Computational Techniques
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Module No. # 05
Regression and Interpolation
Lecture No. # 01

Hello, and welcome to the module five of the computational techniques course, what module five is goning going to cover is essentially, what is known as regression, and interpolation. We have perhaps encountered regression right in our high schools, when we started looking at how to fit a straight line to a bunch of data points, and we have done this regression fair number of times. For example, you have several number of data points, and we need to find out the best fit line that passes through these data points; that is what is known as linear regression. Interpolation is another thing again, what we would have done earlier as well, essentially you are given some amount of data say n number of data points. So, those represent discrete data points in continues set. So, if we want the value at any other point between these among these n data points any other point other than these n data points, we will have to use interpolation.

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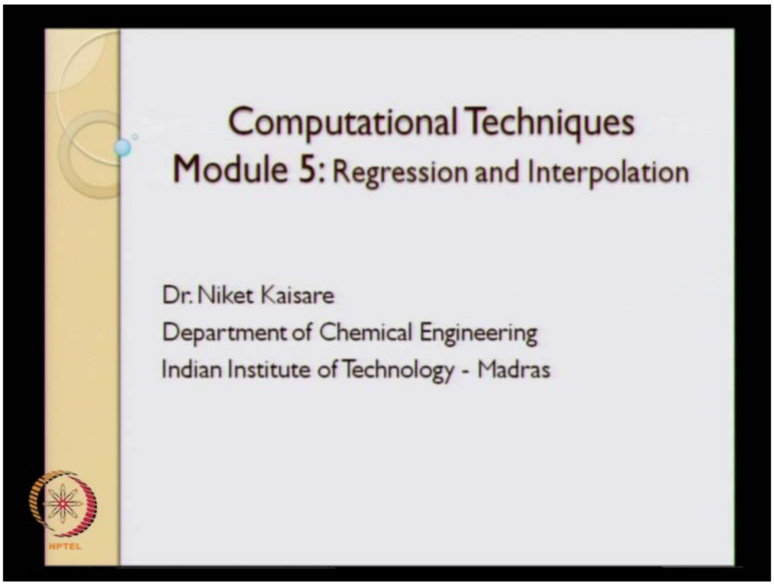

In this particular module is go go through an overview of where regression, and interpolation are going to be used in chemical engineering system systems. And then, we will look at several ways of doing this regression, and then we will continue with several ways of doing interpolation. Each method has it is own advantages or disadvantages or rather more appropriately. It it has a range of applications, where you could use that particular method.

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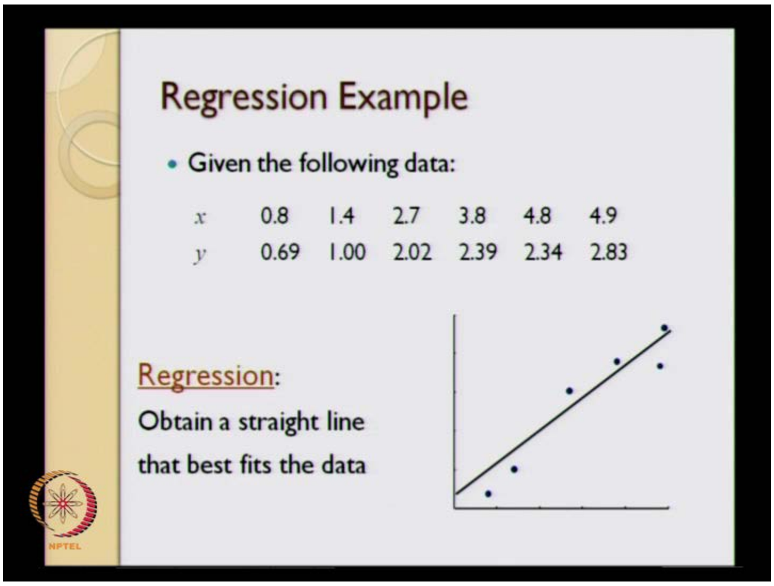

So, let us look at an example. Let us say, we have been given the following data x is the independent variable and y is the dependent variable. And we need to find out a functional co-relationship between the independent variable y, how this particular y relates to this particular x and this is just the data that is given to us. For example, one example could be how that rainfall in the city of Chennai relates to say the temperature that we find are relate to the relative humidity and temperature and things like that. So, just we have an independent variable x, we have a dependent variable y. And we want to find out a functional relationship between x and y that is, what regression is going to be about…

So, what we have done over here is plotted this y against x and these are the six data points. Regression in this particular example is means to obtain straight line that fed best feds the data. In general the regression may we may not necessarily be interested in fitting straight lines. We might be interested in fitting some functional forms to the given data, but in this for motivating examples in the beginning. We will just look at fitting straight lines to to the data.

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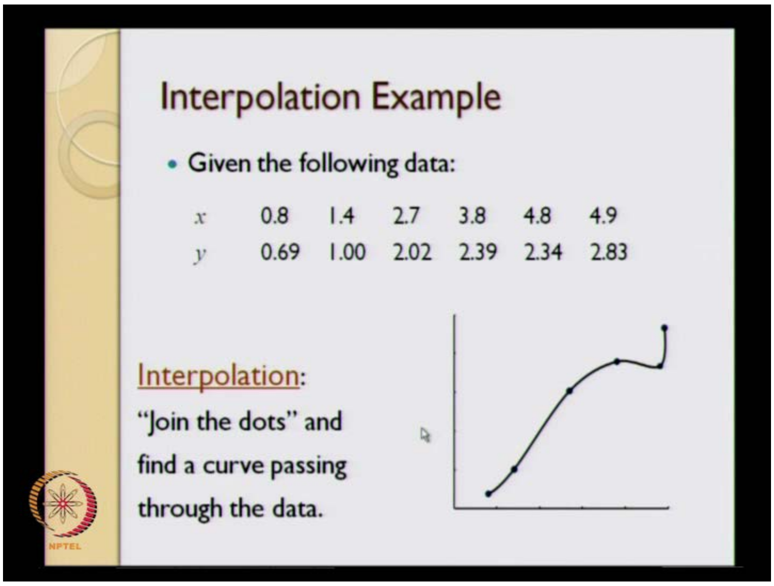

Now, let us look at interpolation case interpolation again, we have been given the same same data as as before and we have plotted the data as before, what interpolation the question we ask interpolation. For example, is given this data let us say, I want the value at x equal to two. So, let us say value at x equal to two, how do I get that particular value. So, in a way interpolation is like joining the dots. It is basically trying to find a curve that passes exactly through all of these points that we have shown over here. If we look at the previous slide and see what we did with regression regression the curve did not necessarily pass through all the data points.

