**Mathematical Modelling and Simulation of Chemical Engineering Process**
**Professor Sourav Mondal**
**Department of Chemical Engineering**
**Indian Institute of Technology, Kharagpur**
**Lecture 57**
**Response surface methodology**

Hello everyone, in this class we are going to talk about stochastic modeling process known as response surface methodology. So, actually this is a Blackbox type of model where we do not need or we do not use or maybe we do not have, that is why we do not use any physical information about the process, but try to connect whatever the parameters are there that we set in the experiment. So, that we set in the or that we see in the system or the operating conditions and what is the outcome or what is the output of that process.

So, it is like connecting the input to the output using certain model which is not at all related to the physics of the system. So, it is not essentially a physical model or a deterministic model, but, there are certain things where you cannot actually describe or you cannot propose such physical laws behind a process and that is where these things are very useful. Most cases, these are like certain cellular reactions or biological reactions, where things are too complex to identify what actually is happening.

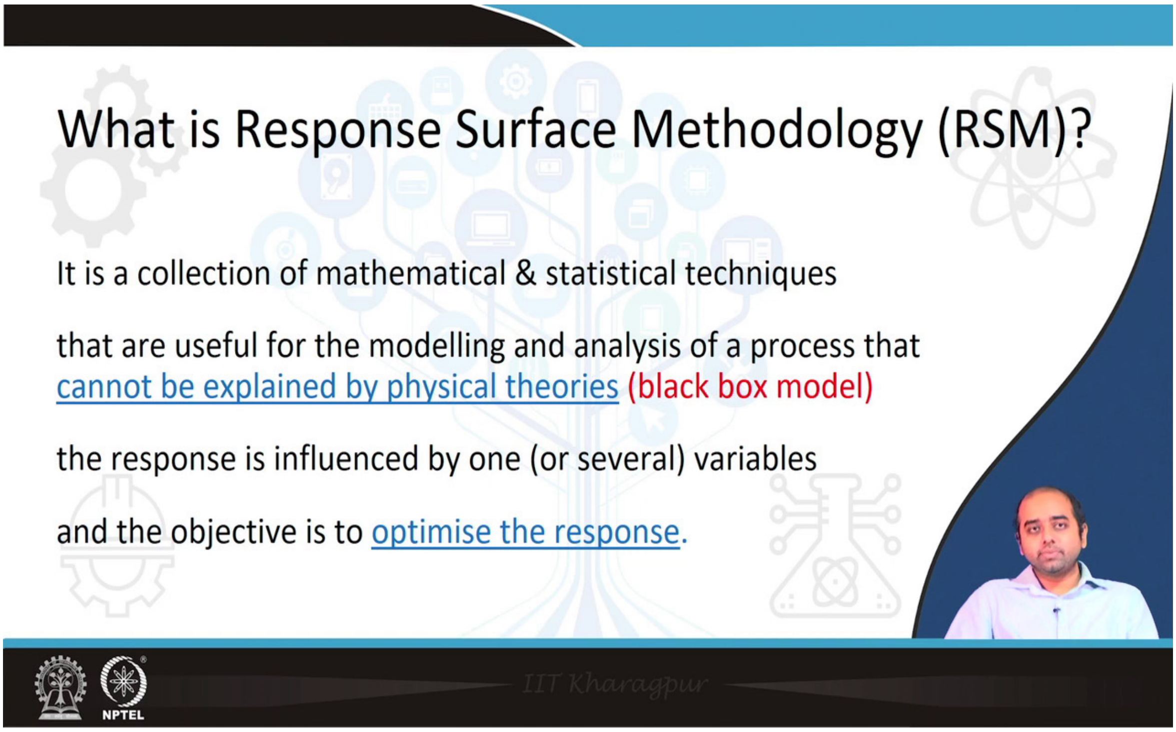
Or for example, there are too much of process variabilities in a system that cannot be actually used to track the process outcome definitively. In that case, we try to fit this model and using certain experimental data, we try to find out what are the model parameters, and that could work or this model could be a generic one in trying to provide answers within certain range of course, as defined by the experimental limits for any combination of the input variables.

