Computational Techniques

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Module No. # 05

Lecture No. # 04

Regression and Interpolation

Hi and welcome to the lecture 4 of module 5. In this module, we were looking at regression and interpolation. In this particular lecture, we are going to move on to interpolation of. For the last three lectures, we have been covering regression; regression is, was basically trying to fit particular functional form or a linear line to the given data. Whereas in interpolation, what we do, is once given the data try to fit a curve that passes exactly through all the data points; instead of trying to fit specific functional form of the curve. There are some standard functions that we employ in interpolation; the objective interpolation essentially is given some n number of data and you want the independent variable value at certain other point, which is not already covered by the data that is given to us.

How can we get that value at the intermediate point? So, the idea is to join the dots in a way, where we have the data points; we will just join the dots and then find out the data value at one of the intermediate points within the data points o; that is the idea behind interpolation.

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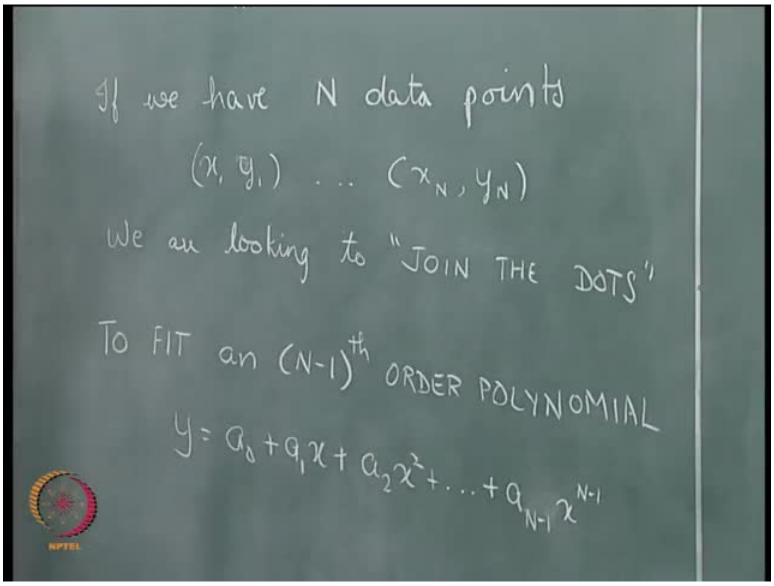

So, the first and straightforward method of doing interpolation is what we looked at in the previous lecture, we saw polynomial fitting. So, if we had N data points, we said that, we can fit up to N minus oneth order polynomial; so, if we fit anything less than N minus oneth order polynomial that it is possible that, we, some of the data will not be perfectly captured by the model, but if we have an N minus oneth order polynomial when we have N data points with us, that name that, particular polynomial will perfectly captured all the data points.

So, the idea is in interpolation or in extension of the polynomial regression to interpolation, is that, if we have N data points x 1, y 1 and so on up to x N, y N. In interpolation, we need a method; we are looking for a method to join the dots that is what we are trying to do an interpolation. The straightforward extension of what we have learned so for, is to fit an N minus oneth order polynomial.

So, the trial polynomial whether that will try to fit will get the form, y equal to a 0 plus a 1 x plus a 2 x squared and so on up to N minus 1 x to the power N minus 1.

So, we have N unknowns, a 0, a 1, a 2 up to a N minus 1; we have N unknowns and we will get N equations, in N unknowns. The equations that we will get is going to be of the formed of some of square errors; if some of square errors is s e, just recollect what we have done in lecture 2 of this module; if s e is the sum of some of square modeling errors, y minus y had. Then the first equation is d s e by d a 0 equal to 0, second equation d s e by d a 1 equal to 0 and so on up to d s e by d a a N minus 1 equal to 0.

So, we have N equations in N unknowns, they will be unique values of a 0, a 1, a 2, at up to a N minus 1, that will give you polynomial N minus oneth order polynomial fit to this data.

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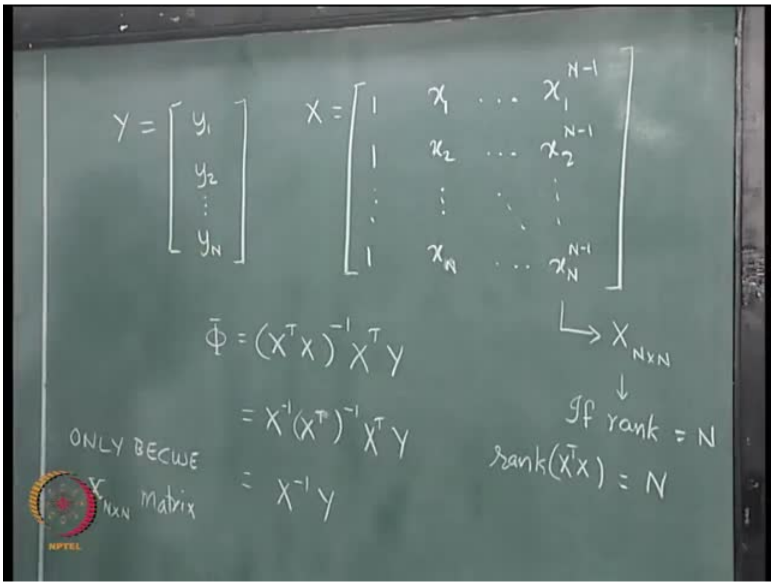

And as we had done before, what we will write our Y matrix as nothing but y 1 y 2 and so on up to y N; our X matrix, if you recall, the first column of X matrix was 1 to 1repeated N minus 1 times that corresponded to a 0, then we would have x 1 x 2 up to x N which correspond to a 1, so on up to x N to the power N minus 1.