So, for example, none of these data points actually this best fit curves passes through it is just a curve that is going to minimize some kind of an error or some kind of a distance between this point and and the straight line that is what we do in regression on the other hand in interpolation. We will get a straight line the sorry we will get a curve that passes through all the data points that we have so, if we want to find out the value at this particular location. We just get this value by reading of from the curve substituting x equal to two in the equation of the curve. And we will get the interpolated value at x equal to two; we will get the value of y.

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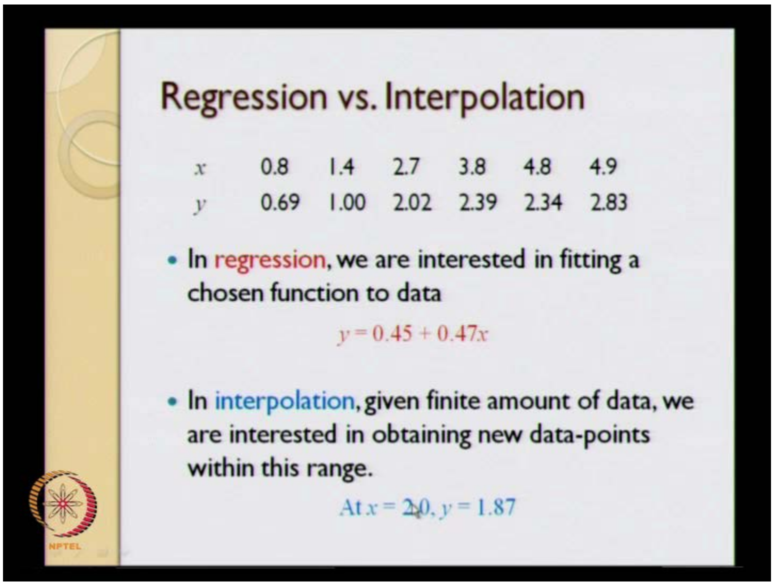

Let us compare regression and interpolation in this particular case specifically what I have done is, I have fitted a best fit straight line to these data points. And in this particular example, I have fitted what is known as spline interpolation both of which we are going to cover in a due course in this particular module. So, in regression we have we fit the chosen function to the data in this particular case, it is a straight line and the equation of the straight line is y equal to 0.45 plus 0.47 x.

In case of interpolation, if given a finite amount of data. We are obtain interested in obtaining new data points within the range again within the range is a very important term over here, because since the data coverage is between 0.8 and 4.9. We will be able to interpolate only within these data points. We would not be able to extrapolate beyond any of these data points. So, what interpolation does is within this these data points. You can, if we are interested in finding the value of the of the independent variable y given a particular dependent variable x we can find that particular value. For example, if we have x equal 2 y will be 01.87. So, this particular point is about one two comma 1.87.

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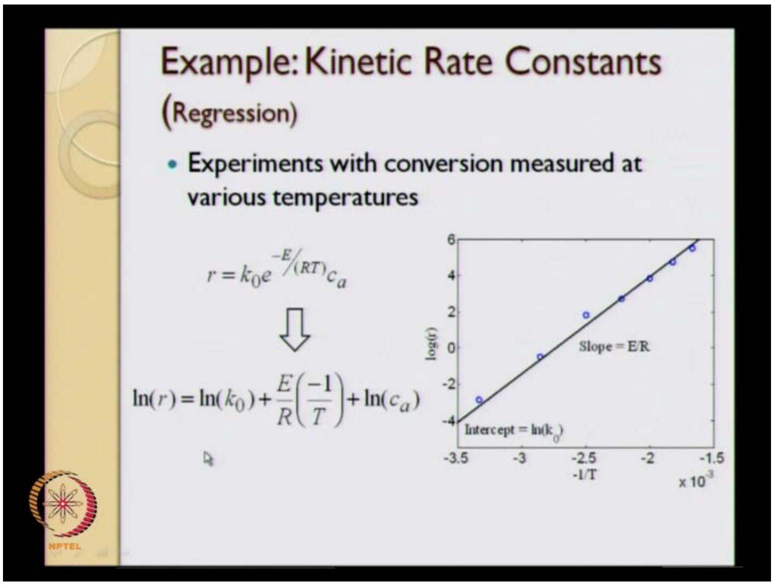

That is what we do in interpolation. Now, let us look at examples, where regression and interpolations are are used and again these are examples these are simple examples these are examples, which you would have done in if some of your courses earlier for example, we have this rate expression. It is a first order rate expression in which the rate depends on the temperature as well as concentration of species a. So, if we carry out this reaction in a batch reactor or say in a continues reactor. And we do that, we run that reaction for certain amount of time and try to figure out the conversions from the conversion that we get we can get the rate, which is essentially going to be the slope of the conversions right in the right before right at the start of this particular experiment.

So, once we have this rate of reaction R and the temperature T basically, what we can do is we can then take a logarithm of this particular function. And once when we take the a logarithm of this this function, we we we will be able to get the k value k value is nothing, but k 0 e to the power minus E by RT and the logarithm of that we will get get to get us log of k 0 and E by R multiplied by minus 1 by T. So, now if we plot log of r as the y axis and minus 1 by T on the x axis what will essentially get is are rather what we should get if this particular functional form is correct is a straight line that passes through the data that we we have over here. The intercept of this straight line is nothing but log of k 0 and slope of this line is essentially E by R.

So, this is an example that we have studied much earlier, while talking about, while finding out rate expression in in chemistry courses some things like that, what we are interested in doing is formalizing the ways in order to get the best line the best line that passes through these points. And we are going to look at a formulation, which is not only going to be finding straight line through y versus x type of data, but when we have multidimensional data as well in that particular case, how do you get the straight line or or any kind of a functional curve passing through the data. So, what we have over here is an inherently it is a non-linear function and we use some transmer transformation. For example, here a logarithm we take in order to transform a non-linear problem into a linear problem. And then we can go ahead and do the regression for this linear regression for this particular example.

