factors was conducted. The five levels of each factor are involved in this design. The coded and actual levels are given in the following table.

Levels of the variables tested

Variables	Coded levels				
	-1.682	-1	0	1.0	1.682
Ammonium sulphate (X_1)	8.3	9.0	10.0	11.0	11.7
Glucose (X_2)	83.2	90.0	100.0	110.0	116.8
Nicotinic acid (X_3)	5.8	6.5	7.5	8.5	9.2

Runs in the example of CCD with 3-factors...

Factorial runs

A	-1	1	-1	1	-1	1	-1	1
B	-1	-1	1	1	-1	-1	1	1
C	-1	-1	-1	-1	1	1	1	1
Y	37.9	39.3	39.8	40.5	38.2	40.0	40.5	41.7

A	$-\alpha$	A	0	0	0	0	0
B	0	0	$-\alpha$	α	0	0	0
C	0	0	0	0	$-\alpha$	α	0
Y	39.8	41.8	38.2	42.4	39.5	39.8	41.3,41.2,41.5, 41.6,41.4,41.4

Star point runs

centre point runs

Analysis of CCD with 3-factors

```
Analysis of Variance for yield
Source           DF    Seq SS    Adj SS    Adj MS        F       P
Regression        9   31.5448   31.5448    3.5050    24.80   0.000
  Linear          3   20.7829   20.7829    6.9276    49.02   0.000
    A             1    5.2452    5.2452    5.2452    37.12   0.000
    B             1   14.6890   14.6890   14.6890   103.94   0.000
    C             1    0.8487    0.8487    0.8487     6.01   0.034
  Square          3   10.3482   10.3482    3.4494    24.41   0.000
    A*A           1    0.5734    1.3455    1.3455     9.52   0.012
    B*B           1    2.4661    3.3528    3.3528    23.73   0.001
    C*C           1    7.3087    7.3087    7.3087    51.72   0.000
