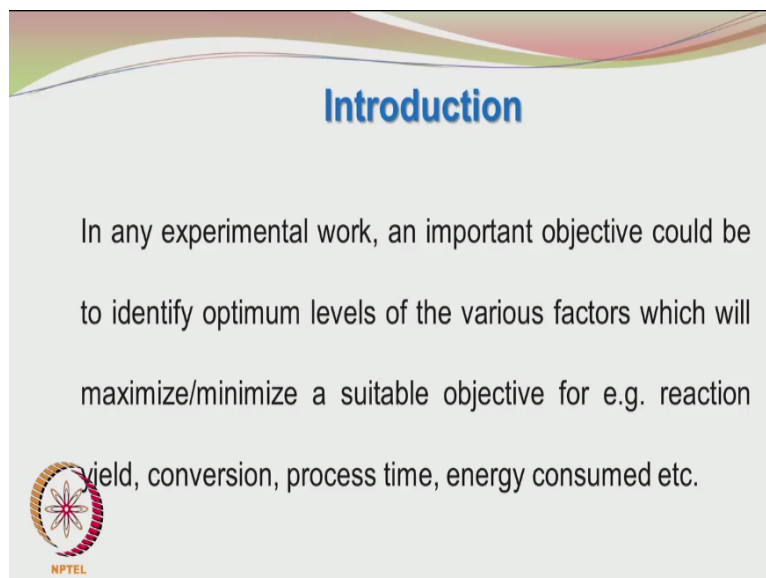


Statistics for Experimentalists
Prof. Kannan. A
Department of Chemical Engineering
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Lecture - 48
Experimental Design Strategies - C


Welcome back. Today we will be looking at new lecture on response surface methodology. Again you might have come across this term when you were reading research papers or books on statistical design of experiments. This is a very popular tool and widely used in the industry. This is simply based on the concepts we have studied until now and involves an optimization exercise.

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Introduction

In any experimental work, an important objective could be to identify optimum levels of the various factors which will maximize/minimize a suitable objective for e.g. reaction yield, conversion, process time, energy consumed etc.

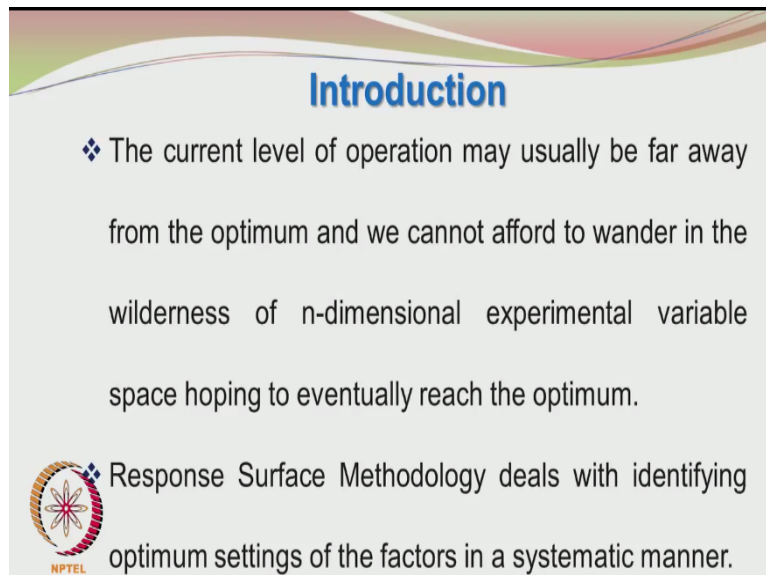
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So the purpose of any experimental work would be to identify optimum conditions for the production so that you want to either maximize the yield conversion to the decide product or minimize the power consumption or minimize the time required to complete the job. So these are all important optimization objectives and now we are adding a new dimension to our experimental design strategies.

We were earlier looking at the issues like rotatability, spherical nature of the design, the scaled prediction variance, variance of the regression coefficients, the analysis of variance, the residual sum of squares, lack-of-fit and so on. The new dimension comes in the form of identifying the direction in which we do the experiments and obtain eventually the optimum conditions.


We also have to ensure that the conditions we have reached are truly optimum. They are maximum conditions if you want to maximize our objective function or minimum conditions if you want to minimize our objective function. We also have mathematical tools available with us to indeed verify we have reached the optimum and not for example a saddle point.

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Introduction

- ❖ The current level of operation may usually be far away from the optimum and we cannot afford to wander in the wilderness of n-dimensional experimental variable space hoping to eventually reach the optimum.

 Response Surface Methodology deals with identifying optimum settings of the factors in a systematic manner.

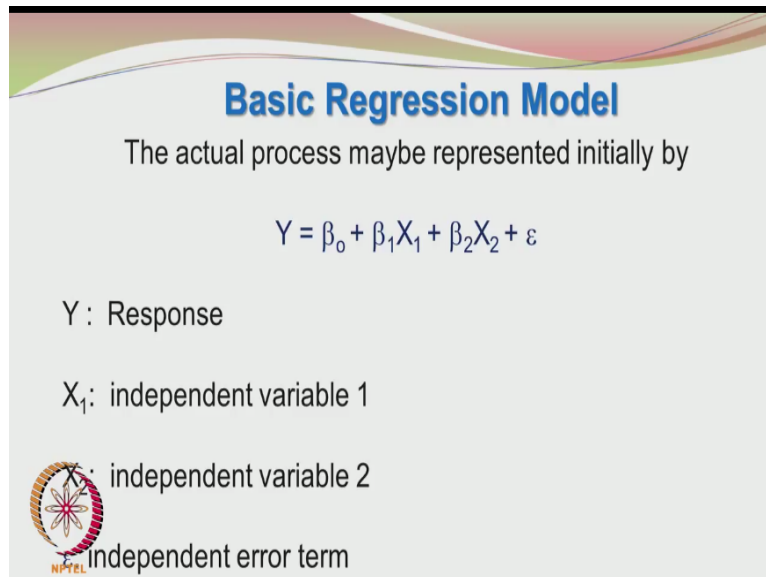
When we start doing experiments, we are really unsure where exactly the optimum conditions are. We cannot afford to wander in the wilderness of n-dimensional experimental space in search for the optimum. A logical procedure is required to find the optimum conditions. So we do some preliminary experiments to get an idea about the features of the experimental design space.

What do I mean by features of an experimental design space? We want to see in the design space of consideration whether only the main factors are contributing or there is interaction between the factors. We also want to see whether there is quadratic terms or curvature effects assuming importance even in our restricted design space. The curvature or quadratic effects manifest themselves in the form of X_1 squared and X_2 squared terms in the model equation.

So we want to first check whether these terms are important. By restricting ourselves to a narrow design space initially, we ensure that we get an idea about the features of the experiment without getting complicated by the curvature or quadratic terms. Even if interaction terms are not there, it is well and good. So the response surface methodology

deals with the identifying the optimum settings of the factors in a systematic and planned fashion.

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A presentation slide titled "Basic Regression Model" with a decorative header. The text on the slide defines the components of a regression equation. The equation $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$ is displayed. Below it, the terms are defined: Y is the Response, X1 is independent variable 1, X2 is independent variable 2 (indicated by a small 'X2' icon), and epsilon is the independent error term (indicated by a small epsilon icon). The NIPTEL logo is visible in the bottom left corner of the slide content area.

Basic Regression Model

The actual process maybe represented initially by

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$$

Y : Response

X₁: independent variable 1

X₂: independent variable 2

ε : independent error term


So let us represent the process initially only in terms of the main factors X1 and X2. We are not considering the interaction between X1 and X2 and when interactions are not considered, then even more complicated terms like X1 squared and X2 squared are not at all considered but this is a simplified model we are starting with but we have to ensure that our model is adequate or correct and the interaction terms and the quadratic terms are indeed not present.

So here Y represents the response, X1 is the independent variable 1 or the factor 1, X2 is the independent variable 2 and epsilon is the independent error term, which is assumed to be normally distributed with mean 0 and constant variance sigma squared. We do not know sigma squared.

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Basic Regression Model

After fitting the model parameters, the model is represented by $\hat{Y} = \hat{\beta}_0 + \sum_{i=1}^2 \hat{\beta}_i X_i$




So after we fit the model parameters, the model is represented by $\hat{Y} = \hat{\beta}_0 + \sum_{i=1}^2 \hat{\beta}_i X_i$. This is the prediction for any coordinate point in the experimental design space.

