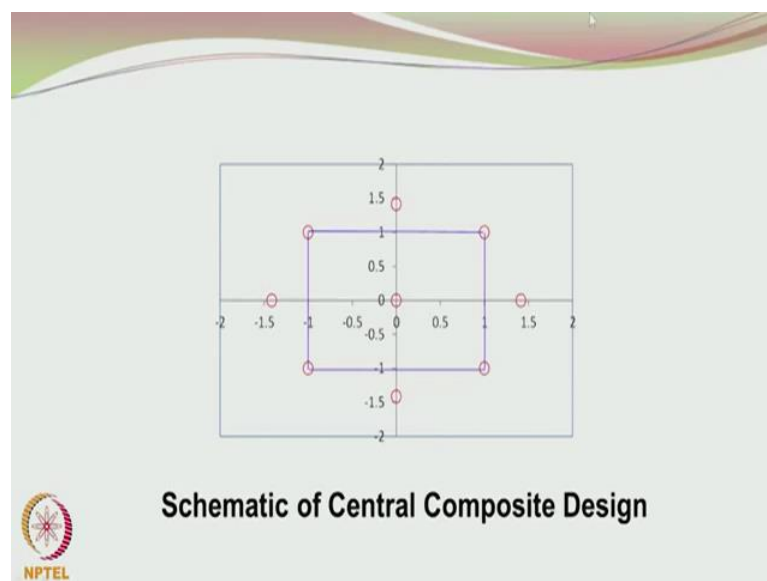


Introduction to Research
Prof. Kannan
Department of Chemical Engineering
Indian Institute of Technology, Madras

Lecture – 05
Design of Experiments

So now, let us look at very popular Second Order Statistical Experimental Design, based on the second order model.

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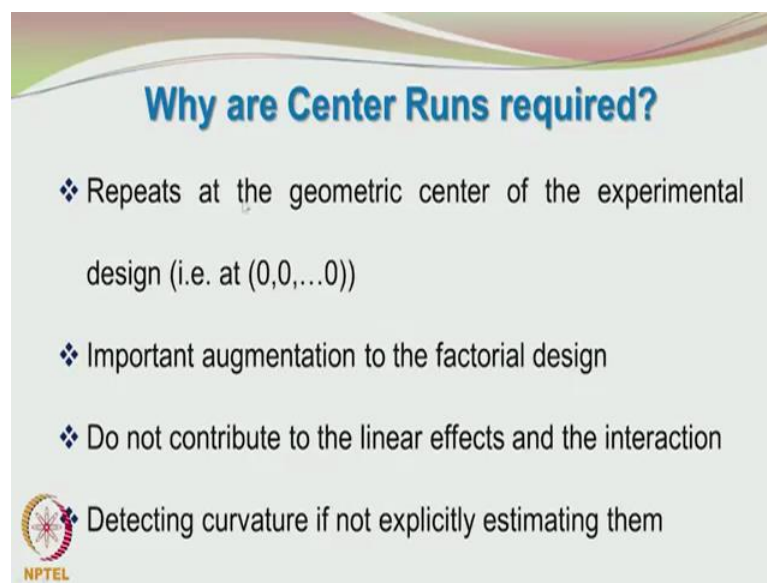
This is the central composite design, you can see that we have a square here; we are talking about 2 factors, 2 variables. So, you have a regular 2 power 2 design, 2 factors in 2 levels so you have 4 settings, this constitutes the square, low-low and then you also have high-high and so on. So, you have an experimental design involving a 2 power 2 factorial designs.

In addition to that, you have the axial points you can see this is the first axial point, second axial point, third axial point and fourth axial point. The first second third and fourth are given arbitrary fashion, so you have 4 runs, 2 power 2. Then, you have 2 k axial points where, k is the number of factors, so you have again 4 axial points that makes it the total of 8. But, that is not all you also have the center point which is the geometric center of the design. I said earlier that, the repeats may be performed at the

factorial points or at the centre points. So, you here you can have 4 or 5 repeats for your experiments.


This is a very interesting and very commonly used design for experiments. There is lot of flexibility, where you want to locate you axial point. You may want to locate at either further or close to the factorial design, depending upon your requirements. What those requirements are? And how do you shift them? You will learn when you do a formal course on the Design of Experiments.