  Interaction     3    0.4137    0.4137    0.1379     0.98   0.442
    A*B           1    0.2112    0.2112    0.2112     1.49   0.249
    A*C           1    0.1012    0.1013    0.1013     0.72   0.417
    B*C           1    0.1012    0.1012    0.1012     0.72   0.417
Residual Error   10    1.4132    1.4132    0.1413
  Lack-of-Fit     5    1.3132    1.3132    0.2626    13.13   0.007
  Pure Error      5    0.1000    0.1000    0.0200
Total            19   32.9580
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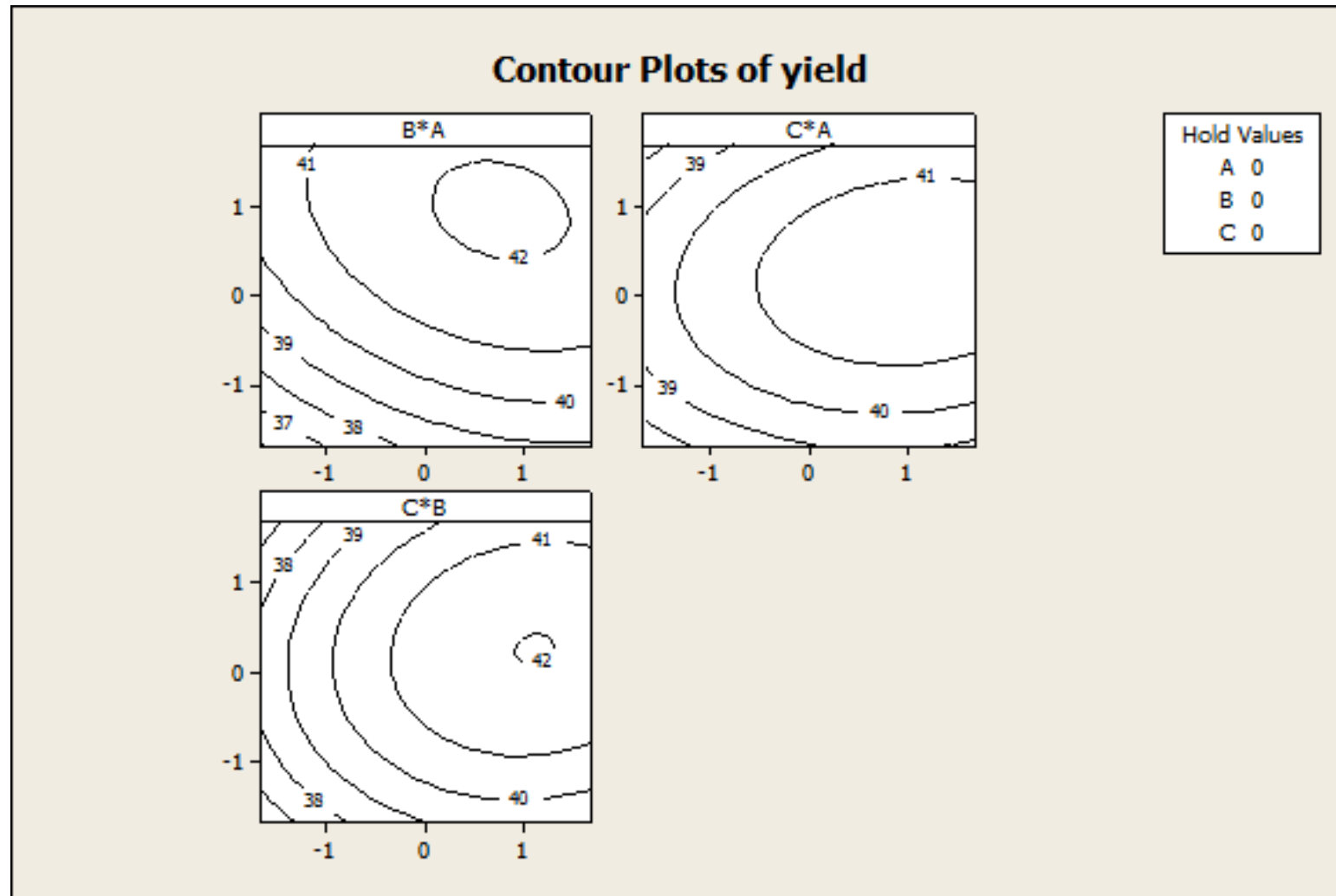
Response surface graphs for CCD with 3-factors..
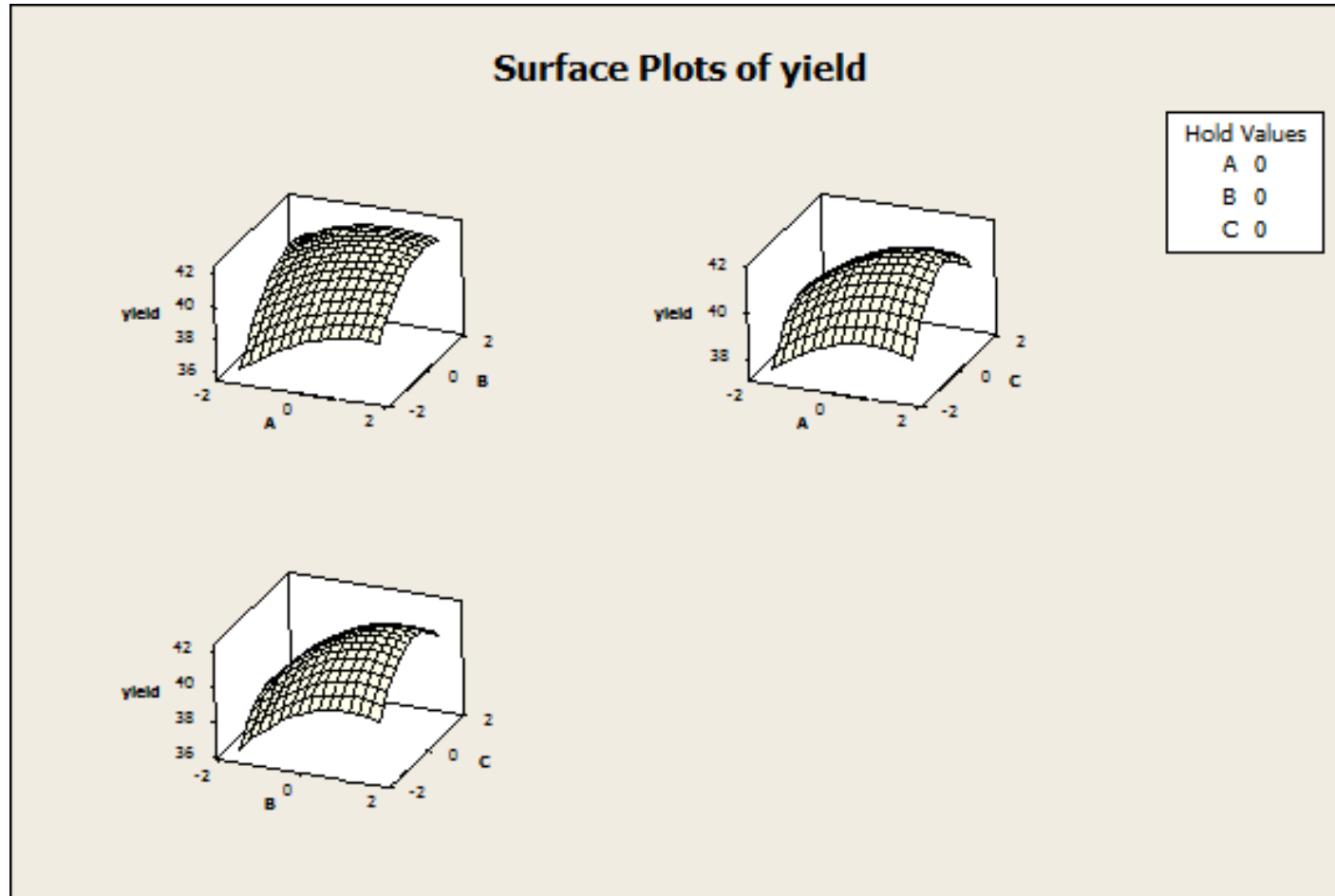
Contour plots for CCD with 3-factors..

CCD and blocking

- When the number of runs is too large to be completed under steady state conditions, you need to be concerned with the error that may be introduced into the experiment. Running an experiment in blocks allows you to separately and independently estimate the block effects (or different experimental conditions) from the factor effects. For example, blocks might be days, suppliers, batches of raw material, machine operators, or manufacturing shift.

- For a central composite design, the number of orthogonal blocks depends on the number of factors, the number of runs, and the design fraction you choose. A central composite design can always be separated into a factorial block and an axial point block. With three or more factors, the factorial block can also be divided into two or more blocks. When you are creating a design, Minitab displays the appropriate choices.

CCD and blocking

- If you add replicates to your design, you can also block on replicates. How this works depends on whether you have existing blocks in your design.

- If your design does not already include blocks, Minitab places each set of replicates in separate blocks.

- If your design already includes blocks, Minitab replicates the existing blocking scheme. The points in each existing block are replicated to form new blocks. The number of blocks in your design will equal the number of original blocks multiplied by the number of replicates. The number of runs in each block stays the same.

CCD and blocking

- If your design already includes blocks but you do not block on replicates, Minitab replicates the points within each block. The total number of runs in the each block equals the number of original runs times the number of replicates. The total number of blocks in the design stays the same.

Rotatable designs

- **Rotatability**: A design is *rotatable* if the variance of the predicted response at any point **x** depends only on the distance of **x** from the design center-point and not on the direction. A design with this property can be rotated around its center point without changing the prediction variance at **x**.