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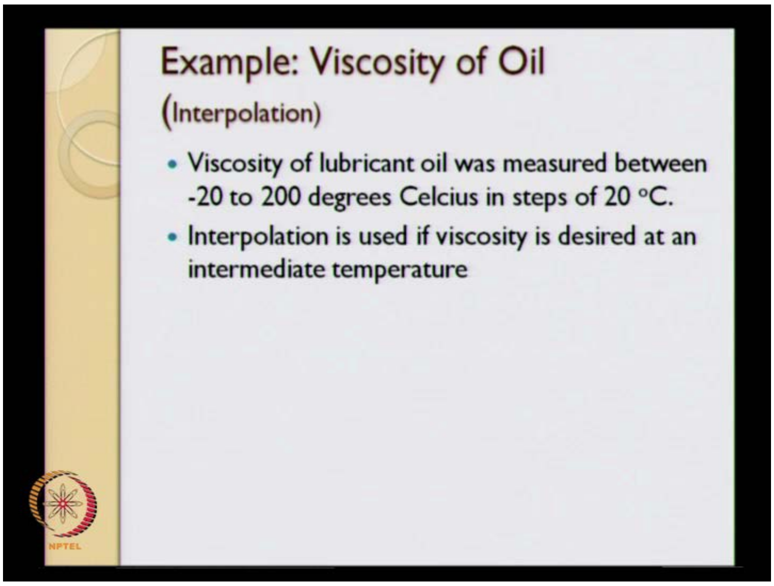

The next example would be interpolation and the viscosity of lubricant oil. For example, will be measured at various different temperatures, but some times the value of the lubricant may not be available at the temperature of of our interest. And if that is the case we might need to use interpolation in order to find out at that particular temperature, what the viscosity of oil is…

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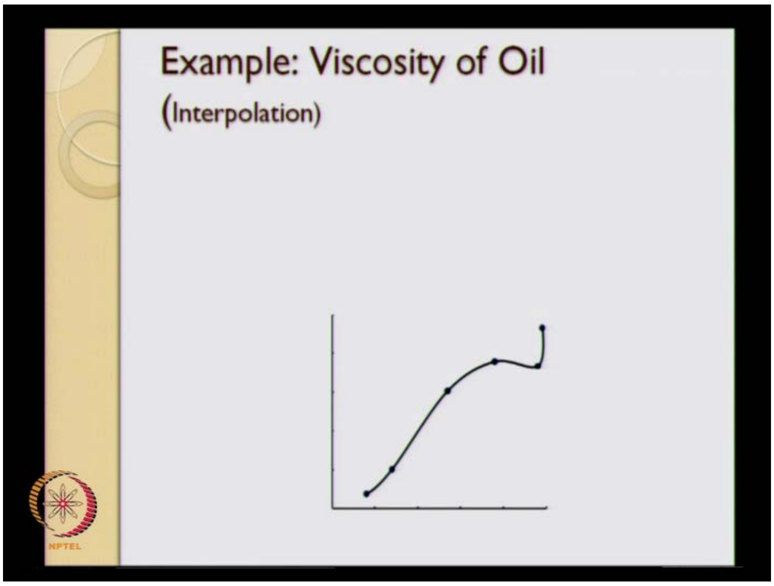

So, just to look at the the example the data that we had previously this is not the viscosity data this is just the same data that we had previously, what we can do is essentially fit all these data fit fit specific type of curves through that through these data points. And one example would be to fit straight lines between each subsequent each successive data points. So, you have a straight line joining this point and this point, you have another straight line joining this point and this point, you have a third straight line joining this points forth one and fifth one.

So, what we have over here is six data points get give us essentially five intervals. And for each of this interval, we fit one straight line that goes through all of and the final curve will eventually go through all of these data point. But this curve that we get finally is composed of five independent straight lines. So, that is one way of doing this interpolation, the other possibility is what is known as spline interpolation. And spline interpolation for example, will fit a curve to each of this subsequent data points. And that that final curve is going to be what is the interpolating curve from, where we can get the data in addition to all of these six data points.

So, for example, the value at x equal to two was 1.87. So, that was just read of from this particular curve.

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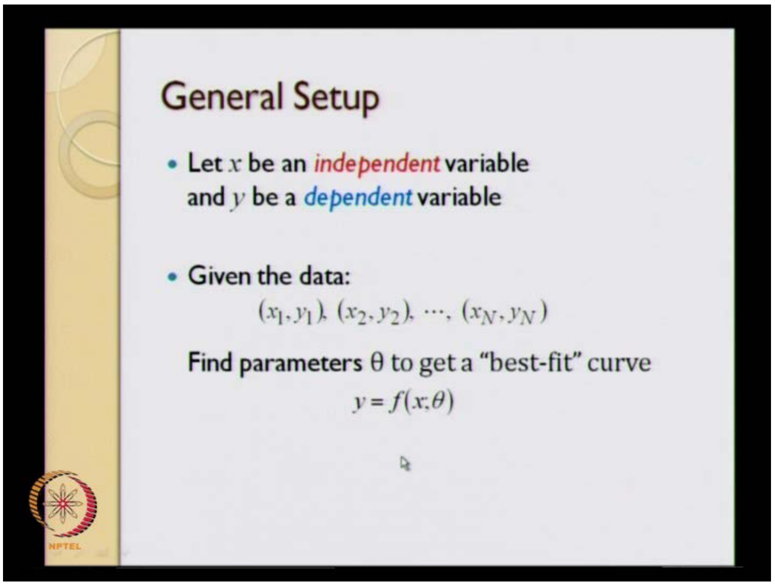

So, that is the difference between essentially interpolation and regression. So, let us now formalize the way of dealing with this interpolation and and regression. So, we have some set of data six data points in this particular case. So, let x be an independent variable and let us y be a dependent variable. And we have been given n capital N number of data points. In this particular case N was six. So, we have been given (x 1, y 1), (x 2, y 2) up to x N y N. We want to find out a best fit curve in some some way or the other on on that curve is given by y equal to f of x semicolon theta, where theta is the set of parameters. So, this is the functional form of that particular curve.

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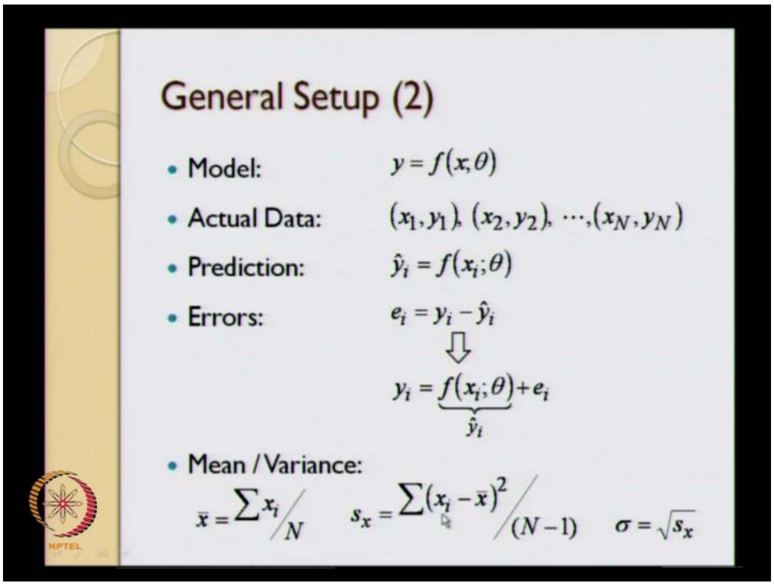

So, the model we will write as y equal to f of x comma theta. So, that is our f x semicolon theta. So, that is the model we are we are interested in we are interested in finding the values of theta that will in some ways best fit give a best fit for y equal to f of x curve. The actual data again to recap consist (x 1, y 1), (x 2, y 2) and so on up to (x N, y N). The prediction is going to be now let us say we we assume certain value of theta. So, we we decide on a function, we assume certain value of theta. Once we substitute the value of x, we will get certain value of the dependent variable y. We call this particular value of dependent variable y with a hat, the hat represents that it is a prediction. Keep in mind that this is the model whereas; this is the prediction from the model. So, what we have done is we have substituted x i over here, and we will get the value of y i.