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Why are Center Runs required?

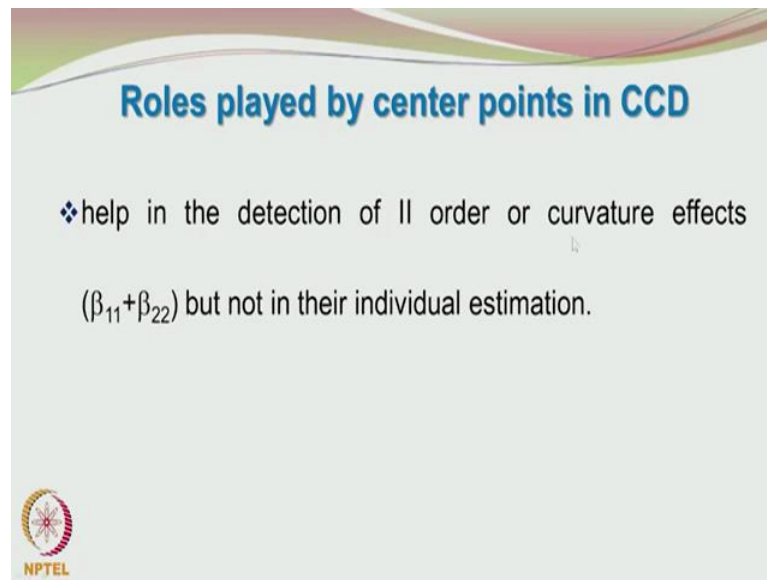
- ❖ Repeats at the geometric center of the experimental design (i.e. at $(0,0,\dots,0)$)
- ❖ Important augmentation to the factorial design
- ❖ Do not contribute to the linear effects and the interaction
- ❖ Detecting curvature if not explicitly estimating them

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So, why do we require the runs at the center? They may represent the repeats **okay**, rather than repeating the experiments at all the factorial points and this may become very expensive especially, when you have very large number factors, doing experiments at the center of the design space is convenient.


As the center of the designs space, is some kind of representation of the overall design. It also represents an important augmentation to the factorial design and it tells whether there is a curvature in the experimental response **okay**. Sometimes, there can be only linear variation with the factors but, sometimes if there is interaction between the factors then you have a curvature or a twist in the planar response curve. It may not be a planar or it may not be a simple, but there may be some kind of curvature. So, to detect this curvature you need the center points. How the center points help you to detect curvature is beyond the scope of this introduction lecture.

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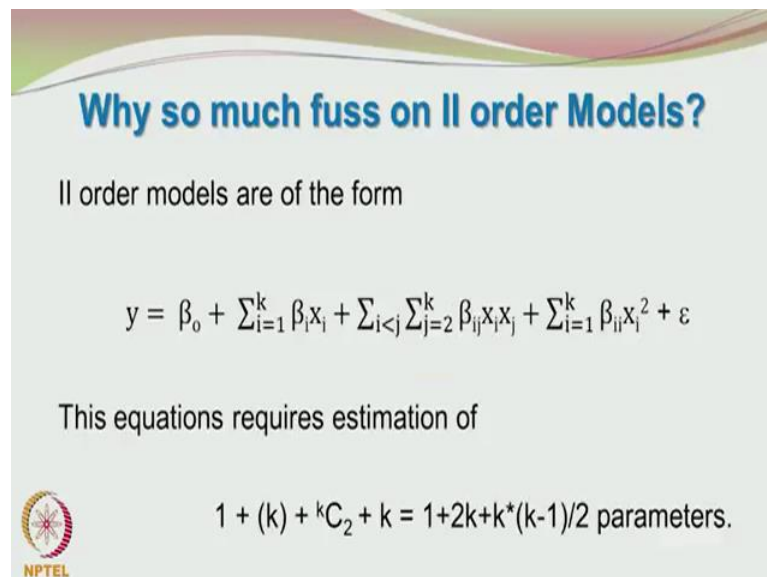
Roles played by center points in CCD

- ❖ help in the detection of II order or curvature effects
($\beta_{11} + \beta_{22}$) but not in their individual estimation.