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The Method of Steepest Ascent (Descent)

Steepest Ascent method is a sequential process where we move in the direction of maximum increase in the response.



If minimization is required, it is called as the method of steepest descent.

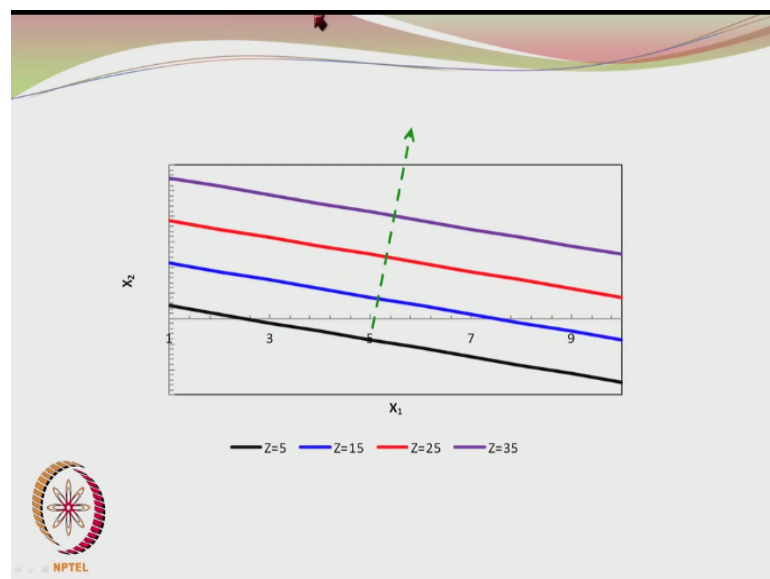
So what is meant by the method of steepest ascent? Even though we generally talk about the method of steepest ascent you may also have to look at steepest descent as well. If your objective function is to maximize or if your exercise is to maximize the objective function then you are looking for the direction of steepest ascent and if your objective function involves minimization, then you are looking for the direction of steepest descent.

So what is steepest ascent? The steepest ascent method is a sequential process where we move in the direction of maximum increase in the response and if minimization is required it

is called as the method of steepest descent. So once we are in the preliminary region, we want to move ahead then we have to move as rapidly or as quickly as possible in the direction where the response is increasing the fastest okay.

So in that way we are hopeful that we would eventually reach the optimum condition as early as possible. So how to identify the direction of steepest ascent in maximization of the objection function problems? We want to look at the direction of steepest descent in the minimization of objective function problems.

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So let us look at process involving only 2 main factors. There is no interaction between the 2 factors and you are having X_1 represented as shown here and we assume that the scale for X_2 is the same as that for X_1 and then what we do is we want to see how to progress the fastest where the response would be increasing very rapidly and you can see that these are constant response values as long as they are in the black line.

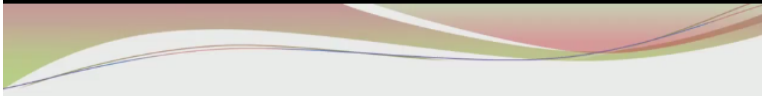
The constant value is $Z=5$, then when you go to the next line this represents locus of all points where the response value is 15, this corresponds to 25 and this corresponds to 35 and as I said earlier the scales are the same on both the axis and if you want to progress along the direction of steepest increase in the responses then we have to take a path which is perpendicular to the lines.

And since only main factors are involved, we are showing the response contours in the form of straight lines. If there were considerable interactions between the 2 parameters X_1 and X_2 ,


the lines here would have become curves. They would have been twisted because of the interaction effects, but fortunately as far as this model is concerned it is a simple one and it is an additive model where only the factors X_1 , X_2 influence the process.

Even the interaction between the 2 factors X_1 and X_2 is negligible. That is why the contours are straight lines and the direction of steepest ascent is given in terms of a line, which is perpendicular to the constant value line.

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- ❖ The direction of steepest ascent is the direction in which \hat{Y} increases most rapidly.
- ❖ It is taken as the line through the centre of the region of interest and normal to the fitted surface.




The direction of steepest ascent is the direction in which \hat{Y} increases most rapidly. It is taken as the line through the center of the region of interest and normal to the fitted surface.

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- ❖ The steps along the path are proportional to the regression coefficients $|\hat{\beta}_i|$.
- ❖ Experiments are conducted along the path of steepest ascent until no further increase in response is obtained.

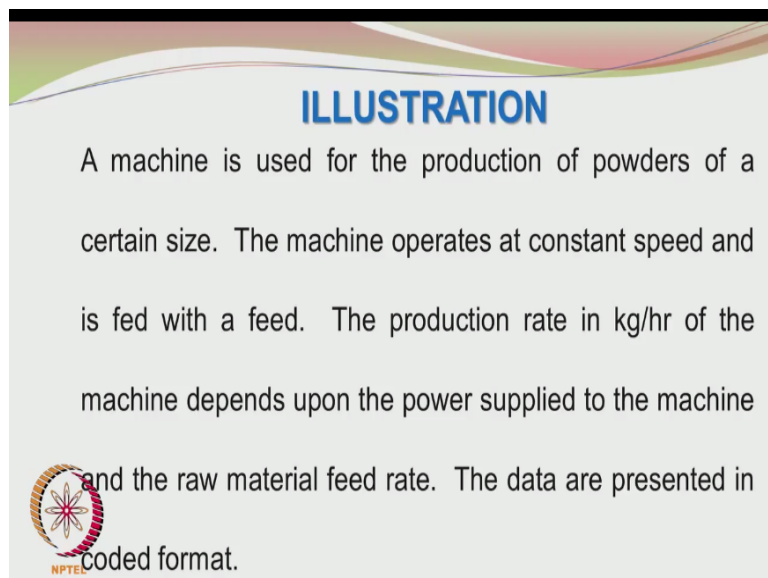


The steps along the path are proportional to the regression coefficients, modulus of β_i . So how do we take the steps along the path of the steepest ascent? Please note that the steps along the path are proportional to the regression coefficients. So we cannot assume equal importance to both the axis. For example, if you are having 2 factors, we are looking at a 2-dimensional space.

And we cannot say that if I move one step in the X_1 direction, I will also move 1 step in the X_2 direction because each factor may not be contributing equally to the process response and hence it is clear that the direction of the steepest ascent would depend upon the relative importance of the two factors and the steps would be determined accordingly. So how long do we conduct the experiments along the direction of steepest ascent?

Please note that we are conducting experiments along the direction of steepest ascent and we are not predicting the responses. So we conduct the experiments as long as the response values are increasing and a point may be reached where the values may begin to drop. So we have reached the conditions where the maximum responses obtained. Then we have to pause here a bit and then reevaluate our experimental design strategy.

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ILLUSTRATION

A machine is used for the production of powders of a certain size. The machine operates at constant speed and is fed with a feed. The production rate in kg/hr of the machine depends upon the power supplied to the machine and the raw material feed rate. The data are presented in coded format.

So let us do this understanding of response surface methodology through an illustration. The problem statement goes like this. Machine is used for production of powders of a certain size and the machine operates at constant speed and is fed with the material. It may be a rock or whatever. The production rate in kilograms per hour of the machine depends upon the power

supply to the machine and the raw material feed rate. The data are presented in the coded format.

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ILLUSTRATION

- ❖ To obtain an idea about experimental error, the experiments have been repeated at the geometric center of the design.
- ❖ The additional role of center points will be explained shortly.

So to obtain an idea about the experimental error, the experiments have been repeated at the geometric center of the design and the additional role of center points will be explained shortly.