Now, because there is an error for example, if we look at if we look at this particular curve so, this particular value the x coordinate is x i and the y coordinate for this value is y i. So, if you if you substitute basically x i into this particular equation of this particular straight line, we will get the value of y, which we obtained from the function at this particular point, which is actually different from the actual data that we had. So, this data point will be called y whereas, this particular predicted value is will be called y hat.

So, we have written the prediction equation in the form y i hat equal to f of x i comma semicolon theta. Now there is an error as we we showed in the previous graph there is an error between the true data value and that value that is obtained through the model. And this error is essentially we will write that as e e subscript i and we just take y i on to the other side, we will get y i hat on to the other side. We will get y i which is the the true value from the data is going to be equal to f of x i comma theta, which is nothing but the model prediction of y i plus the error between the true i i and the module prediction.

And what we are interested in doing is we are interested in finding out methods that will minimize these errors. Before going further, we will also just define a few terms from statistics statistics the mean of data is nothing but sum of that data divided by the total number of data points. It is something that we are all familiar with this is essentially the variance of the data variance of data is nothing but square of this standard deviation which is which essentially gives us how the data is spread with respect to the mean x bar. So, how how much is the spread of x i with respect to x bar is what is given by the variance. And sigma is the square root of variance is nothing but the standard deviation.

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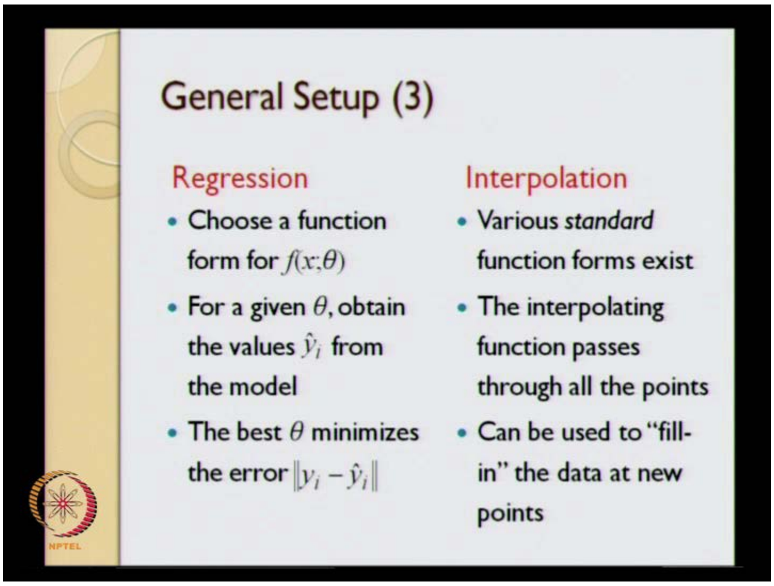

So, again to how is interpolation and how are interpolation and regression going to be different from each other. In regression, what we do is we will choose a functional form f of x. Now, how do we choose the functional form f of x. For example, in the Arrhenius rate rate kinetics the functional form, we choose for excuse me the functional form we choose for the rate of reaction are was nothing but k multiplied by c a and for the rate constant k it was k naught, which is a frequency factor multiplied by e to the power minus E by RT

That is how we choose the functional form form of x for a given value of theta. We obtain the y i hat, which is the module production. And we recursively use some method or we use some kind of a direct method to find out the theta, which minimizes some norm of the error in some way. So, this could be the absolute value of the error sum of the absolute value of the error or it could be the sum of square of error and so on and so forth that is what is going to be our objective is to find out theta that will minimize the error in some form.

As against that in interpolation case, we do not have to choose a functional form there are several standard functional forms that exist and based on the method that we are going to use, we will use one of those standard functional forms for for interpolation. Interpolating function passes through all the data points, which means that the error is going to be 0 for each of the data points. And the the usefulness of interpolation is to fill in the data at new x values whereas, the use of regression is to get a close functional form that can then be used for various purposes. For example, the rate of reaction can be used in order to design cstr or PFR and so on.

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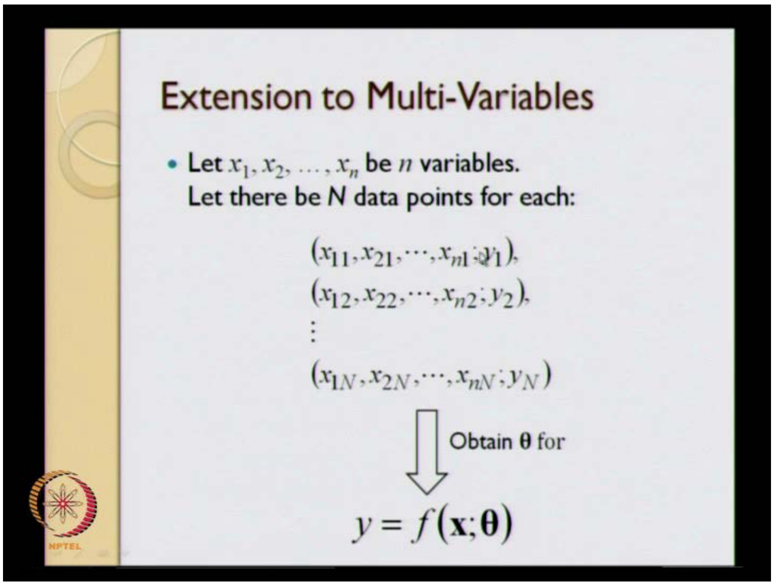

That is the difference between and the silent features of using regression and interpolation. So, after we look at so, initially we look at a single variable case; that means, the output is one variable and the input is a single variable. Next we will extend that particular example to a multivariate case, where x 1 to x n are smaller number of variables and capital N is the total number of data points.

So, we have the data in the form x 1 to x n at data one comma y 1 y x x 1 to x n at data two comma y 2 so on and so forth from x 1 to x n at data N and y N. So, this is what our data would be and our objective in multivariable case. We will be to obtain theta, which is going to be a victorial theta that will give us the best fit for y for a curve y equal to f of x.