So, the center points help to detect the second order or curvature effects. The quadratic terms, it helps to identify whether that beta 11 plus beta 22 is significant or not. But, it **doesn't** help you to estimate individually beta 11 and beta 22. Where did this beta 11 and beta 22 come from?

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Why so much fuss on II order Models?

II order models are of the form

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

This equations requires estimation of

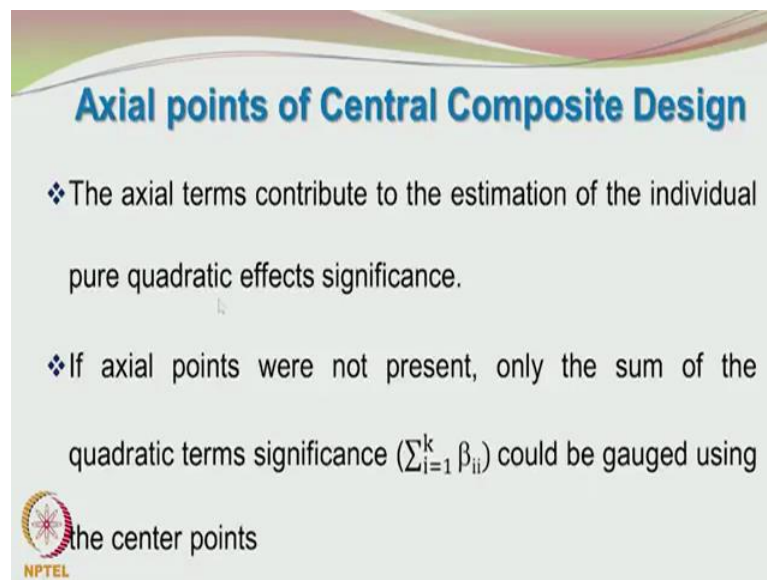
$$1 + (k) + {}^k C_2 + k = 1 + 2k + k(k-1)/2 \text{ parameters.}$$



Let us go back to the model, if you are having only 2 factors then I said, you will have beta 11 x 1 square plus beta 22 x 2 squared. These represent the quadratic terms and also responsible for the curvature, in addition to the interaction terms **okay**. So, to find the


beta 11 and beta 22, you require center points. Even though, you may not be able to find out explicitly beta 11 and beta 22 at least we tell you whether beta 11 plus beta 22 is overall significant or insignificant. If beta 11 plus beta 22 is insignificant then, both the beta 11 and beta 22 are not required to be present in the model.

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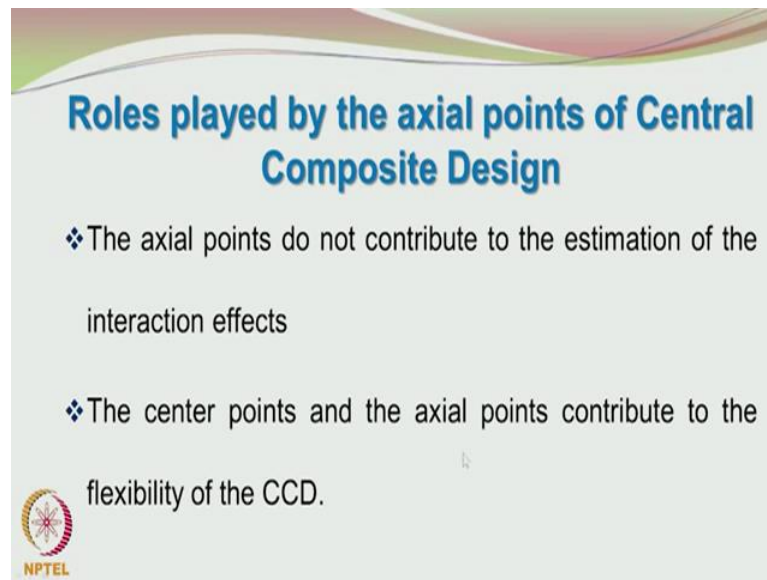
Axial points of Central Composite Design

- ❖ The axial terms contribute to the estimation of the individual pure quadratic effects significance.
- ❖ If axial points were not present, only the sum of the quadratic terms significance ($\sum_{i=1}^k \beta_{ii}$) could be gauged using the center points

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What is the contribution from the axial points? The axial points contribute to the estimation of the individual pure quadratic effect's significance. If the axial points were not present, only the sum of the quadratic terms significance could be gaged using the center points, this is pretty straight forward.