- **Note**: Rotatability is a desirable property for response surface designs (i.e. quadratic model designs).

Rotatable design

- **Rotatable Designs:** If the contours of constant standard deviation of predicted response are concentric circles then the design with this property will leave the variance of $\hat{y}$ unchanged when the design is rotated about the center (0, 0,…,0). Hence it is termed as rotatable design.

- Rotatability is an important criterion for the selection of a RSD. The aim of RSM is optimization and the location of the optimum which is unknown prior to running the experiment. Hence it is desirable to use a design that provides equal precision of estimation in all the directions.

- Any first–order orthogonal design is rotatable.

Rotatable design

- It is desired that the second-order response surface model should provide good predictions throughout the region of interest. That is the model should provide a reasonably consistent and stable variance of the predicted response at points of interest.

- The variance of the predicted response at some point $\underline{x} = (x_1. x_2, \ldots, x_k)'$ is

$$var(\hat{y}) = \sigma^2 \underline{x}'(X'X)^{-1}\underline{x}$$

- It is suggested that a second-order response surface design should be rotatable. This means that the $var(\hat{y})$ is the same at all points $\underline{x}$ that are at the same distance from the design center. That is, the variance of predicted response is constant on spheres
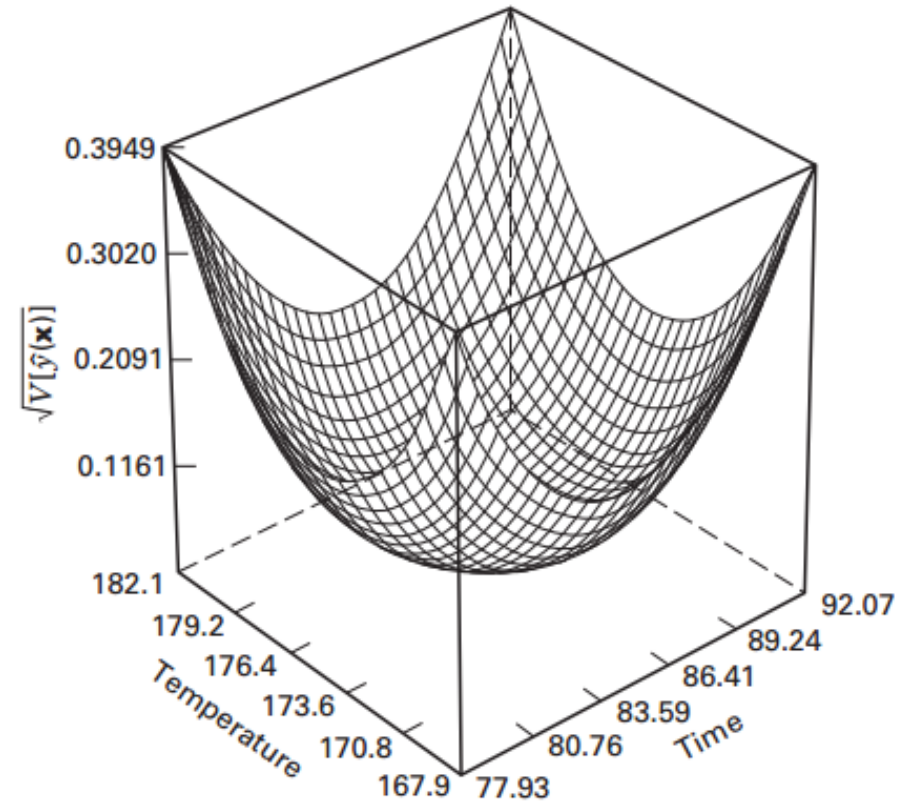
Rotatable CCD and blocking

Contours of constant standard deviation of predicted response for the rotatable CCD