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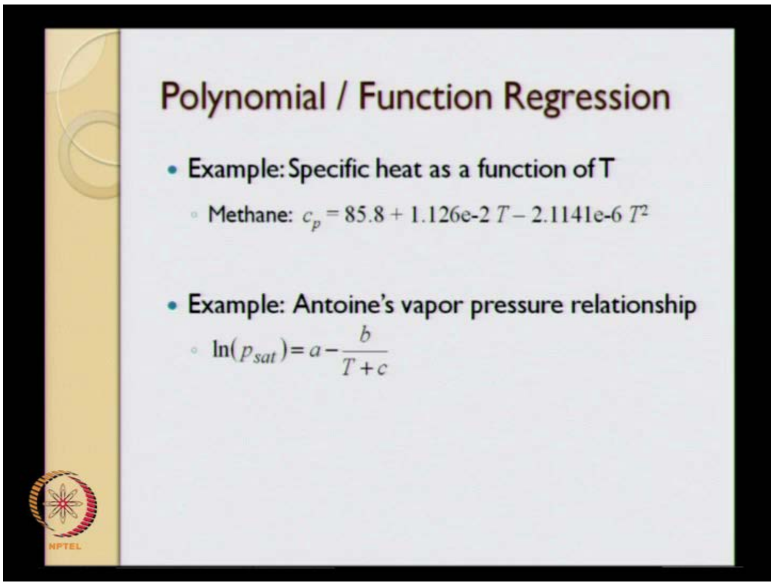

An example of multivariable case is to find this specific heat as a function of temperature. If you go to the NASA's website there is NASA polynomial form of specific heats of several gases and this has been taken from that that that particular NASA polynomial fit. The specific heat of methane the constant pressure specific heat of methane is a given by this particular quadratic function is a 0 plus a 1 T plus a 2 T square as a 0 is 85.8 so on and so forth. So, what we have over here is we are trying to fit a a specific function in order to functional form to the data c p versus T and as we will show later on in this particular module this is an example of linear regression.

Another example is a functional regression, where we want to fit a functional form of this type this is an Antoine vapor pressure relationship log of the saturation pressure is a function of the temperature and a b and c are the three constants in this particular equation. This particular equation as it is formulated is going to be going to require non-linear regression of course, there is an alternative way of formulating this problem also which is going to result in ah linear regression. We will look into that as well how to look do a non-linear regression or functional regression or polynomial regression in this particular module.

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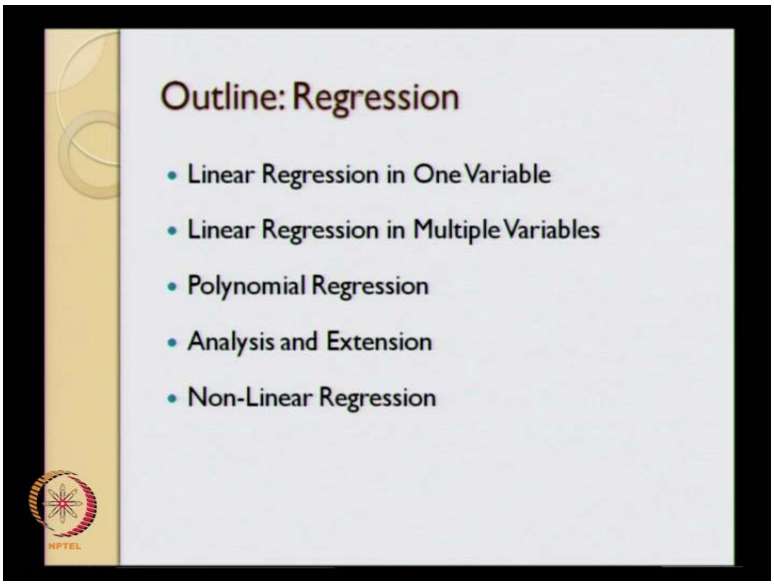

So, to just recap the overall methods that, we are going to use in this particular course. First we will talk about linear regression in one variable, after that we will go on to linear regression in multi variables also known as multi linear regression followed by polynomial regression. We will then analyze these regression methods and look at the extension and then finally, look at the non-linear regression. So, this is the regression part of the of the course. The linear regression is nothing but fitting the curve y equal to m x plus c to the x versus y y data.

But it is actually more than that because for example, we have seen in in one of the earlier slides is we can actually fit a straight line after, we do some kind of transformation to the original function of this type. So, although linear regression per say a single variable case is fitting a straight line to x versus y data it is immensely useful way of doing regression. The next we will we look at is extension to the multi multi regression case, which which is again similar to what we had we had talked about earlier is if y is not just the function of x, but a function of multiple variables.

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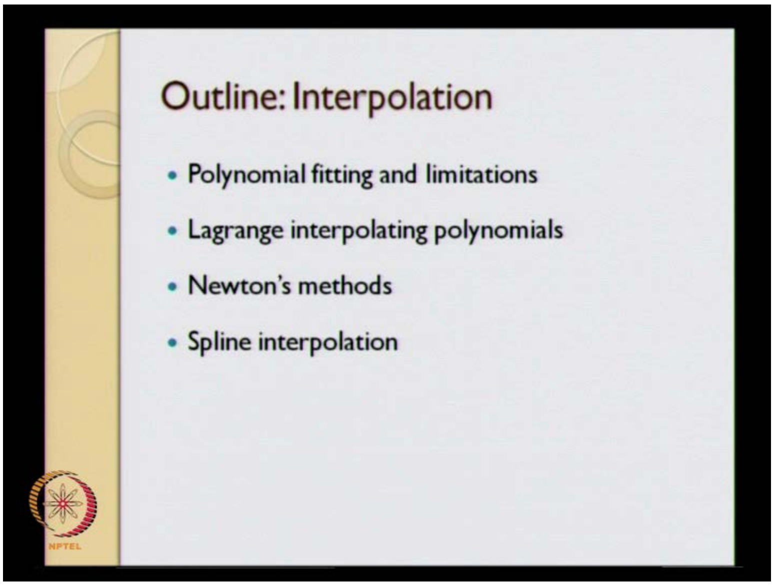

So, that is the overall outline for regression after finishing of regression, we will then go on to interpolation. We will look at a polynomial fitting basically, what we will we will we will say is some of the ideas that we learn from the regression part of this particular module whether we can apply the same idea to the interpolation part. And we will see that we run into certain problems, when we try to do this to do polynomial fitting for in order to get an interpolating polynomial. So, there are alternatives in order to do this interpolation and get rid of some of these limitations and specific methods that we are going to look at is Lagrange's interpolating polynomial and Newton's methods and finally, we will finish of with Spline interpolation.

So, that is the overall over view of our outline of what we are gaw going to cover in this particular module. After doing an overview of what we are going to cover in this regression and interpolation module. We will now just go go and look at the linear interpolation case in single variable and derive the equations, how we can get the values of the slope and the value of the intercept for the single variable case.