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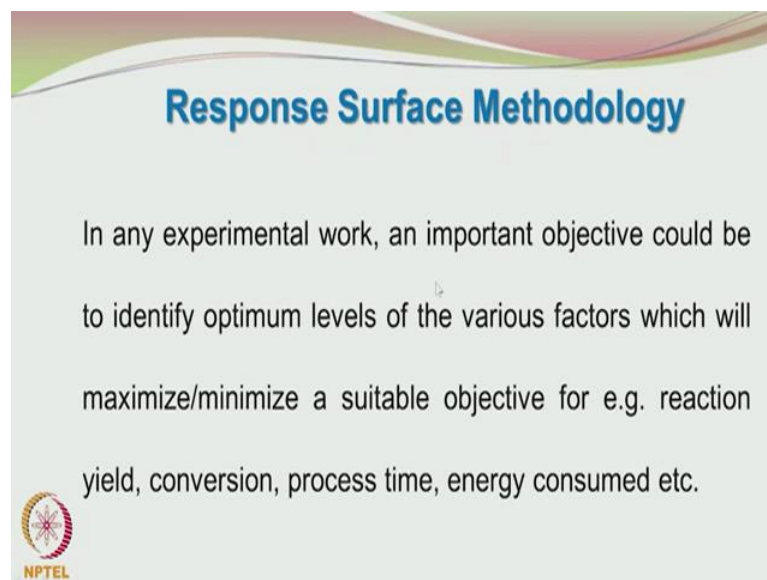
Roles played by the axial points of Central Composite Design

- ❖ The axial points do not contribute to the estimation of the interaction effects
- ❖ The center points and the axial points contribute to the flexibility of the CCD.




The axial points do not contribute to the estimation of the interaction effects. The center points and the axial points contribute to the flexibility of the Central Composite Design.

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Response Surface Methodology

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.

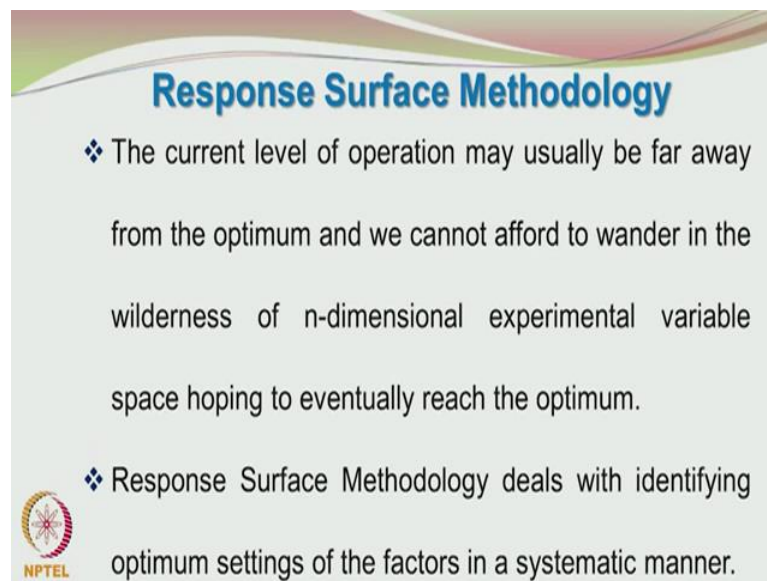


Now, we come into the final topic; Response Surface Methodology. Many industries want to optimize their processes, but did not know where to start and where to end. And, it is not appropriate, especially in the industry to embark on a grand exploratory voyage in the end dimensional space, hoping to sight the promised land sometime or the other.

What **is** important is, first to do a set of screening experiments where you have a preliminary set of experiments and assess the overall trend. And, the Response Surface Methodology then enables you to identify the direction in which you should proceed. In other words, it points to the direction where you should set your experimental factors, so that you are progressing in the correct direction **okay**. Suppose, the goal of your process is to optimize then, the Response Surface Methodology will tell you the direction where the process will be increasing or the process response would be increasing in the fastest manner.