So, you can think this to be sort of a fitting exercise. So, yes, it is it is a sort of sophisticated fitting exercise. And that is true for any kind of Blackbox model, ultimately, you have to use some sort of regression techniques to find out the model parameters, whether we talk about response surface methodology, whether it is artificial neural network, which is something we will cover in this week itself. So, there have to be some sort of regression. But then what sort of model do we create? What is the minimum experimental data set that is needed to find a good estimation of the unknown parameters in the model is something very essential to understand or to relate essential.

(Refer Slide Time: 03:10)

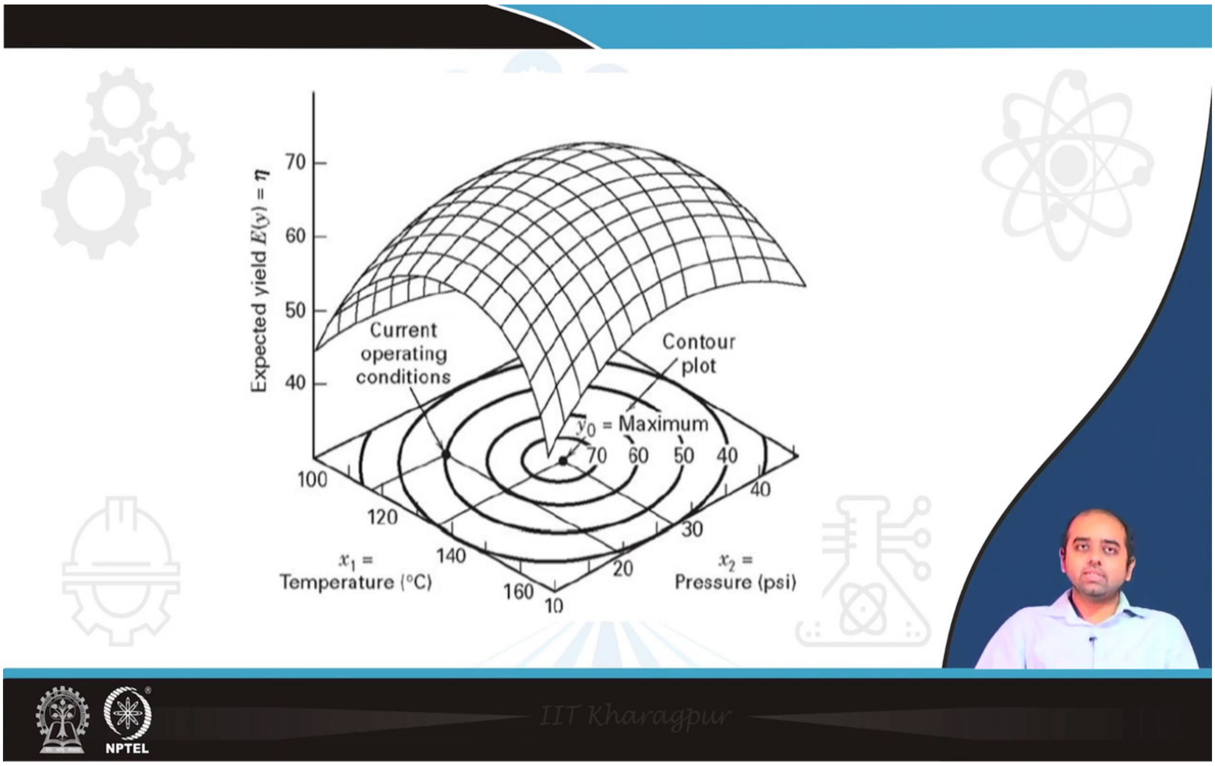

So, in this lecture, we are going to talk about the basics of the response surface methodology, and then we will see the different types of first and second order models that are available, how do we actually pre-process the variables before they are used in the model? And in the next class, we will talk about the design of experiments.

(Refer Slide Time: 03:35)



So, this is essentially as I said, this is a Blackbox model and where there is something which cannot be explained or cannot be described by physical laws, this comes very useful or very handy, and the response or the final output that we see could have an impact of more than one variables and that what makes it very tricky actually. So, using this Blackbox model or this response surface methodology, based on the model that we get, it is actually quite suitable or appropriate to optimize the output. So, let us see that what essentially this means.