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Experimental Data in Coded Format

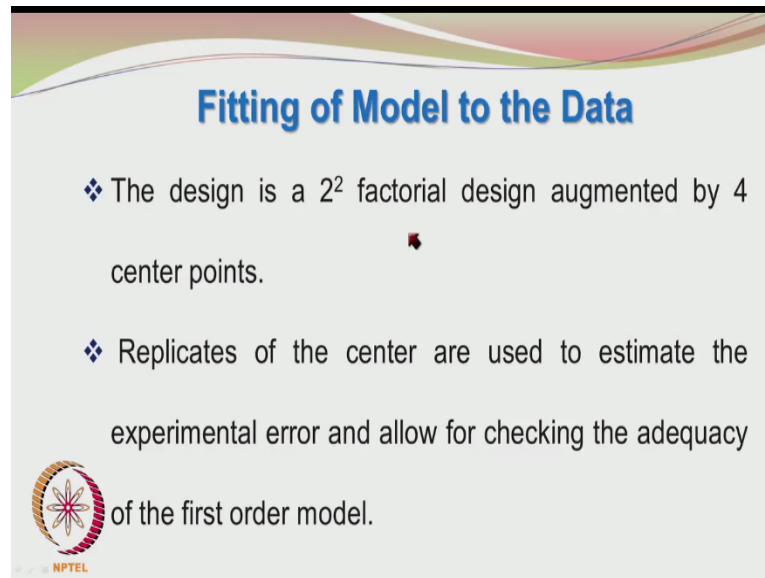
X_1	X_2	Y (kg/h)
1	1	90
1	-1	60
-1	1	66
-1	-1	36
0	0	68
0	0	65
0	0	61
0	0	62

Variance of the center points (68, 65, 61, 62) = 10 a measure of error variance $\hat{\sigma}^2$

So we have the experimental data in coded format. They are given here X_1 , X_2 and Y kg/hour and X_1 and X_2 are not having any units because they are coded variables and they are representing a 2^2 design as shown here 1 1 1 -1 -1 1 -1 -1 settings and the responses are given here and you also have the center points. Repeats are carried out at the center points.


And these are the responses obtained from the 4 repeats. So we calculate the variance of the data obtained at the center points. So we essentially find the variance of 68, 65, 61 and 62 which comes out to be a whole number 10 and this is a measure of the error variance and it is denoted by σ^2 or estimated error variance σ^2 . So this is the estimation of the pure error only due to random factors.

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Fitting of Model to the Data

- ❖ The design is a 2^2 factorial design augmented by 4 center points.
- ❖ Replicates of the center are used to estimate the experimental error and allow for checking the adequacy of the first order model.

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Now the conventional 2 power 2 factorial design is enhanced or augmented by 4 center points and the replicates of the center are used to estimate the experimental error and allow for checking for the adequacy of the first order model. It tells us whether our first order model we have proposed is sufficient or we need to consider the effects of curvature by the addition of the quadratic terms $\beta_{11} X_1^2$ or $\beta_{22} X_2^2$ and $\beta_{12} X_1 X_2$.

This represents the contributions from the quadratic effects. So let us see how to use the center runs to detect whether quadratic effects are significant or not.

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Fitting of Model to the Data

- ❖ Also the design is centered around the current operating conditions of the process.
- ❖ A first order model may be fitted to these data. The fitted model is given as follows



So before we do that let us fit the design based on the available data points.

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Fitting of Model to the Data

$$\hat{Y} = \hat{\beta}_0 + \sum_{i=1}^2 \hat{\beta}_i X_i$$

This first order model assumes that the variables X_1 and X_2 have only an additive effect on the response.



So the first order model which we get is of the form $\hat{Y} = \hat{\beta}_0 + \sum_{i=1}^2 \hat{\beta}_i X_i$. This first order model assumes that the variables X_1 and X_2 have only an additive effect on the response.

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Adequacy of the First Order Model

The 2^2 design with **center points** enables the investigator to

- a. Obtain an estimate of the error
- b. Check for interaction terms in the model (i.e. cross product terms).



So the first order model has center points, it can estimate the pure error, the first order model involving 4 factorial points will not only enable you to find the main effects but also to find the interaction because we are having 4 independent settings for a 2^2 design, we can find the intercept β_0 , then we can find the contribution from factor 1 or the importance of contribution from factor 1 which is β_1 .

And the importance of contribution from factor 2 is given from the β_2 coefficient. So that makes it 3, we have 4 independent settings and so the remaining independent setting may be also used up in the calculation of the interaction term β_{12} that means we are using 4 independent settings to find 4 parameters. We cannot estimate anymore parameters from a 2^2 design.

So even this limited design with center points has enabled us to find a model with main factors and the interaction between the 2 main factors and also it has given us a good idea about the experimental error.

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Adequacy of the First Order Model

The 2^2 design with center points enables the investigator to

C. Check for quadratic effects (curvature).

The replicates at the center points may be used to



estimate the experimental error.

Further the center points are invaluable in telling us whether quadratic effects are important or not. It cannot tell you exactly what those quadratic contributions are. It will only tell whether you need to consider the quadratic terms or you may at present omit the quadratic terms.

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Estimation of Error

The error variance may be estimated using the repeat points made at the center. The usual variance formula may be used here i.e. sum of squares of deviations from the mean divided by $n-1$ where n is the number of



observations

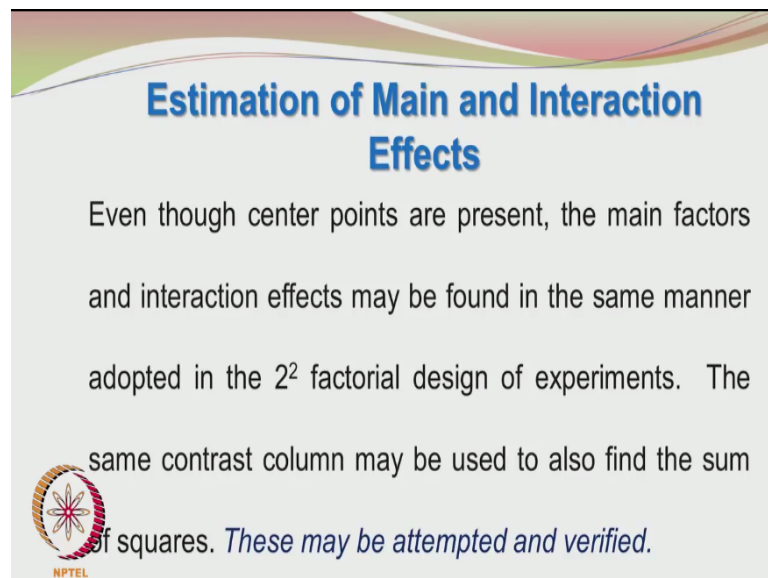
$$\hat{\sigma}^2 = \frac{68^2 + 65^2 + 61^2 + 62^2 - \frac{256^2}{4}}{3} = 10$$

So first let us look at the estimation of error before we go into the testing for the significance of the quadratic terms. Let us do the simple things first which would be the estimation of the experimental error. That is a very straightforward task. We had to just find the variance of the 4 center points. There are different ways of doing it. $\sum (X_i - \bar{X})^2 / (n-1)$ or you may also do $(\sum X_i^2 - (\sum X_i)^2 / n) / (n-1)$.

Well you have come across these kinds of calculations in the previous lectures. Let us take the shortcut formula here. So $\sigma^2 = 68^2 + 65^2 + 61^2 + 62^2$. What are these points? These are nothing but the values obtained at the center. They are the repeat points at the center and 256 would be sum of all these 4 observations. 68 the 65 is 133, 194, 194+62 is 256 so that is what you have here.


And 4 would be the total number of repeats which is 1, 2, 3, 4 and then this 3 represents the degrees of freedom for the 4 data points since we are already calculating the mean from the 4 data points, we lose a degree of freedom there and we have only 3 as the degrees of freedom and we get σ^2 as 10.

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Estimation of Main and Interaction Effects

Even though center points are present, the main factors and interaction effects may be found in the same manner adopted in the 2^2 factorial design of experiments. The same contrast column may be used to also find the sum of squares. *These may be attempted and verified.*

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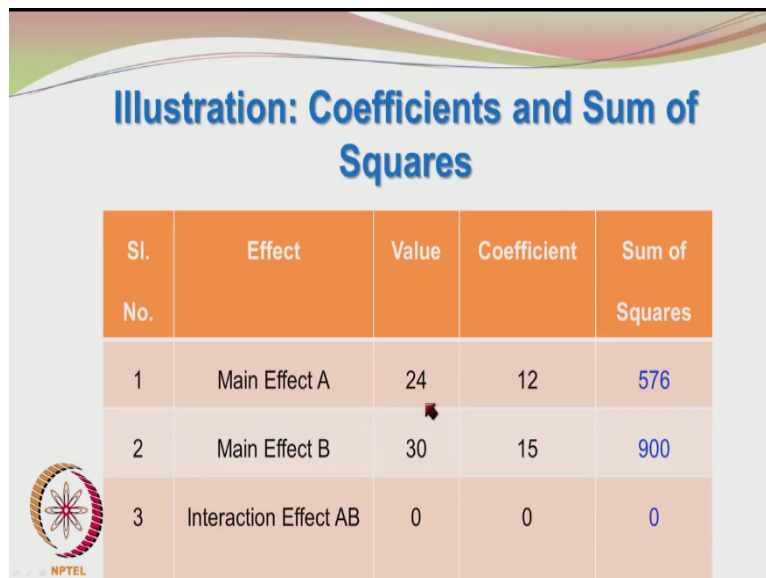
And how do you find the main and interaction effects? To do it in a very economical manner and universal manner, I would suggest you to adopt the regression approach. You have the X matrix and you have the Y vector of responses or the experimental values obtained and you simply use the regression approach to identify the model parameters.