This is very useful, it helps you to decide and plan your next level of experiments. So, 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 example, reaction yield, conversion, process time, energy consumed, etcetera. So, your objective function may be either minimum or maximum. So, you have to proceed in such a manner that, you go to the correct desired condition.

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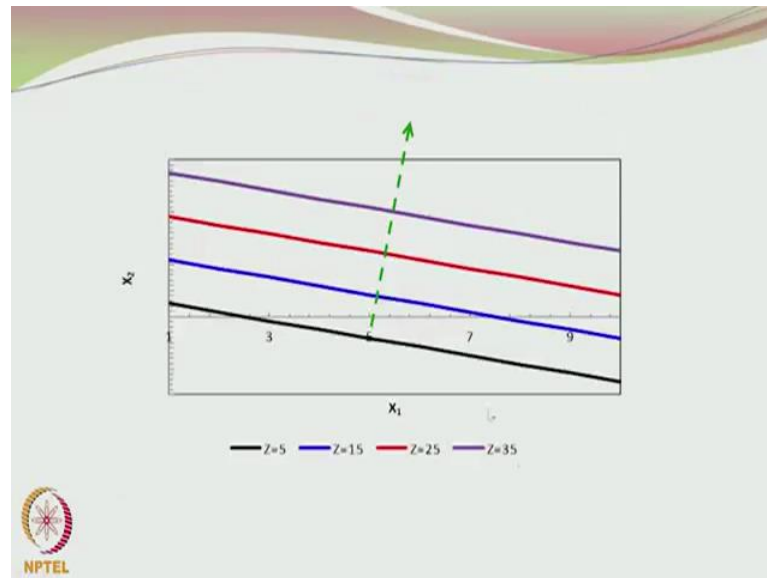
Response Surface Methodology

- ❖ 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.

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So, the current level of operation may be usually far away from the optimum and we cannot afford to wander in the wilderness of the 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.

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So, as I said earlier the Response Surface Methodology helps you to find quickly in which direction the processes increasing the fastest. You have to increase in the process responses what you want. So, if you consider case involving 2 variables, x_1 and x_2 . The method of steepest ascent an optimization tool helps you to know the direction in which the responses are increasing in the fastest possible manner and this is directly shown in terms of the green arrow, for this particular case.


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Second Order Model

The second order response may now be expressed as

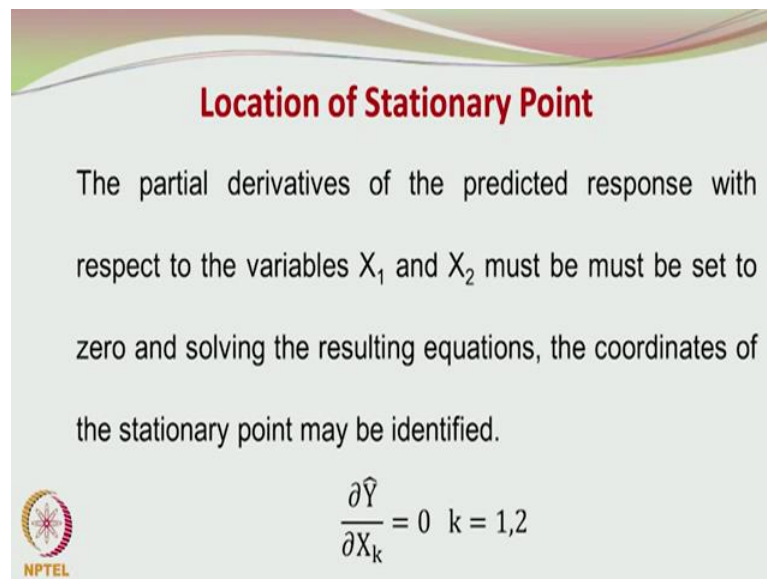
$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{12} X_1 X_2 + \beta_{11} X_1^2 + \beta_{22} X_2^2 + \epsilon$$

The predicted expression is given below

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



So, when you have 2 factors, this is the form of the equation, the true response involving the random error component and this is the model which is being proposed and you have to estimate the beta naught hat and then the remaining parameters beta hat 1 beta hat 2 beta hat 12 corresponding to the interaction, beta hat 11 and beta hat 22 and the last 2 corresponding to the quadratic terms.