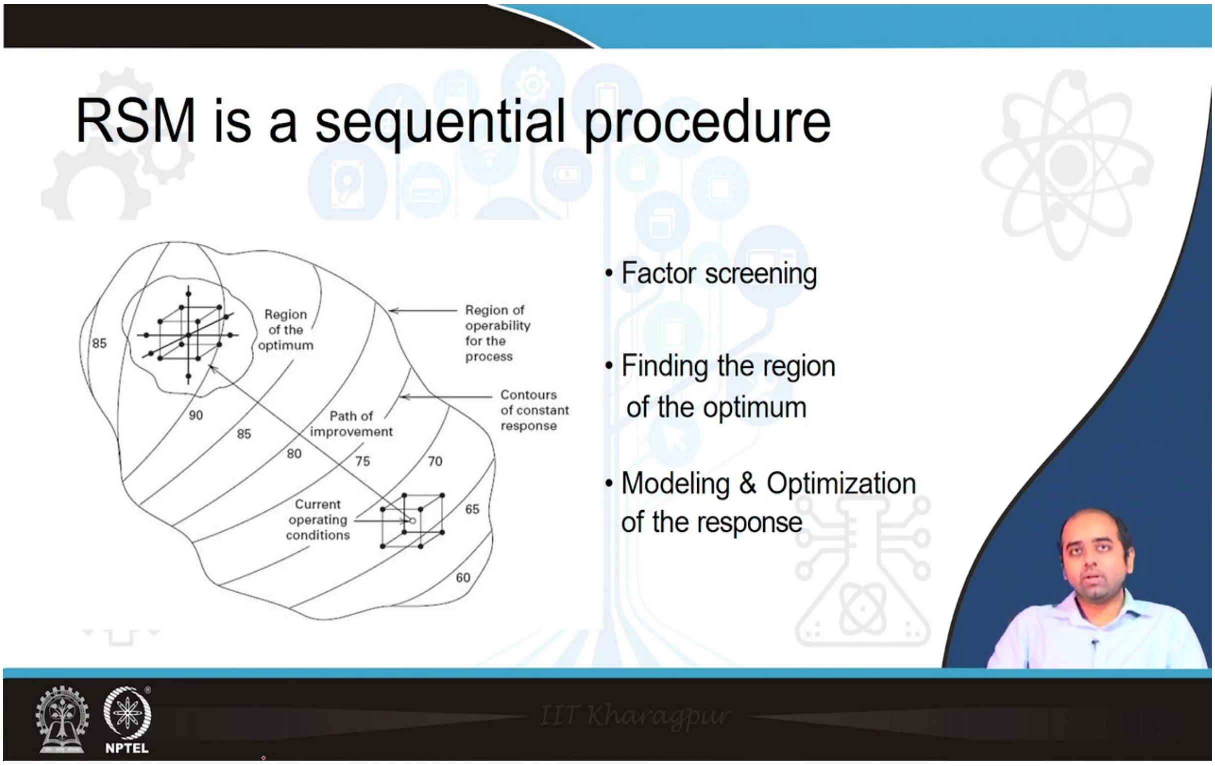
(Refer Slide Time: 04:22)




So, this is an example. For example, let us say we try to see, what is the expected yield of a particular process. Let us say it is a chemical reaction, which is influenced by a gas phase reaction, which is influenced by temperature and pressure. It is quite normal. So, we see that the expected yield has a sort of maximum point, something around here, which is sort of a function of both temperature and pressure. So, experimentally it may not be possible to do a lot of combination of these two process parameters, temperature and pressure and find out this optimum.

So, we can do certain experiments and from there we are hoping that our model can be formulated based on those information or experimental information or the limited datasets that we have and then from there can we predict this sort of optimum point or maximum point.