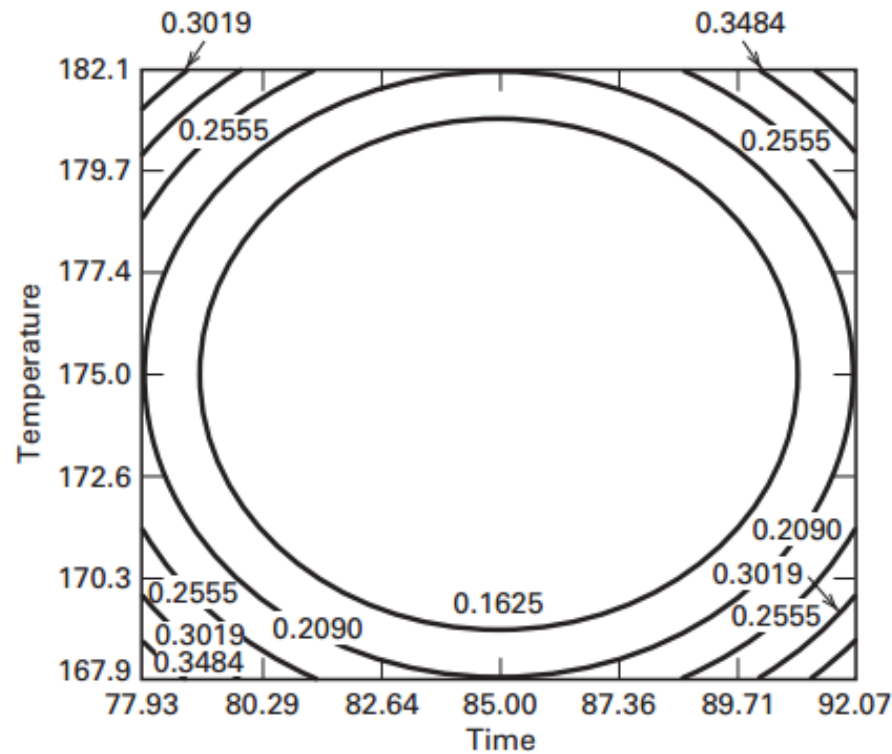
(a) Contours of $\sqrt{V[\hat{y}(\mathbf{x})]}$

(b) The response surface plot

Rotatable CCD

- A central composite design is made rotatable by the choice of . The value of α for rotatability depends on the number of points in the factorial portion of the design. The choice of α yields a rotatable central composite design for,

$$\alpha = \left[\frac{2^{k-f} n_c}{n_s}\right]^{\frac{1}{4}}$$

where f =level of fractionation of 2-level factorial design

n_c =number of replications at each corner point

n_s =number of replications at each star point

Rotatable CCD with 2-factors

- A central composite design with 2 factors is rotatable when $\alpha = \sqrt{2}$

$$\alpha = \left[\frac{2^{k-f}\,n_c}{n_s}\right]^{\frac{1}{4}}$$

$$= \left[\frac{2^{2-0}\times x}{1}\right]^{\frac{1}{4}}$$

$$= \sqrt{2}$$

- Let $n_F = 2^{k-f}$ represent number of factorial runs. Then for $f = 0, n_c = 1$ and $n_s = 1$ the condition of rotatability of CCD is $\alpha = (n_F)^{\frac{1}{4}}$.

Choice of α for Rotatable designs

Determining α for Rotatability

Number of Factors	Factorial Portion	Scaled Value for α Relative to ±1
2	2^2	$2^{2/4} = 1.414$
3	2^3	$2^{3/4} = 1.682$
4	2^4	$2^{4/4} = 2.0$
5	2^{5-1}	$2^{4/4} = 2.0$
5	2^5	$2^{5/4} = 2.378$
6	2^{6-1}	$2^{5/4} = 2.378$
6	2^6	$2^{6/4} = 2.828$

Box-Behnken designs: Designs to fit RSM

The Box-Behnken design is an independent quadratic design

- it does not contain surrounded factorial or fractional factorial design.

- In this design the treatment combinations are at the midpoints of edges of the process space and at the center.