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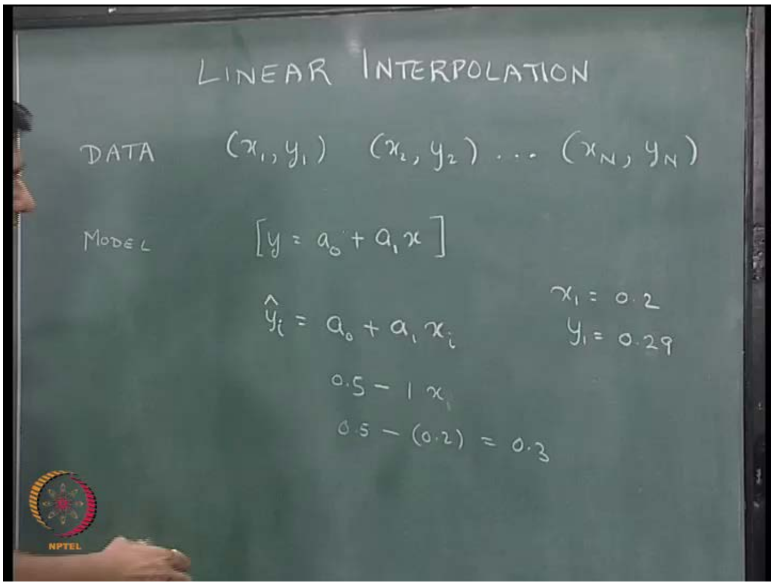

Again for (No audio from 24:49 to 25:00) we have our data (x 1, y 1) (x 2, y 2) and so on up to x N y N. We want to fit a functional form or model form is going to be y equal to a 0 plus a 1 x a a 1 is nothing but the slope and a 0 is nothing but the y intercept for this this particular curve. So, this is the model that we are interested in fitting, when we substitute the value of x i in this particular equation. The value that we will get from the module is we are we are going to call it y i hat is y hat is going to be a 0 plus a 1 times x i. For example, let us cons consider this particular data point. Let us say x 1 value of 0.2 and y 1 value of was 0.3. So, if we substitute the x 1 value of 0.2 and given the values of a 0. So, what I am saying is x 1 is 0.2 y 1 is let us say 0.3 and the functional form over here was let say 0.5 minus say 1 times x. If this was let say the functional form then substituting x equal to x i, we will get 0.5 minus 1 into 0.3 that is 0.2 which is equal to 0.3, which is exactly the same as y 1 that that we had earlier.

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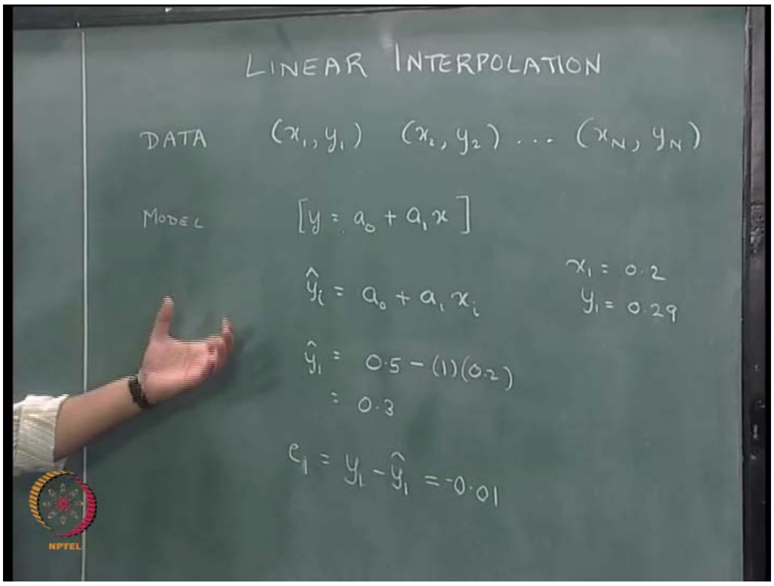

But instead, let us say instead of this let us say the y 1 was 0.29. In that case, when we substitute the values of x x 1 in this particular equation, we will we will get y 1 hat is going to be equal to 0.5 minus 1 into 0.2, which we just obtained as 0.3, which is different from the y 1 hat is different from y 1, this y 1 is data; this y 1 hat is the model prediction. So, the error e i is the difference y 1 multiplied by y 1 hat. And in this in this example that the error is minus 0.01 that is the error in between the data and the model prediction of that particular data.

Previously, when we had taken x 1, and y 1 as 0.2 and 0.3 error e 1 was exactly equal to 0. In general, we need not always get the error to be exactly equal to 0. So, we are going to look at a general case, where the error is going to be certain value e i. So, y i equal to a 0 a 0 plus a 1 x i is as we had said earlier the model prediction.

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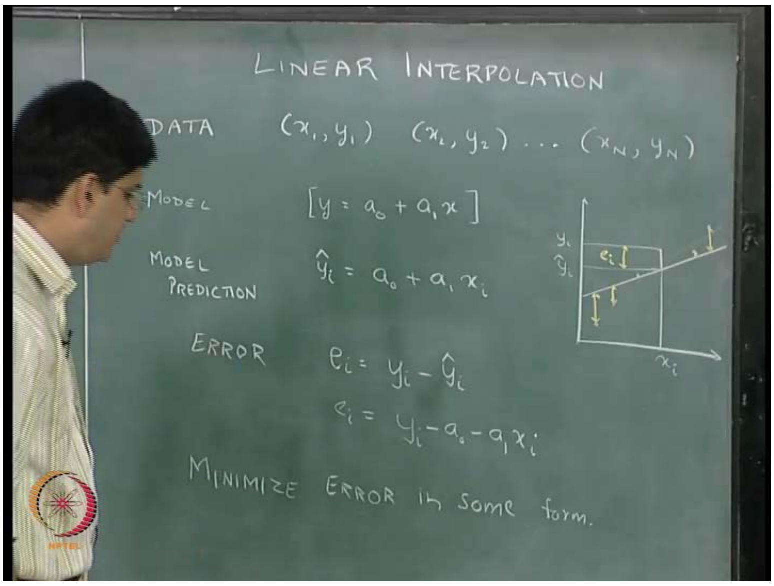

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So, the error is y i minus a 0 minus a 1 x i that is the error for i th point. You will have an error for first point second point and so on up to all all the N points. So, as we had before, let us look at the six data points that we we had we had six data points something like this. So, what let say a given value of for a given value of a 0 and a 1. We will get a straight line as shown over here this clearly is not going to be the best fit line the best fit line is perhaps going to be something something like this. The dotted line is perhaps going to be best the best fit line, but let say this is parti is the particular line that we have we have right now.