So, this is how we will write, we will have this x 1 x 2 so on up to x N and this is x 1 to the power N minus 1; keep in mind, we are fitting an N minus oneth order polynomial x 2 to the power N minus 1 and so on up to x N to the power N minus 1. Just note that, this particular N and this particular N are the same N's; we have N columns and N rows in the X matrix, as the result of this our phi, phi that we had written, so for we had written as X transpose X inverse X transpose Y, that is what we had written. Our phi, now if X has this X matrix, this X is an N by N matrix; if rank of the matrix X is N, then the rank of X transpose Xis also equal to N. And we need the rank X transpose X, so that rank of X transpose X to be equal to N; so that, X transpose X is going to be invertible.

So, if X is invertible and X transpose is also invertible and therefore X transpose X is going to be invertible; this we will be able to write this as X inverse X transpose inverse X transpose Y. Keep in mind, we will, we are able to write this only because X is an N by N matrix and that will give us really phi equal to X inverse Y. So, you get this particular matrix X just invert that matrix multiply with the matrix Y and we will be able to get the values of a 0 a 1 up to a N minus 1; that will give us the perfect fit for the purpose of interpolation.

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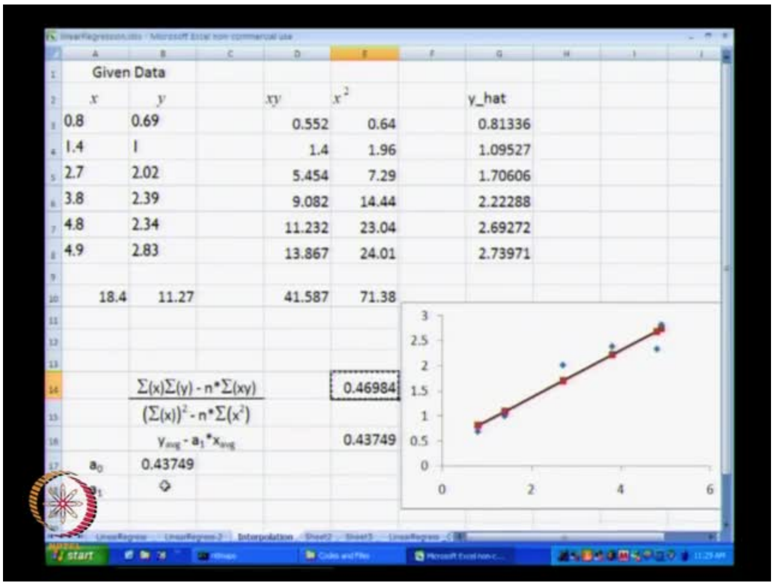

So, what I will do now is, I will go on to excel and we will start off with polynomial regression. Now what I have done over here in Microsoft Excel is pulled up the same work sheet that we used in the previous lecture, to do the linear interpolation. I have just pulled up the same work sheet over here, I will copy this particular work sheet into a separate work sheet and I will copy this into a separate work sheet and we will call it interpolation.

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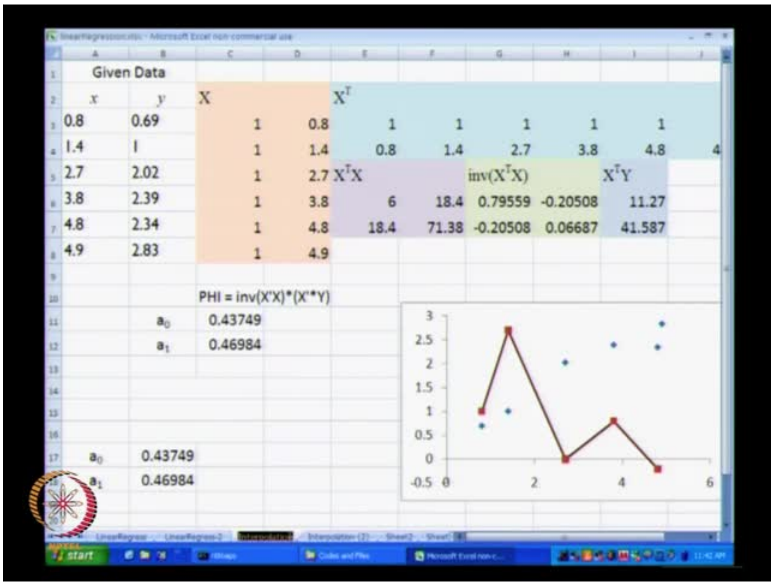

So, this is the data that we were working with; what I will do, is the old values of a 0 and a 1, I will just copy it for our reference, paste special and values, I will get the value of a 0 and the value of a 1, I will copy this also. We will start off by constructing our matrix X. And before, we do that we will just change the font size, so that things are visible to all of you. And change it the usual thing, the Times New Roman font.

The matrix X is, the first row of matrix X contains 1 1 1 1 1 1 repeated N times; N in this case is 6. And the second column not the row the second column of matrix X is nothing but X itself, the various X values. So, I went up here and double clicked on this dot at the bottom and it copied the same values over here. So, this is our X matrix; what we also need to do, is to get the X transpose matrix. So, I will write this as X transpose and format cell superscript; so, we get X transpose, so we will just copy this and paste it as a transpose.

So, what you can do is go on right click and then click on paste special, when you click on paste special this is the overall window that it will open; we want to just paste the values. So, click on the values we do not want to paste the formulae and then there is an option, that we need to switch on transpose and when we click ok basically what we obtain over here is the transpose of X matrix that gets printed over here.

So, this is what we get, now we want to calculate X transpose X; so, X transpose multiplied by X, format this; so, X transpose X, for this we have a function called m mult; that is matrix multiplication m mult. So, when you just start typing it, you will be able to, excel shows you a tool tip, which will tell you what you need to do. So, we need two arrays, the first array is because we want to find X transpose multiplied by X, the first array is going to be X transpose; so that is our first array, the second array, second array is X; so, I will highlight the entire array and I will press enter.