Let us very straightforward and if you have software like MATLAB or Scilab or any software which can do these kind of matrix manipulations routinely then the coefficients may be identified very quickly but from a learning point of view even for this design with the center points, we can identify the main effects and the interaction effects using the factorial design approach.

We use the table of contrast and from that we may identify different effects. We know that once the effects are identified, the coefficients are estimated by dividing the effects/2 because the effects represent the change from going from -1 coded value to +1 coded value a jump of 2 units but our regression equation involves the response when there is a change in 1 unit of a particular factor.

So the effects are divided by 2 to get the coefficients either you use the regression approach or you may use the factorial approach to estimate the parameters. So if you want you can do these calculations since it is only a 2 power 2 design you may do these very easily and you may verify whether the results you obtain are matching with the results which are going to be present.

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The slide features a table titled "Illustration: Coefficients and Sum of Squares" with a decorative header. The table has five columns: "Sl. No.", "Effect", "Value", "Coefficient", and "Sum of Squares". It contains three rows of data. The NPTEL logo is located in the bottom left corner of the slide.


Sl. No.	Effect	Value	Coefficient	Sum of Squares
1	Main Effect A	24	12	576
2	Main Effect B	30	15	900
3	Interaction Effect AB	0	0	0

So when you look the values the main effect is having a value of 24, the main effect B is having a value of 30 and the interaction is having a value of 0 and the coefficient for the different effects or different factors rather are 12, 15 and 0 and the sum of squares again may be easily calculated from the contrast and they turn out to be 576 for A and 900 for B and for AB it is 0.

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ANOVA TABLE

Source of Variation	Sum of Squares	Degrees of Freedom	Mean Squares	F _o	P
A	576	1	576	57.6	0.005
B	900	1	900	90.0	0.002
A*B	0	1	0	-	1
Error	30	3	10		
Total		6			



$$f_{\text{critical}} = f_{0.05, 1, 3} = 10.13$$

We can now construct the ANOVA table and we have the degrees of freedom listed out here. Since we are having 4 repeats, we are having 3 degrees of freedom for the repeats and we found mean square error or the variance as 10 and we also have the mean squares for factors A, B and AB and so you have F_o value as 576/10, for AB it is actually 0. So the probability P value comes out to be 1 for AB.

And so that tells us you can comprehensively reject the coefficient associated with the interaction between A and B but you can see that both effects A and B are highly significant because their P values are very small. The critical f value is given by f 0.05, 1, 3 and that turns out to be 10.13 and since these actual F values are much, much higher than the critical f value, they lie in the rejection region.

And hence you may reject the null hypothesis, which states that the coefficient corresponding to factor A and the coefficient corresponding to factor B are both 0. So we reject the null hypothesis and say that both the factors are significant. Only the insignificant factor is the interaction between the 2 factors A and B.

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Is Interaction Term Necessary?

From ANOVA test (F and associated p value applicable on the interaction term) and even from visual inspection, it may be shown that the interaction term is currently unnecessary.

If an interaction term were to be added then we will have an



additional coefficient $\hat{\beta}_{12}$.

$$\hat{Y} = \hat{\beta}_0 + \sum_{i=1}^2 \hat{\beta}_i X_i + \hat{\beta}_{12} X_1 X_2$$

So from the analysis of variance test from there we get the F and associated p values and perhaps even from visual inspection, which is usually not trustworthy it can be shown that the interaction term is currently unnecessary. If an interaction term were to be added, then we would have had an additional coefficient beta hat 12 and that would have been present here but as far as this model goes we can neglect the beta hat 12 because the interaction effect is not significant.

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Preliminary Model

The fitted model with the interaction term from the usual factorial design analysis in the coded format is

$$\hat{Y} = 63 + 12X_1 + 15X_2$$



So finally we have the fitted model as $\hat{Y}=63+12X_1+15X_2$ and we considered the coefficients are given here. So in the preliminary model in the preliminary designed experiment, we have the model given as shown here.

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Check for Linear Model Sufficiency by Estimating Quadratic Effects

We take the average of the 4 corner points of the factorial design \bar{y}_F and compare it with the average of the center point values \bar{y}_C .



Now let us move on to the checks that are in place for the sufficiency of the linear model. We said that the quadratic effects may be actually important even in this preliminary design space and should we add $\beta_{11} X_1^2$ and $\beta_{22} X_2^2$ or we can get away without adding those model terms that is what we have to check next. So what we do here is quite simple.

We take the average of the 4 corner points of the factorial design \bar{y}_F and compare it with the average of the center point values \bar{y}_C . So if you go back to the table as shown here, so these are all the factorial points and these are the responses at the factorial points and these are all the center points and these are the values at the center points. So if you want to take the average \bar{y}_F it would mean the average of the factorial points.

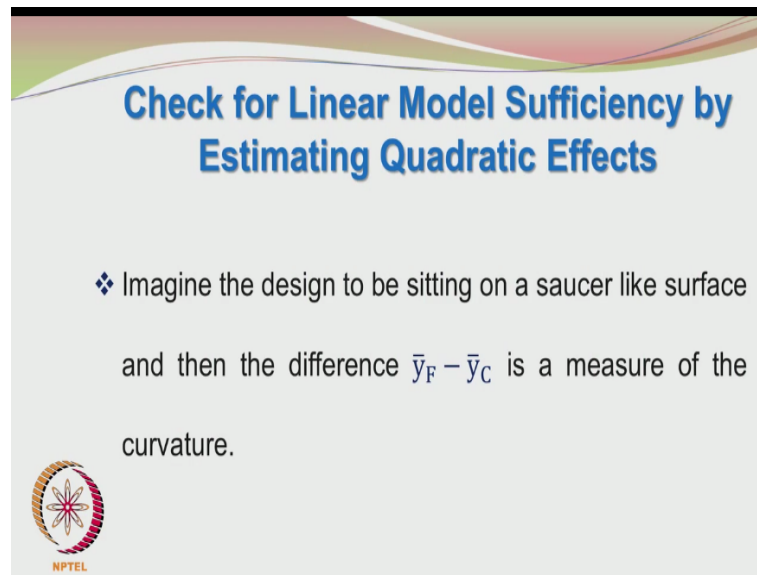
And that would be $152 + 16 + 216 + 36$ is 252 so $252/4$ is 63 and this we saw has 133 194 256 $256/4$ is 64 so the average of the factorial points is 63 and the average of the center points is 64. So the difference between the two is very small. So we can imagine that \bar{y}_F the average of the factorial points is located close to \bar{y}_C which is the average of the center points.

If you are going to have the second order effects of the quadratic effects important, then what would have happened is the center points would have been located very far off from the factorial points. Then, the average of the factorial points would have been quite different from the average of the center points. So if the average is between the center and factorial

points are pretty much the same, then we can understand intuitively that the center points are located very close to the plane containing the factorial points.


In other words, if you look at the model surface you do not see any strong peaks and valleys okay.

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Check for Linear Model Sufficiency by Estimating Quadratic Effects

- ❖ Imagine the design to be sitting on a saucer like surface and then the difference $\bar{y}_F - \bar{y}_C$ is a measure of the curvature.

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So we were looking at the importance of the curvature terms. If you have strong curvature in your design space then the response surface would be characterized by peaks and valleys, which would mean that if you are taking a plane of 4 points, there may be a region in the center which is considerably at elevation with respect to the plane formed by the 4 points. That shows that there is a strong curvature and peak in this experimental design space.

So we are having a center and then we have 4 factorial points. If the center point response is considerably different from the corner point responses, then we may suspect the presence of peak or curvature in the design space between the factorial points and the center points. On the other hand, if the center point values are comparable and very close to the 4 factorial points average, then we may think that they are very close.