(Refer Slide Time: 05:29)

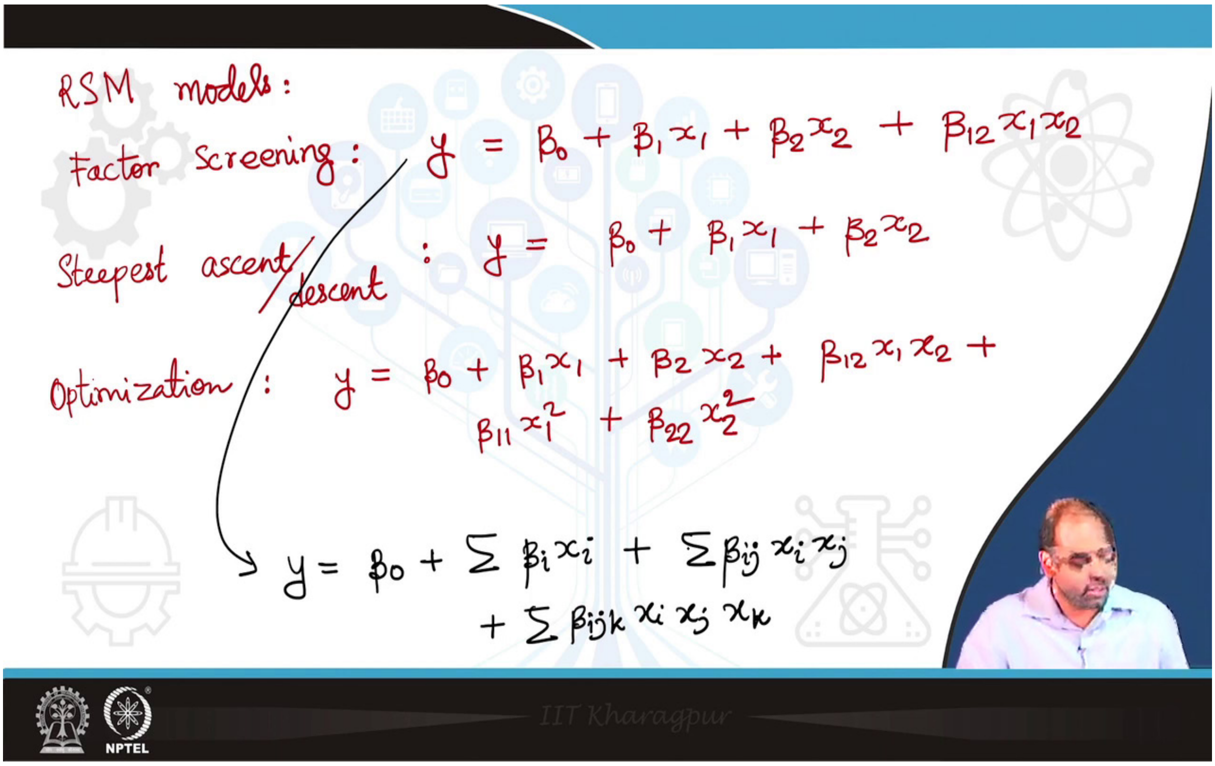



So, the different types of models that are available in this response surface methodology is generally the first order and the second order models. But, before we talk about the model equations, it is very essential to understand that this process of developing the model equation or process of finding out the optimum is a hierarchical process. So, first we try to whatever model we try to prepare, it is very important to understand what are the factors that influence this system.

Second is to find out that which factors or which interactions of the factors is not important. So, unnecessarily we do not want to burden our model with certain terms, which does not contribute much. So, that is what we call as the factor screening. Second is that instead of actually finding the global minimum or global maximum or the global optimum or the local optimum, it is very important or essential, that is what this picture describes that we try to locate the region of the optimum.

So, that is something is generally done by a first order model. We call that as the steepest ascent or steepest descent and these are generally very fast. It is a very fast algorithm or a very fast process and if you move along the direction of the steepest ascent or descent, you can come close to the region of the optimum and final step is to pinpoint or accurately find out the optimum for which second order models generally are useful.

(Refer Slide Time: 07:23)




So, if we try to list down these RSM response surface metrology models, so, for the case of factor screening, we generally, so, this is the output y, the variables that are, this is a bias to the system Beta 0, then the first order terms, let us say we have two process, variables x1 and x2. So, first order terms corresponding to these two and there is an interaction terms x1 x2, like this.