Now, this will just show up on one of the cells, in order to, now X transpose X is a 2 by 2 matrix; X transpose is 2 by 6 multiplied by a 6 by 2 matrix will give it a 2 by 2 matrix; these are things that we need to keep in mind, when using excel that the result of X transpose X is going to be 2 by 2 matrix.

So, when we want to copy this to a 2 by 2 matrix, we will have to highlight an appropriate 2 by 2 area and then click on F2; F 2 allows us to look at the overall equation that we were using. And then control shift enter, what control enter does is, control enter will copy the same formula for each of these cells; what control shift enter does is, it will appropriately modify the formula, keeping in mind that the formula has been written for an array rather than a single cell.

So, again, if you click on f 1 and go for a matrix helpand look at help for Mathmult so I will just click it f 1 and show you, I am not connected to the internet, so do not know whether it will work or not, but let us try to anyway. So, mmult, when you click on mmult, it will show you basically the help for mmult; and then if you just go down and read the help, you will see everything that I have explained over here, explained in this help. So, you can look at this and see for yourself what exactly, I mean, when I am doing the matrix multiplication.

So, now, we have X transpose X, we now want inverse of X transpose X, we want inverse of X and format cells, superscript and this should be Times New Roman.

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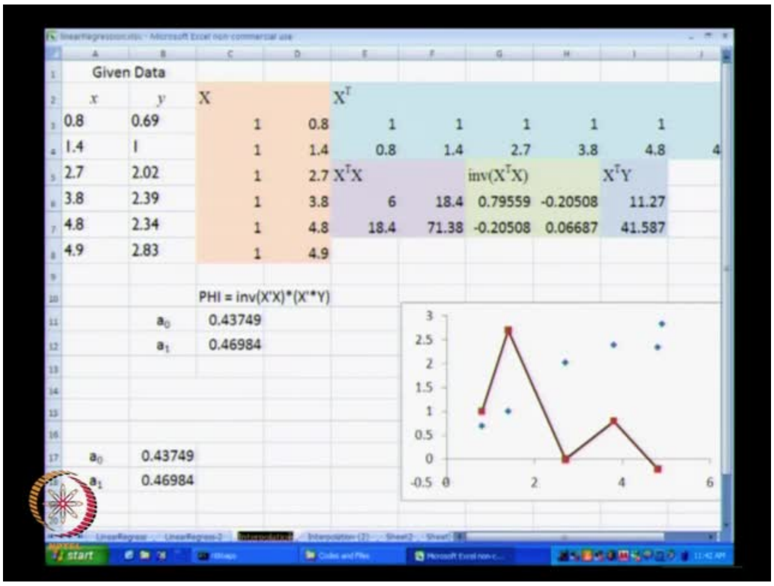

So, this is going to be m, I believe it should be m inverse, inv and m inverse of this particular array close the bracket and press enter and then we can do inverse of X transpose X is also a 2 by 2 array; so, highlight a 2 by 2 region click on F2, control, shift enter and this is inverse of X transpose X. So, that it is clear for us what exactly each array is, I will just highlight this in different colors, should not be putting y hat over here. This is our X transpose and I will highlight this in a different color; this is our X transpose X and I will highlight that in a third color; inverse of X transpose X, I will highlight this with fourth color.

So, now, if we can recall what equation that we had, we had equation as phi equal to inverse of X transpose X multiplied by X transpose multiplied by Y; so what we will do is, we will now compute X transpose multiplied by Y; recall that the matrix Y, Y is a vector which is nothing but what we have over here; so that is what we are next going to calculate. Next we will calculate X transpose Y, right click and say Times New Roman, and right click format cells, superscript and we are done; so, X transpose Y, now X transpose Y is 2 by 6 matrix multiplied by a 6 by 1 matrix, so X transpose Y is going to be a 2 by 1 matrix; so that is going to be equal to mmult that is matrix multiplication of X transpose multiplied by Y and m equal to mmult X transpose; X transpose is this array, Y is this particular vector and this is X transpose Y, the first column of it. Keep in mind X transpose Y is a 2 by 1 matrix; so, we highlight an appropriate size array in excel, click on F2, control, shift, enter and we will get X transpose Y. And phi has to be calculated as inverse of X transpose X multiplied by X transpose Y. And again highlight this and that is going to be equal to phi, I change the font size over here, phi is going to be equal to inverse of X transpose X multiplied by X transpose Y; so, mmult again, this is the first array, this is the second array, close this, press enter highlight the 2 by 1 array, click on F2 and press control, shift, enter.

So, this is the result of a 0 and a 1, our phi matrix that we obtained from this particular method of X transpose X inverse X transpose Y and if we compare it with what we had obtain in the previous lecture in this particular module; we see that in the previous lecture of this module, we had obtained the same value of a 0 and a 1.

So, the objective of this particular exercise was to show that this method inverse X transpose X multiplied by X transpose Y is going to give us exact same result, as we had earlier; that was really the only intention of this particular exercise. So, having done that, now let us go to the interpolation part; interpolation part is where we will built the matrix X which is going to be a 6 by 6 matrix X; and using that particular matrix, we will compute our phi which is going to be a 0, a 1, up to a 5, using just inverse of X multiplied by Y.

So, this is where, I will construct our matrix X; so, what I will do is perhaps just copy this this particular file; once again create a copy after interpolation and this one I will call it polynomial regression what we had done earlier and this I will call this interpolation.