And we do not have any strong peak in the design space we have considered. So with this intuitive understanding we can carry out certain tests. So the first step is to find the difference between \bar{Y}_F and \bar{Y}_C .

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Check for Linear Model Sufficiency by Estimating Quadratic Effects

❖ This comparison helps us to verify whether the response values are close to each other so that they may be thought to lie on the same response plane.



❖ If they are sufficiently different then it is concluded that the quadratic effects may become important.

So if the difference between \bar{Y}_F and \bar{Y}_C is considerable then we can conclude that curvature effects may be important.

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Check for Linear Model Sufficiency by Estimating Quadratic Effects

A quantitative test is recommended as shown below.

The proposed quadratic model is

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \hat{\beta}_{12} X_1 X_2 + \hat{\beta}_{11} X_1^2 + \hat{\beta}_{22} X_2^2$$



What is that quadratic effect of the second order effects? If they are significant then the model should have in addition to the regular intercept, main factors, and then binary interaction. It should also have $\hat{\beta}_{11}$ and $\hat{\beta}_{22}$.

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Check for Linear Model Sufficiency by Estimating Quadratic Effects

\bar{Y}_C = average of center points

\bar{Y}_F = average of corner points

Find $\bar{Y}_C - \bar{Y}_F = \hat{\beta}_{11} + \hat{\beta}_{22}$



So what we are doing here is checking for the linear model sufficiency by estimating the quadratic effects.

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Check for Linear Model Sufficiency by Estimating Quadratic Effects

A quantitative test is recommended as shown below.

The proposed quadratic model is

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \hat{\beta}_{12} X_1 X_2 + \hat{\beta}_{11} X_1^2 + \hat{\beta}_{22} X_2^2$$



The quadratic effects are characterized by beta hat 11 and beta hat 22 with the current experimental design involving 4 factorial points and 4 center points. We are unable to estimate beta hat 11 and beta hat 22 for the simple reason that we do not have sufficient degrees of freedom. So we are not in a position to estimate them explicitly but we may have an idea of the importance of beta hat 11+beta hat 22.

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Check for Linear Model Sufficiency by Estimating Quadratic Effects

\bar{Y}_C = average of center points

\bar{Y}_F = average of corner points

Find $\bar{Y}_C - \bar{Y}_F = \hat{\beta}_{11} + \hat{\beta}_{22}$



And that is given by the estimator $\bar{Y}_C - \bar{Y}_F$. $\bar{Y}_C - \bar{Y}_F$ is acting as an estimator for $\beta_{11} + \beta_{22}$. So we can call $\bar{Y}_C - \bar{Y}_F$ as $\hat{\beta}_{11} + \hat{\beta}_{22}$.

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Check for Linear Model Sufficiency by Estimating Quadratic Effects

This difference in the means is an estimate of the second order term coefficients viz. β_{11} and β_{22} and has to be quantitatively checked



$$\bar{Y}_C - \bar{Y}_F = \hat{\beta}_{11} + \hat{\beta}_{22} = 64 - 63 = 1.0$$

And so the difference between $\bar{Y}_C - \bar{Y}_F$ we saw from our calculations that it is 64-63 and that is equal to 1. So an estimate of $\beta_{11} + \beta_{22}$ has been obtained from $\bar{Y}_C - \bar{Y}_F$ and that turns out to be 1.

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Hypothesis Testing on the Quadratic Effects

$$H_0: \beta_{11} + \beta_{22} = 0$$

$$H_1: \beta_{11} + \beta_{22} \neq 0$$



So the null hypothesis which involves the actual parameters and not the estimated ones please note that. H_0 is given by $\beta_{11} + \beta_{22} = 0$ and H_1 is given by $\beta_{11} + \beta_{22} \neq 0$.

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Hypothesis Testing on the Quadratic Effects

Note that population parameter and not estimators are used in the hypothesis statements. Also note that

$$\bar{Y}_C - \bar{Y}_F = \hat{\beta}_{11} + \hat{\beta}_{22}$$



So we are using the actual population parameters in our hypothesis statements and again to repeat $\bar{Y}_C - \bar{Y}_F$ is used as an estimator for the coefficients $\beta_{11} + \beta_{22}$.

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Hypothesis Testing on the Quadratic Effects

Based on previous exposure to hypothesis testing of means we are now able to conduct a t-test as follows



$$t_0 = \frac{(\bar{y}_F - \bar{y}_C) - (0)}{\text{Var}(\bar{y}_F - \bar{y}_C)}$$

So we can do a t-test which is based upon the estimator $\bar{y}_F - \bar{y}_C$ - the null hypothesis statement which says that $\beta_1 + \beta_2 = 0$ that is why we put 0 here and then we have the variance of $\bar{y}_F - \bar{y}_C$.

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Hypothesis Testing on the Quadratic Effects

$$t_0 = \frac{(\bar{y}_F - \bar{y}_C) - (0)}{\sigma \sqrt{\left(\frac{1}{n_F} + \frac{1}{n_C}\right)}}$$

Converting this into a F-statistic by taking the square of



t_0 we get

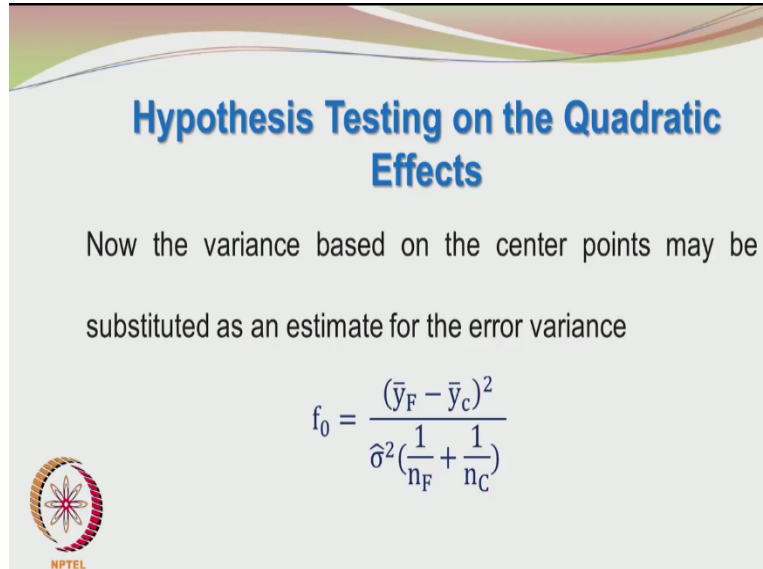
$$f_0 = t_0^2 = \frac{(\bar{y}_F - \bar{y}_C)^2}{\sigma^2 \left(\frac{1}{n_F} + \frac{1}{n_C}\right)}$$

And this may be written as $\bar{y}_F - \bar{y}_C$ whole thing divided by $\sigma \cdot \sqrt{1/n_F + 1/n_C}$ where n is the number of factorial points and n_C is the number of center points and we can convert this t-test into an F test or convert the t statistic into an F statistic by squaring this term and we get $f_0 = t_0^2$ squares which is $(\bar{y}_F - \bar{y}_C)^2 / (\sigma^2 \cdot (1/n_F + 1/n_C))$.

So whatever we have studied in the first phase of this course, hypothesis testing and important probability distributions we are making use now and we do not know sigma

squared but we have an easy solution for that. We have repeats at the center and we can use the mean square error as a surrogate value for sigma squared and we call that as a sigma hat squared.