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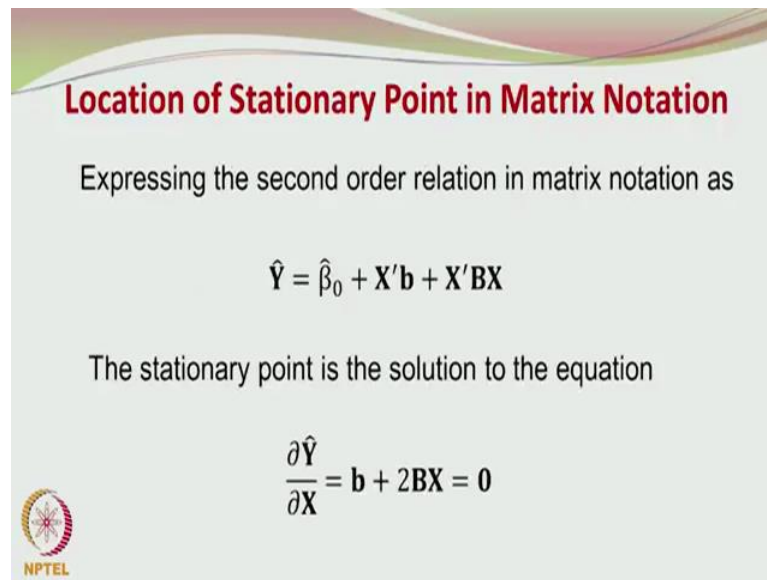
Location of Stationary Point

The partial derivatives of the predicted response with respect to the variables X_1 and X_2 must be set to zero and solving the resulting equations, the coordinates of the stationary point may be identified.


$$\frac{\partial \hat{Y}}{\partial X_k} = 0 \quad k = 1, 2$$

Again, we can use linear algebraic techniques in order to identify the optimum conditions. So, in order to find the stationary points, the so called stationary points, you have to partially differentiate your proposed model with respect to x_1 and x_2 and set them to 0, solve the resulting systems of equations and, or system of equations and identify the stationary conditions.

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Location of Stationary Point in Matrix Notation

Expressing the second order relation in matrix notation as

$$\hat{Y} = \hat{\beta}_0 + \mathbf{X}'\mathbf{b} + \mathbf{X}'\mathbf{B}\mathbf{X}$$


The stationary point is the solution to the equation

$$\frac{\partial \hat{Y}}{\partial \mathbf{X}} = \mathbf{b} + 2\mathbf{B}\mathbf{X} = \mathbf{0}$$


To do this, would be quite tedious especially, when you are having many factors. We may as well use the linear algebra techniques for which several tools are available at present, for example, MATLAB, Scilab and so on, or there is no big deal in writing your own program, if you are having inclination towards that **okay**. So, coming back to our Response Surface Methodology approach, we can represent the second order model in matrix notation as shown here; $\hat{\beta}_0 + \mathbf{X}'\mathbf{b} + \mathbf{X}'\mathbf{B}\mathbf{X}$. And, the stationary point of the solution can be **obtained** by differentiating this in matrix terms, to get $\mathbf{b} + 2\mathbf{B}\mathbf{X}$ and we get the stationary conditions by equating this to 0. Again, all the bold terms indicates that they are vectors and matrices and not the regular usual scalars.