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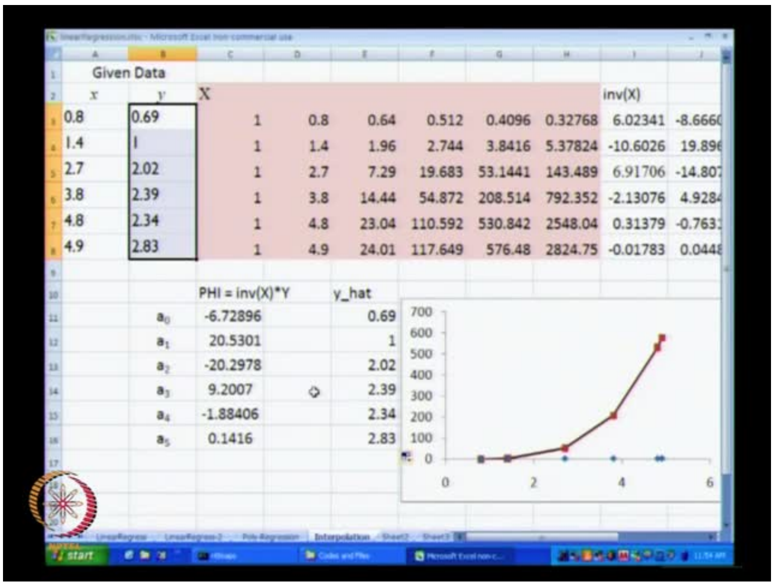

Now, what we need, we do not need all of this, I will just delete it, no fill. So, this is our matrix X, the matrix X will be 1 1 1 1 1 1 then x 1, x 2, up to x N; then we will have x 1 squared equal to x 1 to the power 2, x 2 square and so on; then we will have x 1 to the power 3 x 2 to the power 3 and so on; we will have equal to x 1 to the power 4 and finally to the power 5.

And we will highlight this entire thing and have it the same background. So, this is our matrix X1, so the first column is 1's, the second column is X's, the third column is X squared, the fourth column is X cube, the fifth column is X to the power 4, and the last column is X to the power N minus 1. So, this is our X matrix, our Y vector is just what we have over here. And our phi in this particular case will not just be a 1, a 2, but instead it will be a 0 to a 5; so, format cells, some of the cells are merged, so I will unmerge those cells. And just drag it a 4, a 5 and I will just delete this, this as we had seen gets change to nothing but inverse of X multiplied by Y.

So, what we need to do is to compute inverse of X and again I will increase the font size over here equal to MINVERSE and select this entire array, press enter, and now go ahead and I will expand this.

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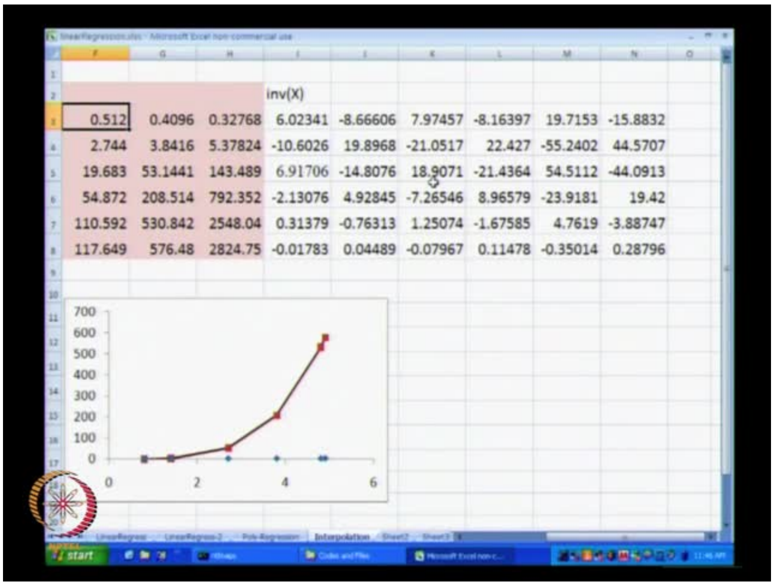

So, select a 6 by 6 array over here, so I have selected 6 rows 2 3 4 5 6 columns, press F2 and then press control, shift, enter and this is now going to be our inverse of X. And our phi is nothing but inverse of X multiplied by Y mmult, function mmult and we have to choose the 6 by 6 array which is inverse of X, in that is what I am doing over here, the vector Y

So, mmult of the inverse of X, Y, we will give us the first value of, that is a 0; we then highlight the 6 rows of the phi vector, click on F2 and then control, shift, enter and what we will get is really, so what I am doing over here is changing the font size.

So, what we get now is a 0, a 1, a 2, up to a 5, so the equation of the polynomial is going to be a 0 plus a 1 x plus a 2 x squared plus a 3 x cube plus a 4x to the power 4 plus a 5x to the power 5. So, let us see what our y hat are going to be, y hat is going to be nothing but a 0 plus a 1 multiplied by x plus a 2 multiplied by x to the power 2 plus a 3 multiplied by a cubed plus a 4 multiplied by x to the power 4 plus a 5 multiplied by x to the power 5.

So, we have a 0 over here, a 1 x plus a 2 x squared plus a 3 x cube plus a 4 x to the power 4 plus a 5 x to the power 5; Microsoft excel found an error, so let us look at this F2.

So, a 0 plus a 1 x plus a 2 x square plus a 3 x cube plus a 4 x to the power 4 plus a 5 x to the power 5. Remember what we did earlier, so if we drag and drop this downwards, what is going to happen, is really, what we will end up getting if we drag and drop this downwards, is instead of a 0 plus a 1 x it will be this value plus this value plus this value and so on, as a result of this we have to put dollar signs for all of our a 0, a 1, a 2 and so on. So instead of C11, will have to put C dollar 11, C dollar 12, C dollar 13, C dollar 14, C dollar 15, C dollar 16.

And now when we drag it down, we will essentially get our y hat; now, when we check our y hat and compare it with the actual values of y; observe what we find is that y hat and the actual values of y are one and the same; we are getting exact same values of y hat as we got for the value of y. So, what happens over here is that, this particular polynomial fit is going to exactly lie or exactly pass through all these points; that is what we get in this particular case, what I will do is, I will just get the overall curve for this particular, now that we have this out of way.

So, this is y hat, now what I want to draw is, I want to draw a curve a between x equal to 0.8 and x equal to 4.9; so, I will take new values of x and new values of y hat ,is what I will take over here; so, x is a 0.8, 1.0, 1.2 and so on.