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Hypothesis Testing on the Quadratic Effects

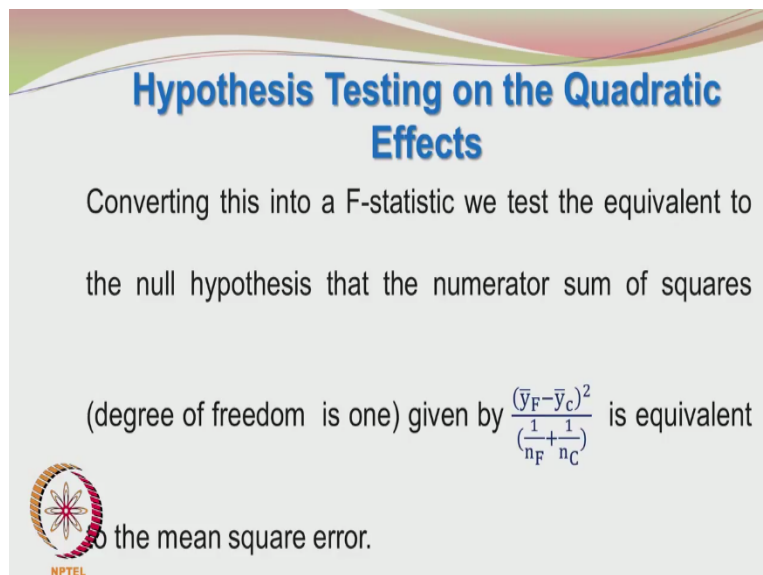
Now the variance based on the center points may be substituted as an estimate for the error variance

$$f_0 = \frac{(\bar{y}_F - \bar{y}_C)^2}{\hat{\sigma}^2 \left(\frac{1}{n_F} + \frac{1}{n_C} \right)}$$

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So now the variance is based on center points and it may be substituted as an estimate for the error variance and so you have $f_0 = \frac{(\bar{y}_F - \bar{y}_C)^2}{\hat{\sigma}^2 \left(\frac{1}{n_F} + \frac{1}{n_C} \right)}$

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Hypothesis Testing on the Quadratic Effects

Converting this into a F-statistic we test the equivalent to the null hypothesis that the numerator sum of squares (degree of freedom is one) given by $\frac{(\bar{y}_F - \bar{y}_C)^2}{\left(\frac{1}{n_F} + \frac{1}{n_C} \right)}$ is equivalent to the mean square error.

 NPTEL

So converting this into an F statistic, we test the equivalent to the null hypothesis that the numerator sum of squares, degrees of freedom is 1 given by $\frac{(\bar{y}_F - \bar{y}_C)^2}{\left(\frac{1}{n_F} + \frac{1}{n_C} \right)}$ is equivalent to the mean square error.

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Hypothesis Testing on the Quadratic Effects

The F-statistic is tested with 1 and n_c-1 numerator and denominator degrees of freedom respectively.



So this F-statistic is tested with 1 and n_c-1 numerator and denominator, degrees of freedom respectively.

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Hypothesis Testing on the Quadratic Effects

$$SS_{\text{pure Quadratic}} = \frac{n_F n_C (\bar{Y}_F - \bar{Y}_C)^2}{(n_F + n_C)}$$

$$= \frac{4 \times 4 \times (1)^2}{(4 + 4)} = 2$$

$$F = \frac{SS_{\text{pure Quadratic}}}{\hat{\sigma}^2} = \frac{2}{10} = 0.2$$



So how do you calculate the sum of squares of the pure quadratic? So when you simplify this particular expression which is given here, we get $n_F \cdot n_C \cdot \bar{Y}_F - \bar{Y}_C$ whole squared / $n_F + n_C$ which is number of factorial points 2^2 which is 4, number of center points 4 and $\bar{Y}_F - \bar{Y}_C$ whole squared is 1 squared / 4 + 4 which is 8 that turns out to be 2.

So when you divide sum of squares of the pure quadratic by sigma hat squared, we get 2/10 which is equal to 0.2 so the F value is 0.2.

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Hypothesis Testing on the Quadratic Effects

This f-ratio is small ($P=0.685$) and hence pure quadratic effects may be neglected. Hence, both the main effects are significant while the interaction and pure curvature are



And this F value is associated with the P value of 0.685, which is very high and tells that the curvature terms is insignificant because the P value is much higher than 0.05 so both the main effects are significant while the interaction and the pure curvature effects are not significant.

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Direction of Steepest Ascent

$$\hat{Y} = 63 + 12X_1 + 15X_2$$

$$X_2 = -4.2 - 0.8X_1 + 0.06667\hat{Y}$$



So we can say that the model may be well represented by $\hat{Y} = 63 + 12X_1 + 15X_2$. In order to find the direction of steepest ascent what we do is we convert this into X_2 versus X_1 form. When we do that we can show very easily that $15X_2$ is $\hat{Y} - 12X_1 - 63$ so $X_2 = (\hat{Y} - 12X_1 - 63)/15$ which is $-4.2 - 0.8X_1 + 0.06667\hat{Y}$.

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Direction of Steepest Ascent

The contour lines are drawn for constant \hat{Y} and the search direction is normal to the straight line defined by the above expression.



So what we have to do is use this equation to find the path of steepest ascent. So what we do here is we draw contour lines for constant \hat{Y} using this equation. We fix \hat{Y} at a certain value and then draw this line then we fix \hat{Y} at another value and draw another line. This way we can generate sufficient number of contour lines in the experimental design space of interest.

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Direction of Steepest Ascent

The slope (m_1) of this equation is -0.8. Since the slope of the line normal to this line (m_2) is defined according to $m_1 m_2 = -1$ we get

$$m_2 = -1/(-0.8) = 1.25$$

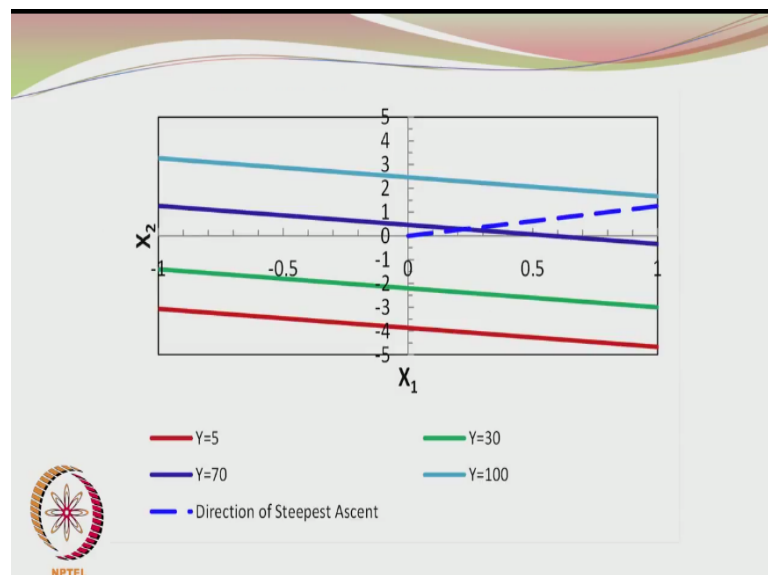


And what is the slope m_1 of this equation? The slope is given by -0.8 because we are plotting X_2 versus X_1 where Y is a parameter and it is kept at different, different values. So the main important defining relationship is between X_2 and X_1 and if I take the slope of this particular equation dX_2/dX_1 would be -0.8.

And that is the slope and if you want to find the direction normal to this slope, then we have to find a slope which is bearing a relation $m_1 m_2 = -1$, m_1 is the slope of the original line, m_2 is the slope of the new line in the direction of steepest ascent. To get the slope of the line in the direction of steepest ascent, we have to find m_2 and the relation is $m_1 m_2 = -1$. Since m_1 is known we can easily find out m_2 .

So the slope m_1 of this equation which was given before that is $\hat{Y} = 63 + 12X_1 + 15X_2$ or X_2 is $-4.2 - 0.8X_1 + 0.06667$. So the slope initially is -0.8 and we have to find m_2 the slope of the line of steepest ascent such that the relation $m_1 m_2 = -1$ is satisfied. This equation comes in the normal calculations. So here we get $m_2 = -1/-0.8$ which is 1.25 .

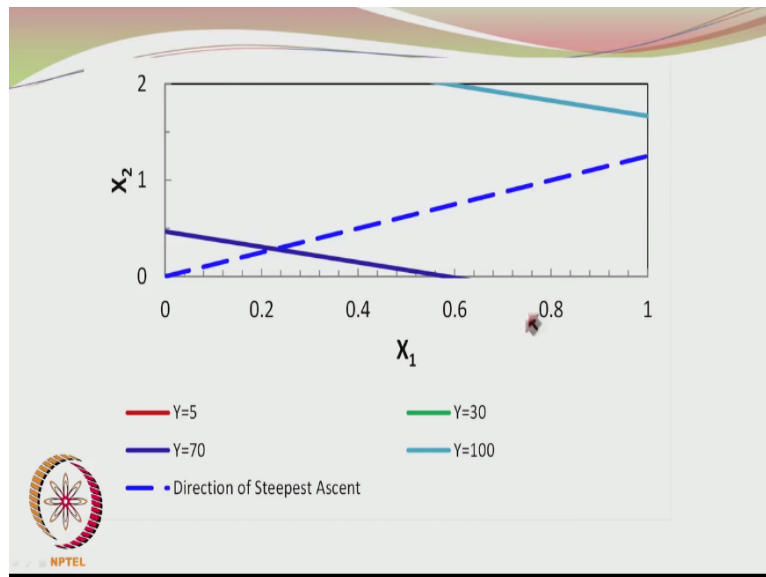
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So here we are sketching the responses, we are fixing different responses for Y , Y is 5, Y is 30, Y is 70 and Y is 100. So these are different responses and you can see that for each of this response Y , there is a line so for $Y=5$ we have this line, for $Y=30$ we have this line, for $Y=70$ we have this line and $Y=100$ we have this line and all of these lines have a slope of -0.8 . In order to identify the direction of steepest ascent, we have to find a line with slope of 1.25 .