- These designs require 3 levels of each factor.
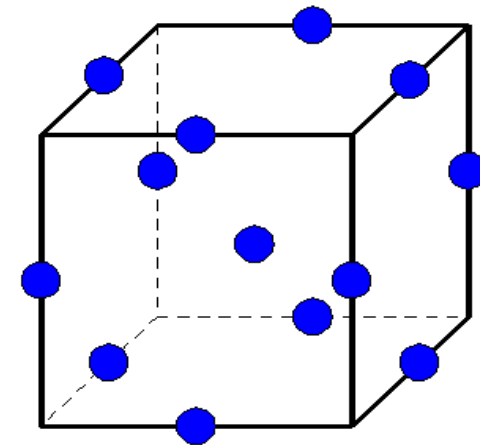
What are Box-Behnken designs?

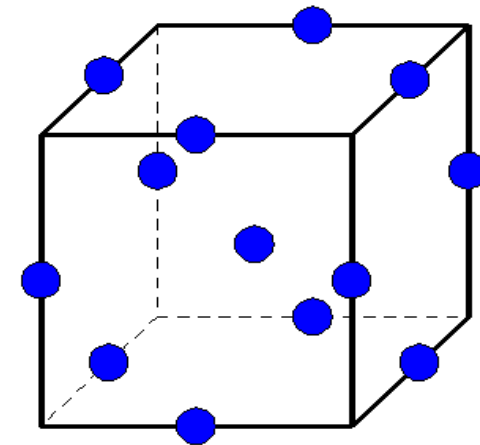The Box-Behnken design is an independent quadratic design

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- In this design the treatment combinations are at the midpoints of edges of the process space and at the center.

- These designs require 3 levels of each factor.

About Box-Behnken designs

- Box-Behnken designs are response surface designs, specially made to require only 3 levels, coded as -1, 0, and +1.

- Box-Behnken designs are available for 3 to 10 factors.

- In this design three factors can be evaluated, each at three levels.

Number of runs required by CCD and Box-Behnken Designs

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

Plackett-Burman design: Screening designs

What is a PBD?

- It is one of the screening experimental designs with many advantages.

Advantages of PBD:

- One can study N-1 factors using N runs.

- They are able to detect significant main effects using very few runs.

Key Features of Plackett-Burman designs

- These are a class of 2-level designs.

- They have $k = N - 1$ variables and N runs

- The number of runs, N, needs only be a multiple of four but not powers of 2.

  i.e. $N = 12, 20, 24, 28, 36, \ldots$

- Interactions between the factors are ignored.

- Last run uses all $-$ signs in the layout.

Layout of Plackett-Burman design

- Layout is a matrix of +1 and/or -1

- The number of columns represents # of factors

- The number of rows represents # of runs

- Columns represent Factor.

- Row represent the runs of experiment

- +1/-1 indicate the high/low level of the factors in the respective run.

- Subsequent rows to first row are circular right shift of preceding row

- Last row = all (-1)

Example of Plackett-Burman design

Run	Input Parameters (factors)							Response
	A	**B**	**C**	**D**	**E**	**F**	**G**	
1	+1	+1	+1	-1	+1	-1	-1	
2	-1	+1	+1	+1	-1	+1	-1	
3	-1	-1	+1	+1	+1	-1	+1	
4	+1	-1	-1	+1	+1	+1	-1	
5	-1	+1	-1	-1	+1	+1	+1	
6	+1	-1	+1	-1	-1	+1	+1	
7	+1	+1	-1	+1	-1	-1	+1	
8								
9								
10								
11								
12	-1	-1	-1	-1	-1	-1	-1	

Plackett-Burman designs

When to use PBD?

- If one knows based on foreknowledge that there are *no interactions*.

- If one is interested in screening important factors affecting the response among many factors.

- if one is for some reason is only interested in main effects, than Plackett-Burman designs are preferred.