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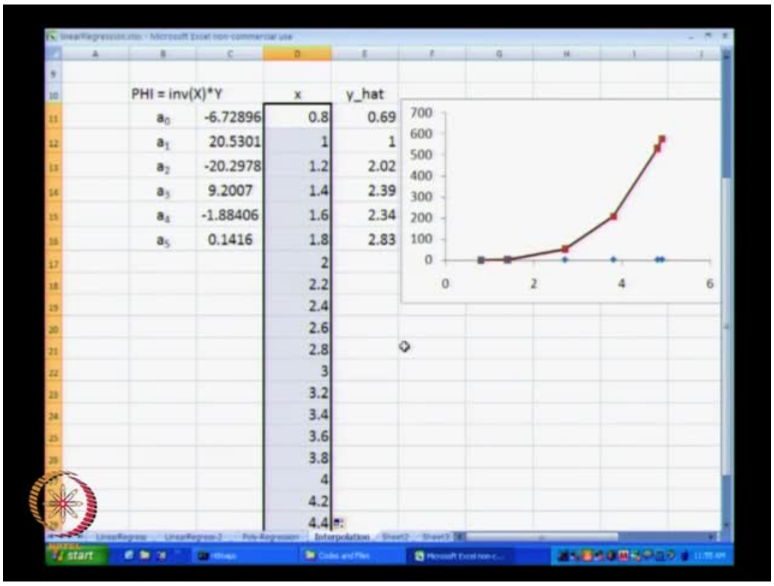

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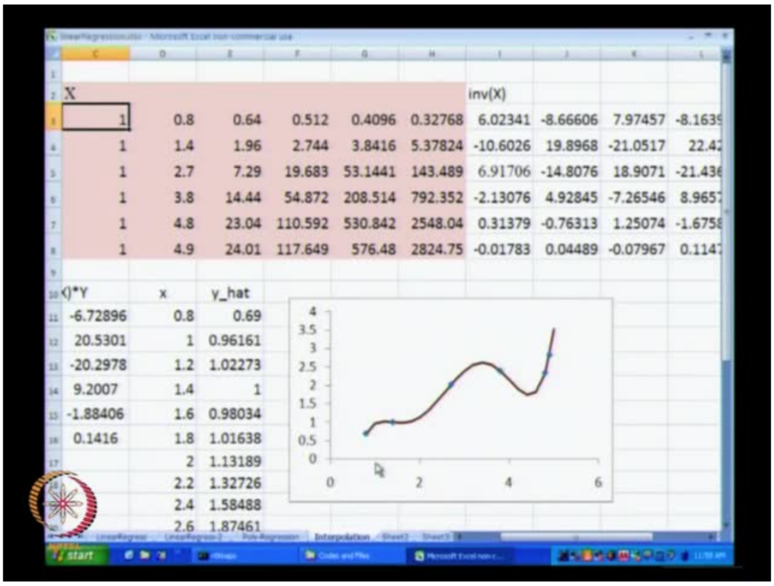

So, I will just select this and drag on until a reach 5 and y hat all I need to do is, just drag, all I have to do is drag these guys over here and my equation will be recomputed. Now, let us see what our equation is, our equation is a 0 plus a 1 multiplied by this x plus a 2 multiplied by this x squared plus a 3 multiplied by this x cube, so on and so forth;

that is our y hat, I will delete these values, I will click on this and double click at this particular edge.

So, this is our x, this is our y hat and I will plot this on this particular curve that we had over here; I will take this value move it here, take this value and move it here, and I will just format this data series to remove the blocks; so, the marker options is no marker that format data series go to marker options, I do not want any marker over here. So, this is the curve, now what we will do is, just expand this particular data and just expand this over here.

So, let us look at what we got true interpolation, and this, the blue dots where the original data points that we had, and this polynomial this fifth order polynomial fit is what I shown by the red curve. If you see the fifth order polynomial fit, although this fifth order polynomial fit exactly passes through each of these six points, six data points that we had; we clearly, it does not do a very good job of following all these data. For example, you will see that this particular data beyond this point is almost flat however in order to fit this particular polynomial, this fit goes to a value much lower than that and then comes back up.

So, we are sure whether this particular interpolating function that we have gotten is a good function or not; for this example, actually the problem was not very large, simply because this was a 6 by 6 matrix X of this sort. 6 by 6 matrix is really the largest value of X that the largest size of the matrix X, that we need to go for, if we want to do polynomial interpolation. What we see in this particular example is that, while polynomial interpolation works, polynomial interpolation is not necessarily a best case situation to have; for example, if you take an eighth order polynomial fit, we will not be able to get a good polynomial fit, simply because the matrix X becomes a very poorly condition.

As a result of this, and again this is not something I am going to demonstrate in these lectures, but the one thing that you can see with, which becomes immediately obvious why this is a problem is one part of, the matrix is of order one whereas the other part of the matrix is of order 1000; this itself does not, mean much, but this is kind of a reason why this particular overall matrix becomes very yield conditioned, the matrix X becomes very yield conditioned.

So, we did the polynomial interpolation part, just for the sake of completeness just to show that this is one possibility that one can use in order to do interpolation. What we will, now look at is several methods, which use certain known functional forms for doing this interpolation. So we will start off with Lagrange interpolating polynomials go on to Newton's interpolating polynomials.