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Matrix Notation Explained

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \cdot \\ \cdot \\ \cdot \\ X_k \end{bmatrix} \quad B = \begin{bmatrix} \hat{\beta}_{11} & \frac{\hat{\beta}_{12}}{2} & \dots & \frac{\hat{\beta}_{1k}}{2} \\ & \hat{\beta}_{22} & \dots & \frac{\hat{\beta}_{2k}}{2} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \hat{\beta}_{kk} \end{bmatrix} \quad b = \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \cdot \\ \cdot \\ \cdot \\ \hat{\beta}_k \end{bmatrix}$$


So, what is the form of the X vector, the B matrix and the small b vector? We came across all these, in this equation so we have to identify the form for all these. So, you have X as the vector, comprising of the different factors starting from X 1 so on to X k. Then, you have the B matrix, given in terms of these coefficients and what is this beta hat 11? I already told you, what beta hat 11 is. So, this is beta hat 11, beta hat 22. So, you can easily show that this is the form of the model. It might be interesting for you to find out, why some of these terms in the capital B matrix are divided by 2. So, I think **it's** worth the effort to find out the reason. I **will** leave it to you. Then you have the b matrix, which again comprises of the parameters to be estimated and it is given in this particular form.


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Location of Stationary Point in Matrix Notation

Solving the above equation we get

$$\mathbf{X}_s = -\frac{1}{2}\mathbf{B}^{-1}\mathbf{b}.$$

The predicted value of Y at this stationary point is

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



So, when we want to use this matrix method, we solve this particular equation and then we identify the stationary condition in a very simple way, minus half times the B inverse times the small b vector **okay**. So, that will give us the stationary conditions and then using those stationary conditions, we can give the estimated predicted value of Y by using this relationship.

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Nature of the Optimum Solution

Check the eigenvalues of **B**.

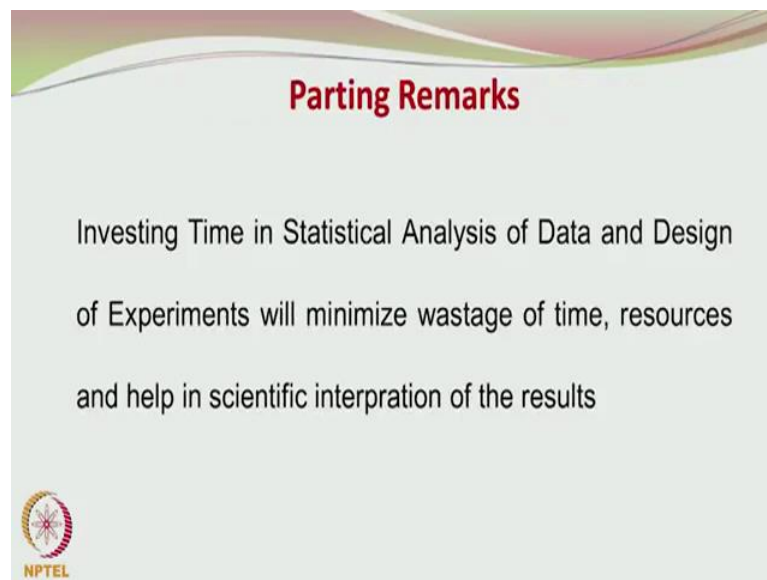
If all the eigenvalues are positive (negative), and the stationary point is within the region of exploration, the stationary point is a minimum (maximum).



So, whether the optimum obtained is maxima or a minima, you can again use or sort of linear algebra tools we can check the eigenvalues of the capital B matrix. So, we find the eigenvalues of this matrix.

So, if the eigenvalues are all positive then, the stationary point in the region of exploration is a minimum, if the eigenvalues are negative then we have hit up on the maximum. Again, there will be some complications when you have 1 eigenvalue and which is positive and another eigenvalue which is negative, I will not get **into** these complications, but I think there is sufficient unexplored, uncharted territory as far as the student is concerned which he can get into and learn at his own pace.

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So, we are coming to an end of the introductory series of lectures. It has been **a** real pleasure to talk about the various concepts associated with the Design of Experiments. I **didn't** only focus on the various experimental designs because I felt to appreciate and understand the experimental design and also to understand, then analyze and present the results from the experimental design concepts, proper introduction into the basics of statistics and probability is also necessary. So, I covered lot of ground talking about normal distribution, the random variable, the sampling distributions of the means, the chi square distribution, the f distribution, the hypothesis testing concepts, believe me all these will come in your Design of Experiments analysis and knowing them would be a good investment, so that you can better appreciate the Design of Experiment concepts.

I have also given NPTEL lectures on this fascinating subject. You are welcome to look at that for getting further information and understanding on this fascinating subject.

Thanks for your attention.