In that parti in that case, let us look at graphically what the error e i really means I will just erase the dotted line that I had I had drawn. So, let us look at the forth point forth for the forth point basically this is the value x i this particular value is y i hat, y i hat is the value that we obtain from the module prediction that is by substituting the value of x i in the equation of that straight line and y i is the actual data. So, this particular vertical distance is the e i. So, what we have is essentially for each of the data points, we have this vertical distance as e 1, e 2, e 3, e 4, e 5 and e 6.

So, the objective of any kind of regression technique is going to be for the regression technique will choose to minimize (No audio from 31:19 to 31:27) minimize the error in some form. And the way, we have learnt in so far the way that the thing that works the best with respect to minimization essentially is to minimize the square of error. So, if you were have to minimize the square of error.

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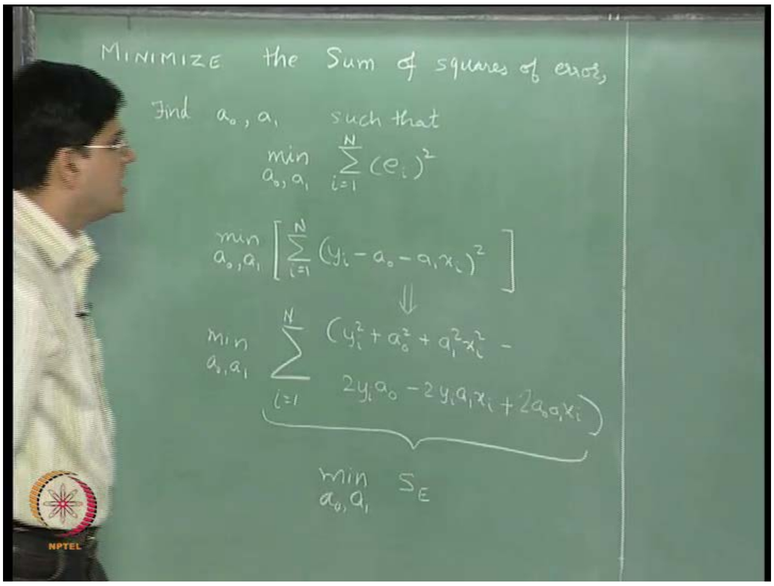

(No audio from 31:53 to 32:10) So, what we want to do is we want find a 0, and a 1 such that…

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So, this is essentially our problem statement is we want find the values of a 0, and a 1; such that the sum of square of errors in the data, and the model prediction of the data is minimized. So, let us substitute the the form that we had for e i in this particular equation. So, we will get (No audio from 33:01 to 33:14) forgot the summation sign over here, summation i equal to 1 to N, y i minus a 0 minus a 1 x i the whole squared. So, this particular term, if if we look at within the summation sign, this particular term is going to expand as y i squared plus a 0 squared plus a 1 x 1 x a 1 x i the whole squared, multiplied by two times this term and this term with the negative sign, multiplied by two times this term multiplied by this term with a negative sign, multiplied by two times this and this term with a positive sign, because there are two negative signs, which which cancel of.

So, this particular term can be expanded as y i squared plus a 0 squared plus a 1 squared x i squared minus 2 times y i times a 0 minus 2 times y i a 1 x i plus 2 times a 0 a 1 x i summation i equal to 1 to N minimize a 0 a 1. Now how do we find the value of a 1 a 0 and a 1 that minimizes this this particular function. So, let us just lo look at the the equivalent problem (No audio from 35:05 to 35:16) to find some x that minimizes g of x the x that minimizes the g of x. We are going to take dg by dx the slope and equated to 0 this will give us either the minima or the maxima for this particular g of this particular value g of x.

So, in this particular case, since it it is a function of two variables. We want to find out this particular guy over here differentiated take a partial differentiation with respect to a 0 and equated to 0 and take a part partial dipre differentiation with respect to a 1 and equated to 0. It is the same problem as we had stated over here, since this is sum of square of errors, we will write this as S E and our problem is to minimize are to find a 0 and a 1 that is going to minimize S E

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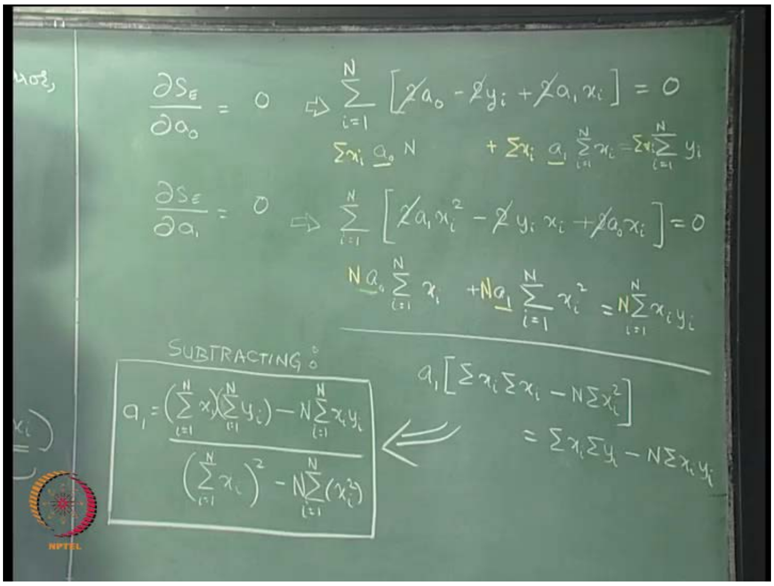


As we we just just said less than a minute back the way we are going to do this is to take partial differentiation of S E with respect to a 0 and equated to 0 take a partial differentiation of S E with respect to a 1 and equated to 0. What we mean by partial differentiation with respect to a 0 means that we hold a 1 constant and differentiate the overall equation. In this case, we hold a 0 constant and differentiate the overall equation. Keep in mind in this particular problem x 1 x y 1 x 2 y 2 and so on up to x N y N are data that have been given since it is data that have been given those for the purpose of differentiation have to be treated as constants.

So, this is a constant term for the purpose of differentiation this term depends on a 0, this does not depend on a 0. So, d by d a 0 of this term will be 0 so on and so forth. So now, we start differentiating this term. Now, keep in mind that differentiation operator essentially is a linear operator. So, you can take the operator with in the summation sign. So, what we will do is, we will keep the summation sign outside summation i equal to 1 to N and let us look at this particular expression over here

Now, we are differentiating with respect to a 0. So, this term will go away there will be 2 times a 0 term this will go away 2 times y y i term 2 times y i a 1 x i this will again go away because there is no a 0 over here and they will be 2 times a 1 x i term. So, the terms that we will we will we will retain in our a 0 in d S E by d a 0 are these these three terms. So, this particular term is going to be 2 times a 0, the second term is going to be 2 times y i, when we differentiate with respect to a 0. So, minus 2 times y i and the third term that we have over here is going to be 2 times a 1 x i (No audio from 39:05 to 39:14) equal to 0, and we will we can cancel of these two's over here.