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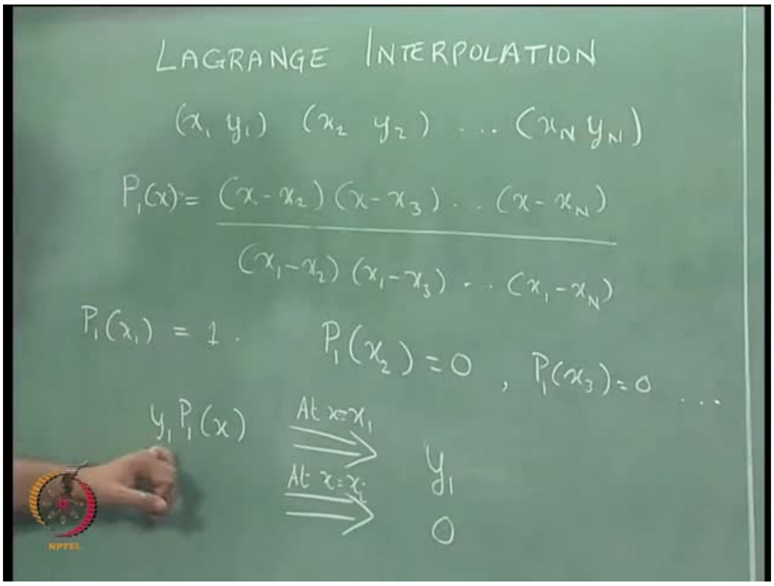

So, let us now talk about other ways of doing interpolation, the multi linear regression in the polynomial regression does work; however it is not a good method in order to do interpolation. So, we will look at several alternatives to do interpolation and the first alternative we will look at is, lets define a polynomial; so, again we have the data x 1,y 1 x 2, y 3, and so on up to x N, y N.

Let us define a function and let us call that particular function as P 1; let us define P 1 equal to x minus x 2 multiplied by x minus x 3 and so on up to x minus x N divided by x 1 minus x 2 x 1 minus x 3 and so on up to x 1 minus x N; let us define this as P 1 x.

So, now, if we substitute x equal to x 1 in this particular equation, so, you substitute equal to x 1 in the equation, we will get this as x 1 minus x 2 divided by x 1 minus x 2 multiplied by x 1 minus x 3 divided by x 1 minus x 3 and so on up to x 1 minus x N divided by x 1 minus x N.

So, the value of P of 1 at x equal to x 1 is nothing but 1. Now, let us see the value of P 1 for x equal to x 2; for x equal to x 2, we will have x 2 minus x 2 as 0; so, it does not matter what we get in rest of the numerator, because this guy is 0 and none of denominators are 0; we will get P1 of x 2 equal to 0, P1 of x 3 equal to 0, and so on.

So, if you look at the interpolating polynomial P 1, then P 1 is equal to 1 when x 1 equal to 1; when x 1 is going to be equal to any of these data points P 1 is going to be equal to 0.

Now, let us consider a value y 1 multiplied by P 1, y 1 multiplied by P1 x, at P 1 equal to x 1, this particular value is going to be y 1; this is an important property that we need to keep in mind.

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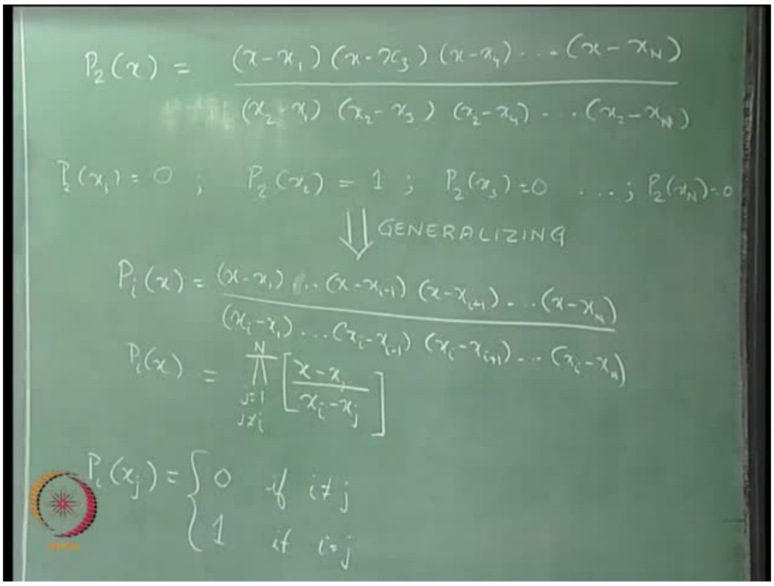

So, y 1 multiplied by P1 x, at x equal to x 1, is y 1 at all other points its equal to 0. Just as we have P 1, let us construct another polynomial P 2; so, P 2 of x we will write as x minus x 1 multiplied by x minus x 3 and so on up to x minus x 4 and so on up to x minus x N, whole thing divided by x 2 minus x 1 multiplied by x 2 minus x 3 multiplied by x 2 minus x 4 and so on up to x 2 minus x N.

So, this is our P 2 of x when we substitute x equal to x 1 in this particular equation, then P 2 of x 1 is going to be, we have this x 1 minus x 1 term as 0, none of the other terms are 0 in this particular polynomial; since, there is an 0 in the numerator and no 0 in the denominator P 2 of x 1 is going to be 0.

Now, let us look at P 2 of x 2, P 2 of x 2, we will have x 2 minus x 1 which will cancel from here, x 2 minus x 3 will cancel here, x 2 minus x 4 which will cancel here, and so on up to x 2 minus x N which will also cancel; so, P 2 of x 2 is going to be equal to 1, P 2 of x 3 is going to be equal to 0, and so on up to P 2 of x N equal to 0.

So, now you are generalizing all these polynomials, a polynomial P I, we will write that as x minus x 1 and so on up to x minus x i minus 1 multiplied by x minus x i plus 1, we are missing the term x minus x I, the only term that is not present over here is x minus x i, this thing divided by x i minus x 1 and so on up to x i minus x i minus 1 x i minus x i plus 1 and so on up to x i minus x N.