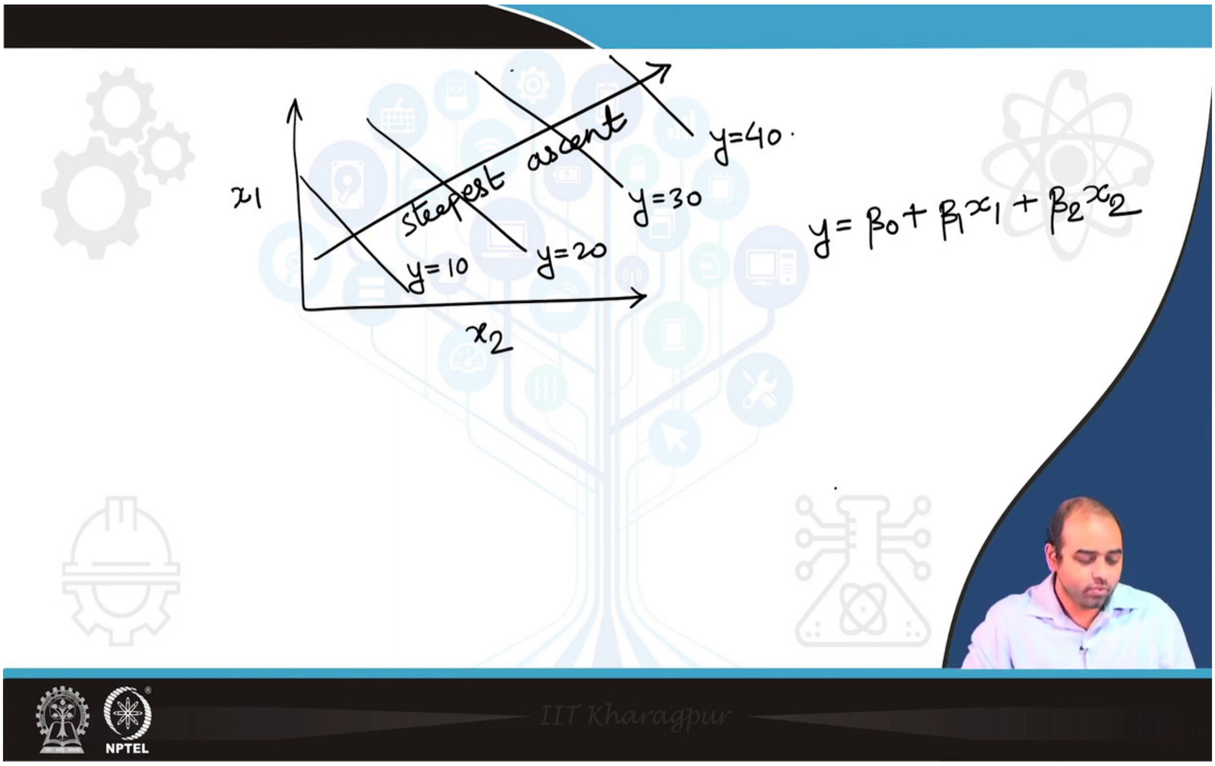
So, this is an addition, so, these will help us to determine like, if we try to fit this equation to the experimental data, it will try to then estimate these constants, beta 0, beta 1, beta 2 and beta 1 to these four constants and then try to find out that which of these constant is very small or very insignificant and that can help us to determine that which factor is unimportant in the problem.

So, it may happen that beta 1 2 is very small compared to the other terms. So, then we know that this interactive term is not important. So, these factors will be screened out. So, this is what we call factor screening, that is sort of the first stage. Next is the steepest as I said, steepest ascent or decent. This is useful when we try to find out the region near the optimum parameter and this is always a first order model.

This model or this equation will help you to find what is the region along the maximum or close to the region of the optimum. And finally, for optimization once you reach to the optimum region, we generally use the optimizing equation which is essentially a second order model. So, the second order model can you essentially give you the optimized location. So, this includes all the first order, the interaction terms and the second order terms.