And the line is represented here. Since the scales are not the same in both X and Y axis, you can see that this line is not exactly perpendicular to the lines but it is slightly at an angle but it still represents the direction of steepest ascent because it is drawn with the slope of $m_2 = 1.25$ right.

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So this is a close-up view of the same figure which is showed previously and it can be seen that this is the path taken in the direction of steepest ascent and the slope of this particular line is 1.25. I am drawing this line starting from the center of the design, which is the origin and so you can see that for every one step along the X_1 direction I am taking a step of 1.25 along the X_2 direction.

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Direction of Steepest Ascent

It is important to remember that the values are in coded format.

This means that for an unit step of 1 unit along X_1 direction we have to take a step of 1.25 units along X_2 direction.



Now I have the direction of steepest ascent and please remember that the values are on the coded format. So persisting in the same coded format if I take a step of 1 unit along the X_1 direction, I take a step of 1.25 units along the X_2 direction, not the Y direction, Y is the response. If I take a step of 1 unit along the X_1 direction, I take a step of 1.25 units along the X_2 direction.

Please note that the step size in each of the two directions need not be the same because the regression coefficients are different. There is a different weightage given factor 1 and different weightage given for factor 2 and hence the direction of steepest ascent also has to respect these different weightages and when you are doing experiments in real life, please keep a track on your actual experimental value corresponding to the coded variables okay.

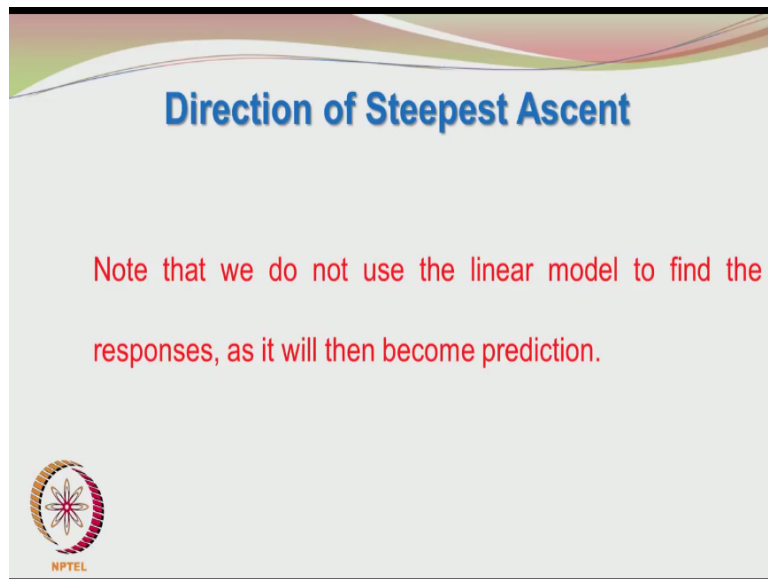
Sometimes when you are going along the direction of steepest ascent, you are going 1, 1.25 and 2, 2.5 and so on the response may be increasing all the time but you may not be able to go beyond a certain point for the simple reason because the pump would have saturated or the flow rate would have hit its maximum upper bound. So you have to stop at that particular point.

So in some cases you cannot do experiments indefinitely until you get to the true optimum because you may hit a bound crossed by the boundaries of your experimental design. You may not be able to cross the boundary for various practical reasons. So what I am trying to say here is when you are going along a particular direction in the coded format keep also a track on the actual values.

We know that the coded format is done in order to put the factors independent of units and assign them equal importance. Now once you have a coded value, you should also have the uncoded value. In one of my earlier lectures, I have given you the formula for converting coded values into uncoded values and vice versa.

Please refer to that. So when you are going along this direction of steepest ascent, please make sure that you are not hitting a bound created by the constraints of your experimental program.

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Alright and another important thing is in the direction of steepest ascent you are doing the experiments, you are not using the prediction model which you had developed earlier. The prediction model was carried out over a narrow design space and you ensured that there is no curvature effects present in that narrow design space and then it also help you to identify the path of the steepest ascent.

So from that preliminary region, you are going along the path of steepest ascent and that is helping you to proceed as quickly as possible but once you have crossed that -1 $+1$ boundary corresponding to that narrow design space, you should stop using the model prediction. You should actually perform experiments along the path of the steepest ascent and from the experimental responses decide when to stop okay.

I have hit my bounds, so I cannot go further on from here so I will stop or I am reaching an optimum response value and I will pause here to reevaluate my design strategy. So if you are lucky enough to get into the second stage where your responses showing a maximum value and then declining, you want to stop at that point and pause a bit and reevaluate your design strategy.

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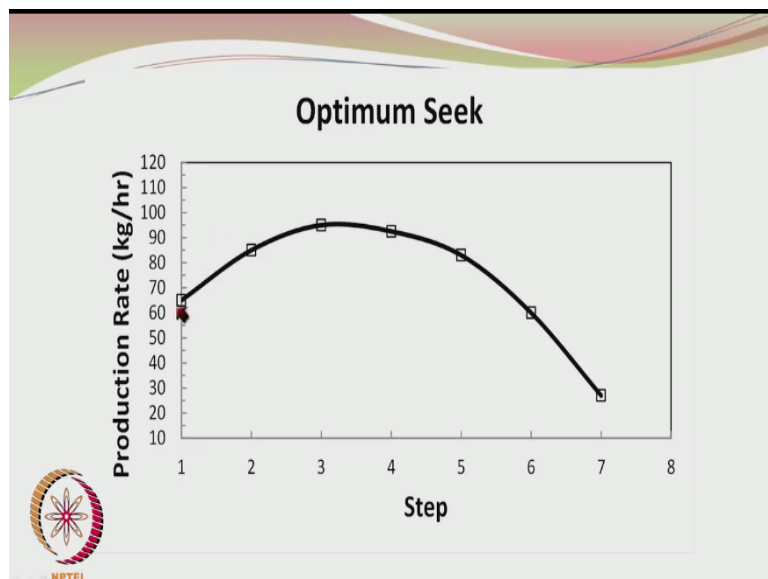
Direction of Steepest Ascent

The experimenter has to meticulously do the experiment and measure the responses. He proceeds according to the table given in the next slide. The observed yield increases until a value of about 95 observed at (2,2.5) and then starts decreasing.



So the experimenter has to meticulously do the experiment and measure the responses. He proceeds according to the table given in the next slide. The observed yield increases until a value of about 95 observed at 2, 2.5 in the coded format and then starts decreasing.

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So that particular figure is as follows. This is where you started and then when you proceed you find at the third step you are having a maximum value corresponding to about 95 and then the value start declining. The production rate in kilograms per hour has reached maximum of 95 at about the third step and remember that you are going for 1 unit along the X1 direction, you are going 1.25 units along the X2 direction.

So this is the point where you have to pause a bit and reevaluate your design strategy.

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Direction of Steepest Ascent

❖ Hence the engineer should re-evaluate the strategy on experimental optimization at this maximum point.