The short hand notation for writing P i is nothing but P i is product of j going from 1 to N j not equal to i x minus x j divided by x i minus x j; that is the short hand notation for writing P i of x. So, this, these are, what are known as the Lagrange polynomials, the property of Lagrange polynomials is P 2, for example, P 2 of x 1 was 0, P 2 of x 2 was 1, P 2 of any other x we are between x 1 to x N was equal to 0. As a result the property that we have is P i of x j is going to be equal to 0, if i not equal to j and is going to be equal to 1 if i equal to j. So, this is a very important property that, that we have for the Lagrange polynomials.

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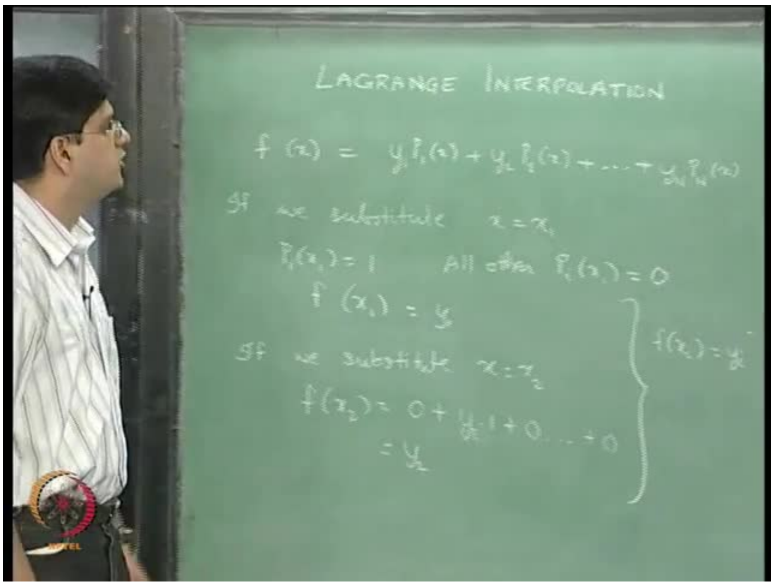

Let us, now construct f N minus 1 of x as y 1 times P 1 x plus y 2 times P 2 x plus so on up to y N time P N x; let this be the function that we have obtain. Now, what happens if we substitute x equal to x 1, P 1 of x 1 is equal to 1, all other equal to 0.

So, our f N minus 1, this represents the N minus one th order function polynomial function form that we have fit to the data; f N minus 1 of x 1 is or we will just drop the subscript N minus 1, for sake of simplicity, so f of x 1 is nothing but y 1 multiplied by 1 plus 0 y 2 multiplied by 0 plus y 3 multiplied by 0 and so on and so forth; so, f of x 1 is nothing but y 1.

So, what if we substitute x equal to x 2, if we substitute x equal to x 2, our f of x 2 is going to be 0 plus y 2 multiplied by P 2 of x 2 which is 1 plus y 3 multiplied by 0 plus y 4 multiplied by 0 and so on; so, f of x 2 is also equal to y 2, so on and so forth when we generalize this, what we will find is f of x i is going to be equal to y i. What does f of x i equal to y i, mean, f of x i equal to y i is simply means, that this particular function f passes through all the points x 1, y 1 x 2 ,y 2 x 3, y 3 so on up to x N, by N.

So, that is what the Lagrange interpolating polynomial is going to do; so, just to summarize what we get with Lagrange interpolating polynomial, I will just erase this and summarize.

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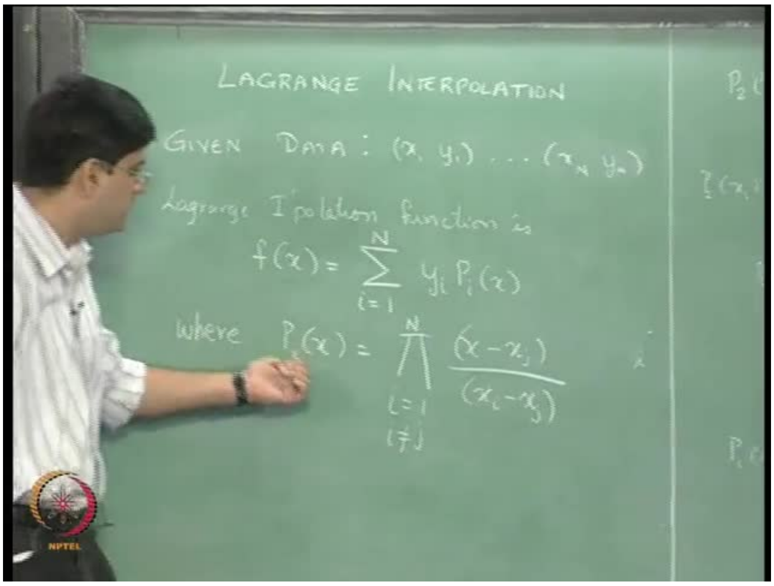

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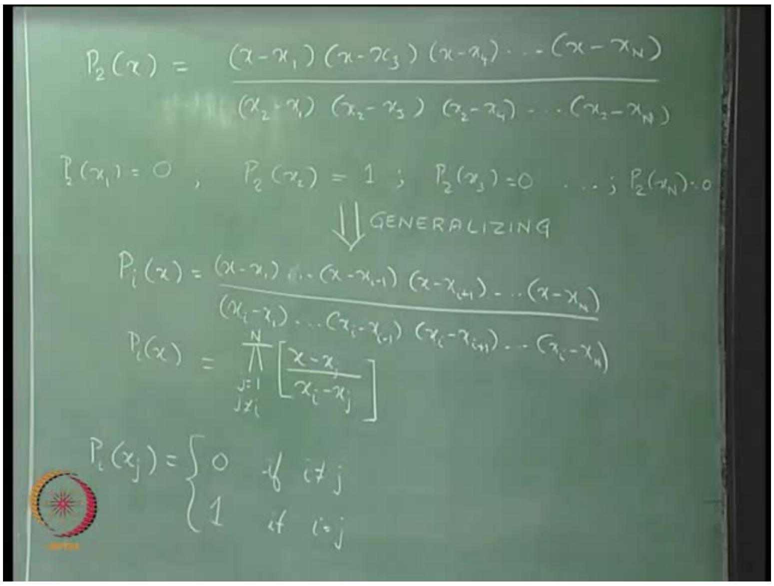

So, this is what we have done with respect to the Lagrange interpolating polynomial function, Lagrange interpolating function f of x is nothing but y 1 P 1 plus y 2 P 2 plus y 3 p 3 up to y N p N and our P 1, P 2, P 3 are essentially given by this particular formula. If we go on to this part of the board, this is exactly the same formula that we had derived; what it means is P i is nothing but product of x minus x 1 x minus x 2 up to x minus x N without having the term x minus x i and in the denominator we have x i minus x 1 x i minus x 2 and so on up to x i minus x N, except the term x i minus x i.