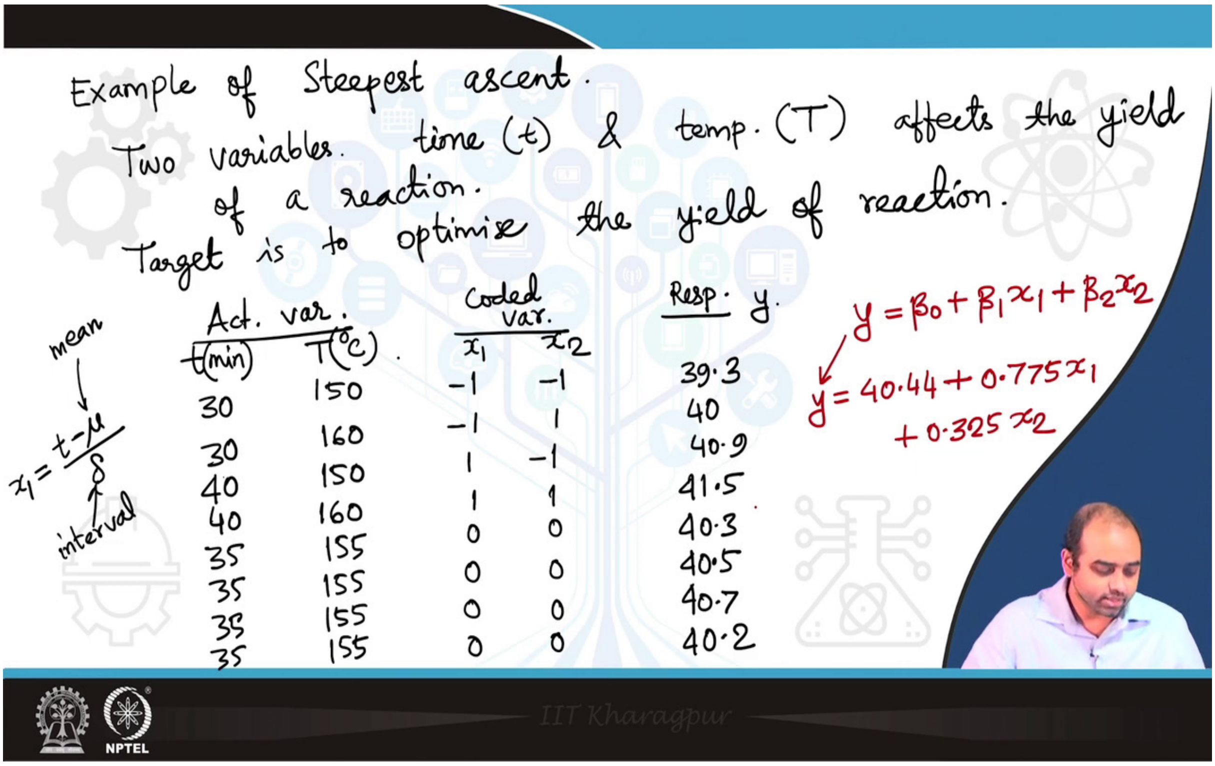
So, I hope all of you realize this, in the case of let us say if you are having a case of more than two variables then you can say for example, if there are more than two variables, then this factor screening would be equal to beta 0 plus sigma beta i x i let us say if there are more number of these variables then you have beta ij xi xj plus beta ijk xi xj xk, this is for three variables right this would be how it will look like and four variables, we have another terms. The number of terms will go on increasing as you have more number of variables or independent variables or perhaps parameters in the system. So now, let us quickly talk about little bit on the steepest ascent also.

(Refer Slide Time: 11:36)




So, the steepest ascent is you can think of this, something like this, let us say you have x1 and x2 and if you try to draw contours or phase diagrams of constant y values, let us say y is equal to 10, this is like y is equal to 20, y is equal to 30, y is equal to 40, then this equation y is equal to beta 0 beta 1 x plus beta 2 x2, if you follow these paths of constant y, this will lead you to the part of the steepest ascent. So, this helps you to determine that which is the region where the Y is increasing or the output is increasing based on this first order process. And this would be always in a straight direction or over a straight-line path because this is a first order linear model.

(Refer Slide Time: 13:01)




A quick example of real-life process. Let us see an example of steepest ascent. Let us say two variables, one is time and called as t and another is temperature, called as capital T affects the yield of the process, yield of a reaction and the target is to optimize the yield of the reaction. So, target is to optimize the yield of reaction. So, you have our data set, data set let us say the actual variables. So, let us list down some realistic values, t in terms of let us say minutes and this is in terms of centigrade, whatever.