So, that will be our first equation. So, our first equation is going to be now a 0 is is a value, which does can be taken out of this summation sign because a 0 is one particular value for while while we are trying to do this parti this summation. So, this a 0 summation i equal to 1 to N of 1 is going to lead us to a 0 multiplied by N minus summation of y i i equal to 1 to N plus we take a 1 out of the summation. So, we will have a 1 summation of x i is going to be equal to 0. So, that is the first equation, what we will do is we will take summation y i on to the other side and retain the terms in a 0 and a 1 on to the left hand side. So, we will take summation y i on to the other side and we are summing over from i equal to 1 to N. So, this is going to be our first equation.

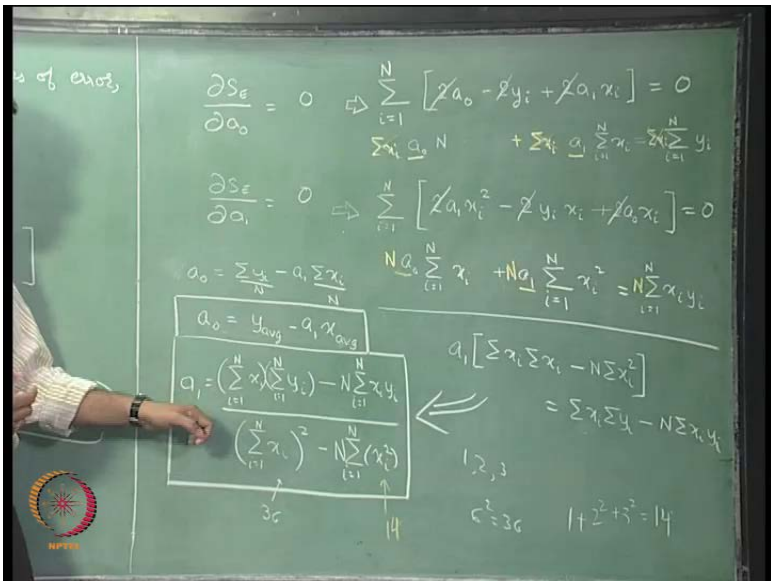
Now, let us look at the second equation. The second equation is going to be obtain by differentiating S E with respect to a 1. Again this particular term is going to vanish away this will be retained and this will be 2 times a 1 times x i squared. This term is going to vanish, because there is no a 1 term over here, this is going to be retained and this term is going to be retained. So again, we will have like before we will have three terms that get retained. So, the first term that is retained is to so, let us let us look at. So, in this particular term, we will have 2 times a 1 times summation of x 1 squared. So, we have again this summation i equal to 1 to N outside and in there we will have 2 times a 1 multiplied by x i squared.

The second term is minus 2 times y i x i and the third term is going to be plus 2 times a 0 x i we are differentiating this term with respect to a 1. So, we will have 2 times a 0 x i equal 0. And again we will discard this this twos so, we will have we will rearrange it again. So, that a 0 is our first term a 1 becomes our second term and so on. So, we will have some a 0 times summation of x i i going from 1 to N. The second term is going to be plus a 1 summation i equal to 1 to N of x i squared and what we do over here is we will take the x i y i term on to the right hand side. So, that is going to be equal to summation x i y i i equal to 1 to N

So, now what we have is we have two equations in two unknowns. The two unknowns are our a 0 and our a 1 these are the two two unknowns and we have two equations and then we can we can solve these two equations we can solve this equation by. So, in this particular equation we will multiply by summation of x i and this equation will multiply by by N. So, multiplication by N I will I will write that using a different color chalk. So, we multiply this entire equation by N and we will get N times a 0 times this plus this equal to N times this. And then in this particular equation, we will multiply by summation of x i. So, we multiply this by summation of x i and this particular also we will have this multiplied by summation of x i.

So now, what we will do is this equation minus this equation will lead us.(no audio from 44:19 to 44:29) So, this and this term will vanish away, we will have a 1 multiplied by summation x i multiplied by summation x i minus N times summation x i squared will be equal to summation x i multiplied by summation y i minus N times summation x i y i.(no audio from 45:09 to 45:22) So, this will lead us to a 1, a 1 is going to be equal to summation x i multiplied by summation y i minus N times summation x i y i (No audio 45:37 to 46:06) divided by summation x i summation x i minus N times summation x i squared (No audio from 46:12 to 46:32) and this that N term over there. So, this is going to be our a 1. And we can use this particular equation to get our a 0.

(Refer Slide Time: 47:02)



So, our a 0 (No audio from 46:55 to 47:04) N times a 0 is going to be so, just ignore this yellow terms over here, because remember this yellow terms had come because we had multiplied this entire equation with summation x i. So, ignoring this yellow terms what you will get is summation of y i minus a 1 times summation of x i is going to be equal to N times a 0. So, we have summation y i minus a 1 times summation of x i. And now, you divide throughout by N, we will have summation of y i divided by N minus a 1 times summation of x i divided by N. If you recognize this this is nothing but average of x i and this is nothing but average of y i. So, a 0 is going to be equal to y i avg minus a 1 times sorry not y i avg y a v g minus a 1 times x avg.

So, this is how we will get the value of a 0, this is how we will get the value of a 1. So, given N data points x 1, y 1, x 2, y 2 up to x N y N. We first find out summation of x i, we next find out summation of y i, we find out summation of x i times of y i and summation of x i x i squared. The difference between for example, this term and this term is that, we square the x i is first and then sum them up whereas, in this particular case we get summation of x i and then square of that that particular summation of x i. So, for example, if we have the value of x i as say 1 2 and 3 then summation of x i squared x i the whole squared is going to be 1 plus 2 plus 3 that is 6 squared that is 36 that is essentially this particular term whereas, this term is going to be 1 squared plus 2 squared plus 3 squared that is 1 plus 4 plus 9 that is 14. So, this particular guy is going to be 14 whereas, this particular guy is going to be 36.

So, that is the difference between summation x i the whole squared and summation of x i squared. Same difference over here also, we find the summation of x I, we find independently the summation of y i and multiply the two, minus the summation of the product x i y i. So, x 1, y 1 plus x 2, y 2 plus x 3, y 3 so on and so forth is what this terms is actually indicates. So, that is what we have for today for linear regression what we will do in the next class is going to be to extend this linear regression in one variable to linear regression in multiple variables. So, not just we we not just the data x versus y, but we have multiple independent variables then how to do the linear regression.

Before, we do that we will take Microsoft excel, and show one example the same example that we saw in the in our power point slides. We will take that same example in order to do get the values of a 0, and a 1. And then we will find out an alternative, which and more general way of doing this linear regression. And then talk about linear regression for functional forms such as polynomial regression or functional regression that is what essentially we will be doing in the next lecture, thank you.