❖ He performs experiments around this point after



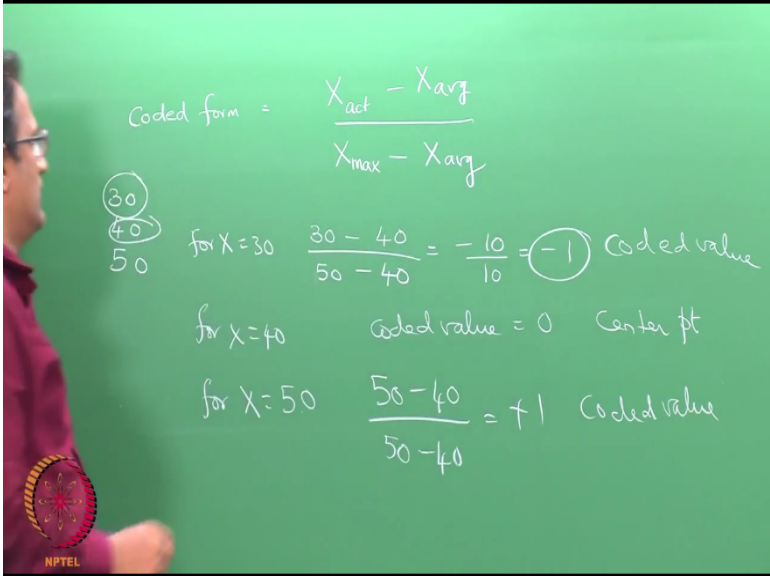
recoding the input variables to the -1 to +1 range.

So what we do is once you have reached that optimum location, you will be having a new set of coordinates corresponding to that. There again you recode your experimental settings as -1 and +1. Again this is very straightforward and this helps us to carry out the design on a uniform basis. So that we do not have odd numbers, odd values like 1.27, 3.56 and so on. We are always working with -1 +1.

So whenever we adopt a new experimental design strategy, we have to recode those experimental settings as -1 +1 format but we have to keep track on all the transformations so at any point we should be able to convert the coded values into the actual uncoded experimental settings. That is what is of interest to the experimenter and these things are done very easily.

I will just go to the board and tell you how the coding and uncoding is done.

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Coded form = $\frac{X_{act} - X_{avg}}{X_{max} - X_{avg}}$

for $X=30$ $\frac{30 - 40}{50 - 40} = -\frac{10}{10} = -1$ Coded value


for $X=40$ Coded value = 0 Center pt

for $X=50$ $\frac{50 - 40}{50 - 40} = +1$ Coded value

So a thing in coded form is very simple. This is the actual X value-X average/X max-X average. So let us say that you are having data points 30, 40, and 50 and if I am looking at 30 then it would be 30-average of 30, 40, 50 is 40/max is 50-40 and this turns out to be 30-40 is -10/10 which is -1. Now when I am having 40 this is corresponding for X=30. This is -1 coded value.

And for X=40, its coded value=0 which is the center point for that particular X and for X=50, we have 50-40/50-40, which is +1 as the coded value. So for any experimental set of data we are able to convert it into -1, +1 coded format.

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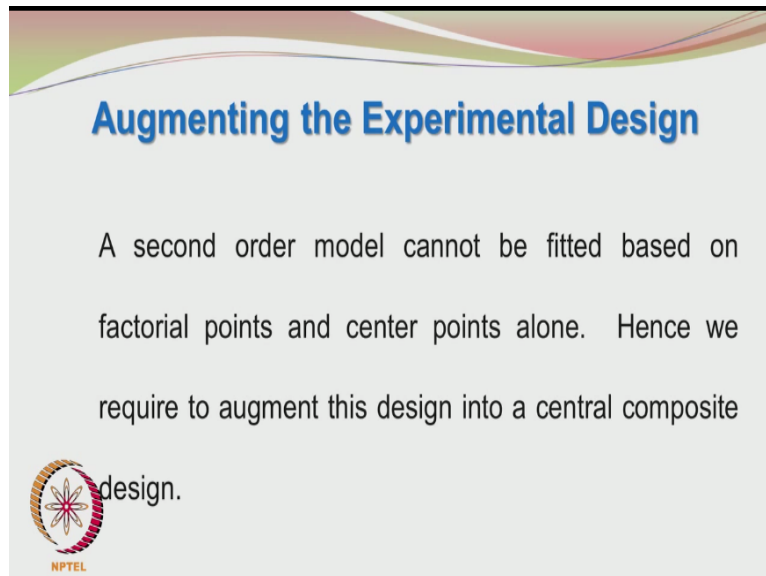
X_1	X_2	Y
0	0	65
1	1.25	85
2	2.5	95
3	3.75	92.5
4	5	83
5	6.25	60
6	7.5	27

So in the new so called optimum location we are again recoding our values and we get the responses as 85, 95 and 92.5 so at 2 and 2.5 we are getting the maximum response 95. So

these values are now coded values and those coded values are 1, 2, and 3 okay. This is the original coding. Now we have to recode these values as -1, so 1 will become a new -1, 2 will become a new 0 and 3 will become a new +1.


Similarly, 1.25 will become a new -1, 2.5 will become a new 0 and 3.75 will become a new +1. So this methodology I showed in the board can be adopted to code these values into -1, +1 format.

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Augmenting the Experimental Design

A second order model cannot be fitted based on factorial points and center points alone. Hence we require to augment this design into a central composite design.



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So now we are in a new situation where we are hit a maximum. This itself indicates that there is a curvature and a peak and a valley kind of region in the new experimental design space. So a simple model involving the main factors and the interaction between the two main factors will be definitely insufficient. So we have to capture the quadratic terms or the peak and valley coefficients correctly and efficiently.

And for this reason we cannot stick with the original factorial design and the center points, we need to augment the original factorial design with axial locations. So we are now going in for the central composite design where we add axial points in addition to the existing factorial points and center points.

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Central Composite Design

In addition to the previously used setting, the analyst uses $(X_1=\pm 1.414, X_2=0)$ and $(X_1=0, X_2=\pm 1.414)$. The complete design is shown in the table given on the next slide.

This design is called as the **central composite design**



And for two factors, the axial points are located at $+\text{ or } -\sqrt{2}$ 0 and $0 + \text{ or } -\sqrt{2}$.

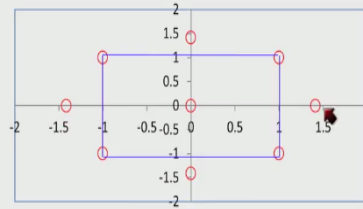
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A	B	P
-1	-1	85
1	-1	126
-1	1	64
1	1	92.5
-1.414	0	77
1.414	0	123
0	-1.414	101
0	1.414	66.1
0	0	93.5
0	0	95
0	0	91
0	0	96

And this is the design matrix for the central composite design and you can see that in the recoded format we have the factorial point shown in green color, the axial points shown in blue color and the center points shown in red color and when we do experiments at these conditions, these are the production rates obtained.

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Central Composite Design



So at this point, we can also show it graphically or in the form of a figure, you can see that these were the factorial points and this represents a center points or central points and then these represent the axial points and they are located at -1.414 $+1.414$ $+1.414$ and -1.414 . So these are the axial points. So in addition to the factorial points and center points, we have the axial points and this represents the central composite design strategy.

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Second Order Model

The second order response may now be expressed as

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{12} X_1 X_2 + \beta_{11} X_1^2 + \beta_{22} X_2^2 + \epsilon$$

The predicted expression is given below

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \hat{\beta}_{12} X_1 X_2 + \hat{\beta}_{11} X_1^2 + \hat{\beta}_{22} X_2^2$$



And what is the second order model we are testing with? Second order model we are testing is $\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{12} X_1 X_2 + \beta_{11} X_1^2 + \beta_{22} X_2^2 + \epsilon$ the error term or the predicted expression or the prediction equation is given as $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \hat{\beta}_{12} X_1 X_2 + \hat{\beta}_{11} X_1^2 + \hat{\beta}_{22} X_2^2$.

So this completes our initial discussion on the response surface methodology. We will be looking at another example involving the central composite design and we will see how to estimate the β_{11} and β_{22} and we can also see whether these particular additional terms are significant or not and once we have done that we also have to locate the optimum condition.

It is not enough that we identify the optimum condition; we have to characterize the optimum condition also. First, we have to tell whether the obtained optimum condition is a maximum or a minimum. Sometimes, it can even be neither. You may be sitting on a saddle and there may not be any change in the value along a particular direction, so that may also happen, we do not know.

And even though we may have hit an extremum point we have to see whether it is a maximum or a minimum and some mathematical tools are available with this and we can use them. This is a very important aspect of experimental design and perhaps represents the ultimate point in experimental design strategies. So we have done experiments in efficient manner, planned manner using factorial design concept.

And now we have added an additional dimension to the entire exercise by using design of experiments to find the optimum location. So we will continue in the next lecture with the suitable example involving the central composite design. Thanks for your attention.