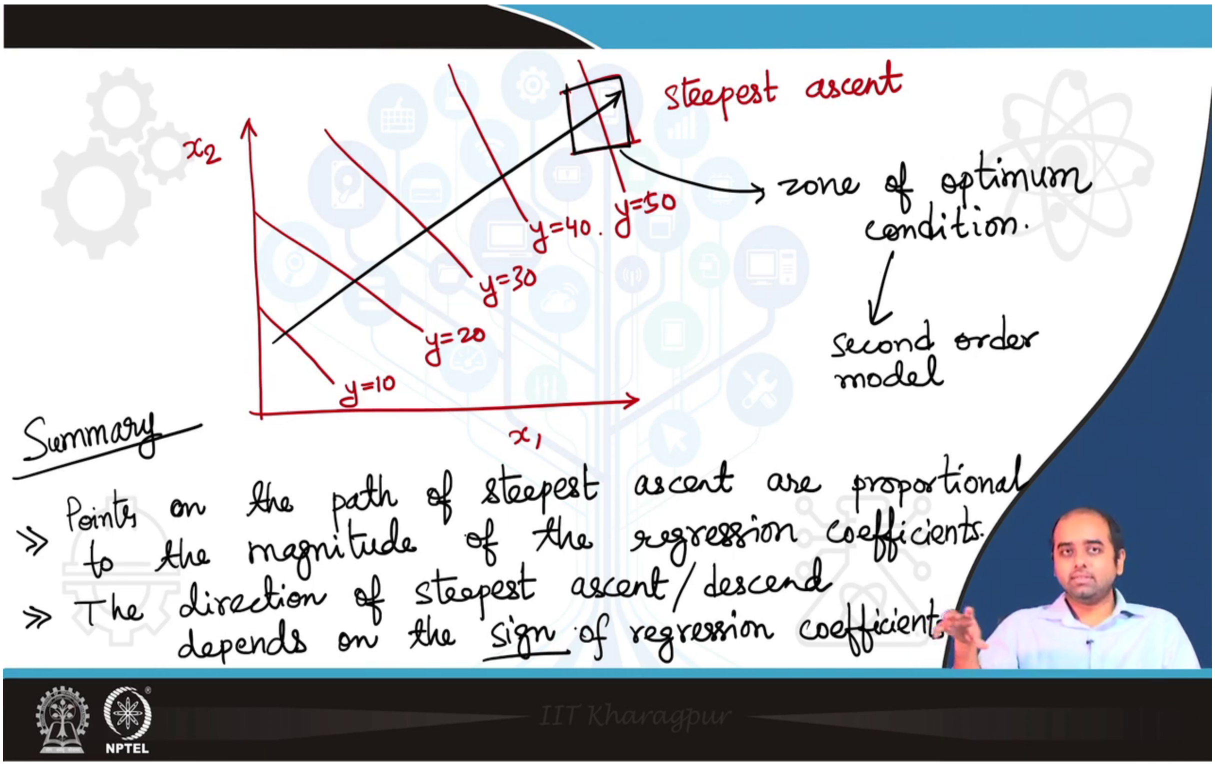
So, let us say it is like 30, 30, 30, 40, 40, 35, 35. So, there are five 35s and then here I am having 150, 160, 150, 160 and these are all 155. So, generally the actual variables are not directly used. This is something what we call as the normalized variables or coded variables. So, I would prefer to use the coded variables because that is something which is used. You can think of this to be as the normalized, dimension less or whatever.

So, the coded variables let us say x1 and x2, so, X1 represents the actual time and x2 represents temperature. So, this coded variable for the x1, I am getting for the first case as minus 1 minus 1, then plus 1 so, plus 1. So, how I am getting this coded variant? Simple, just do a normalization of let us say x1 is equal to this value of t minus mu by delta. So where, mu is the mean and this is the interval if I divide, so, the interval that is here is like 5 degrees and mean is 35.

So, with that if I do I will get this coding. So, similarly, I can also do so, this coded variable as for the temperature also, the temperature also you can see that the mean is 155 and temp difference is 5 degrees. So, which is minus 1, then I have 1, then I have 1, minus 1 1 and the rest all are 0, response, let us call that response as y. So, the y is actually given by something of some realistic numbers, 39.3, then you have 40, then you have 40.9, 41.5, 40.3, 40.5, 40.7, 40.2.

This is something what we see in the response. So, in this case, if you try to fit a model satisfying this relation, so, it is linear regression of two variables. So, all of you know these regression techniques that is something which you have already studied in your numerical method score. So, if you do this over this data set, you will be getting beta 0 as 40.44, then something like 0.775 x1 plus 0.325 x2, this is something we expect to get.

(Refer Slide Time: 18:30)



And this is something that if you try to plot this graph based on that equation for different values of your x1 and x2 over the range of minus 1 to plus 1 let us say or minus 2 to plus 2, then you can have different regions of y is equal to 10, like this, y is equal to 20, then you will get y is equal to 30. It is possible to get. So, you will see that this is the path of the steepest ascent and this will land you up to the region right let us say we want, we are expecting that after that it is very far away, any further change.

So, this is the zone of optimum condition that we can expect. Of course, this first order model cannot give us the optimum condition for which you need the second order model, but we know that the zone or the limit of the second order model is maybe restricted only to that region. So, this helps us in narrowing down the region of the model over which I mean then if if I say that this is the narrow zone I need, so, I can only select my variables and do some more experiments focusing around that region.

So, for example, I do not have any clue about what could be the possible optimum point and I cannot map the entire two parameter space like three parameters would be like a three-dimensional space in fact, we are having three operating condition or three process variables. And things become more complex when you have four variables. So, even with two variables, I do not know that what is the region over which I can expect to find the optimum.

So, steepest ascent helps us to locate that region and from there let us say now, I know that this is the region where this optimum value is expected. So, then I can choose my x1 and x2 or whatever, this time and temperature around that region or select around that region or try to monitor my, this reaction or process for this combination of the variables and try to get some more points or some more refined points in that region, where I can apply the second order model, is not it? where I can apply the second run model. Is not it?

The second order model of course, will need more parameters or more experimental values, because it has more number of unknowns in the regression equations to be quantified. So, necessarily it will require more number of experimental data points. Now, I may focus all my resources into that small region or into the region essentially which is bounded by the values of these process parameters to find out that, that is the location at which the optimum is expected to be found out and I can have more experiments on that region or the values of the parameters in that region and get some more data points there and not do an overall scanning of the entire phase space.

So, this essentially a phase space plot, where you draw the values of your response with respect to the process variables. So, it is a two-dimensional plot with two variables. If you have three variables, then it becomes a three-dimensional plot and the combinations increases. So, this steepest ascent actually helps us to find out that where is the zone where which we can expect to find the optimum and then you do more experiments on that part of the mind, on that part of the region, bounded by these process variables and apply the second order model.

So, in summary for the steepest ascent, these points on the path, so I can write down the summary of the steepest ascent model as points on the path of steepest ascent are proportional to the magnitude after regression coefficient, and second is the direction of steepest ascent or the direction of the steepest ascent or descent, depends on the sign of regression coefficients, is not it?

So, this is the summary of the steepest ascent process and this is something which helps us to determine that in which path, on which direction depending on the sign of the regression coefficient, this will proceed towards to. So, I hope all of you found this class to be quite useful. In the next class, we are going to talk about the design of the experiments and how we can, depending on the kind of model we are choosing, whether it is a 1$^{st}$ order model or whether it is a second order model, what are the possible design of experiments that can be devised or the minimum number of experiments can tell us to have a more accurate prediction of these regression coefficients.

So, I hope all of you like this class, and this is something which is actually quite relevant for the case of processes where you do not have definitive models or you do not have definitive physics which govern the process phenomena and this sort of Blackbox model what we call as response surface methodology, which is essentially nothing but first order and second order equations, can help us to relate the input and the output.

So, depending on how many number of different process variables you are having it can be single variable to dual variable or triple variable regression. And the more number of unknown variables you have, the more number of unknown coefficients in the regression also needs to be determined. So, this generally works very best for the case of up to 3 parameters I would say. Beyond three parameters, you do not get reasonable, the number of requirements of the experimental data becomes too large and then we generally move towards other methods, for example, neural networks.

So, response surface methodology is very good for up to 3 unknown process parameters. So, we will talk about the design of experiments in the next class, and that will help us to determine that how the experimental data points are determined for the first and second order models. Thank you and see you everyone in the next class.