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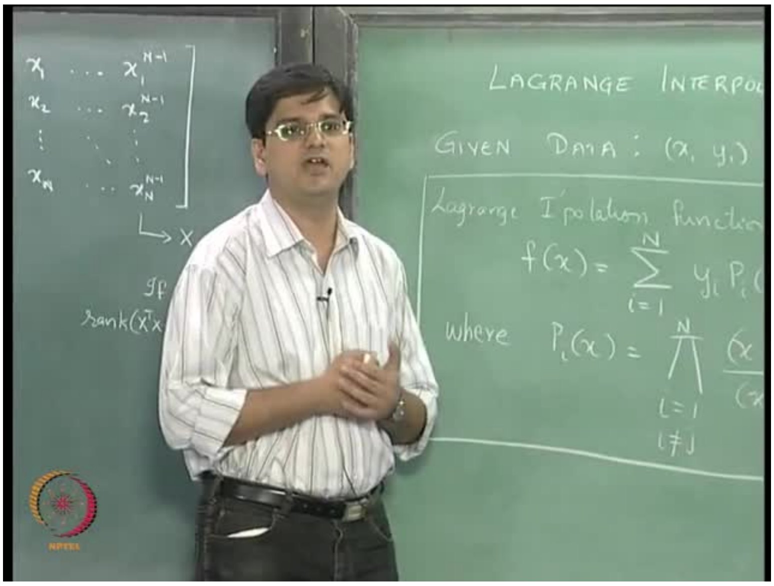

So, this is what the polynomial p 1 means and this is the short hand notation of Lagrange interpolating polynomials. So, this is what we have time for in this particular lecture; what we have covered in this lecture is we started off with a polynomial regression polynomial regression, we solved one particular example for polynomial regression to show that the polynomial regression method gives us exact same result as the linear regression method. We solve that particular problem in Microsoft excel and what we found over there is that the solution inverse of X transpose X multiplied by X transpose Y gives us the same results as we had obtain in the lecture 2 of this particular module

After that we extended that idea for polynomial fit through fit and N minus oneth order polynomial to N data points.

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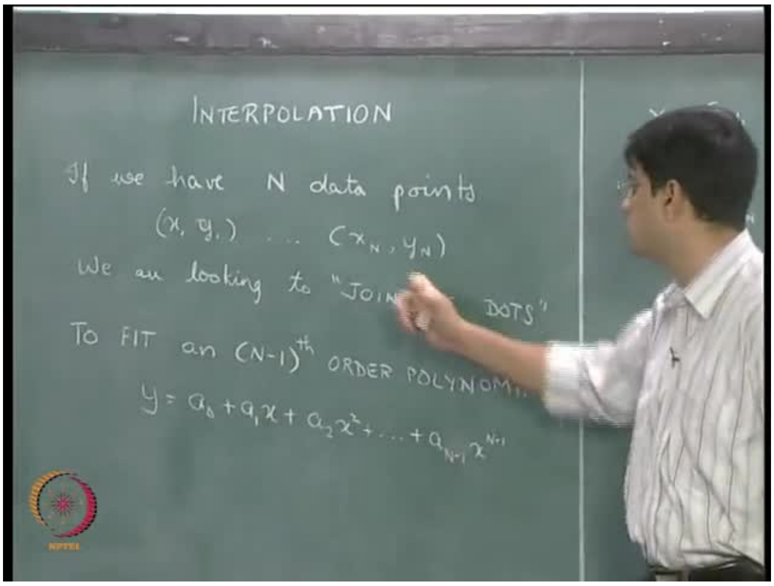

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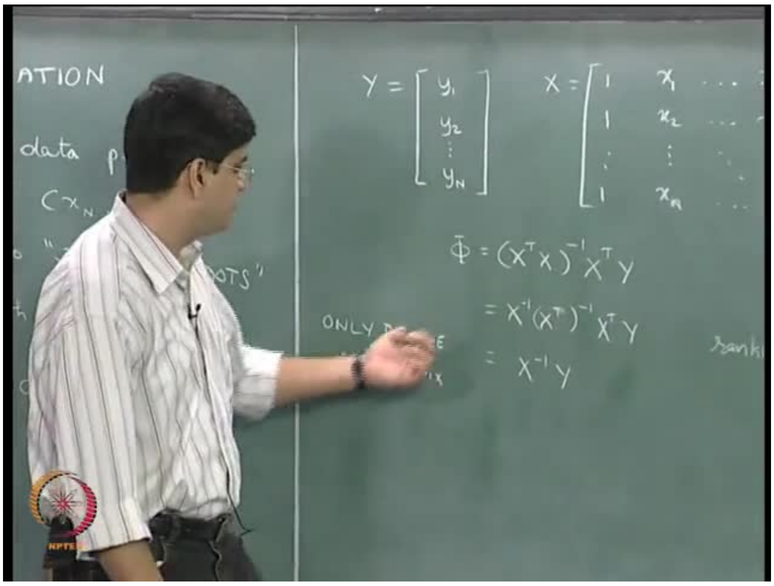

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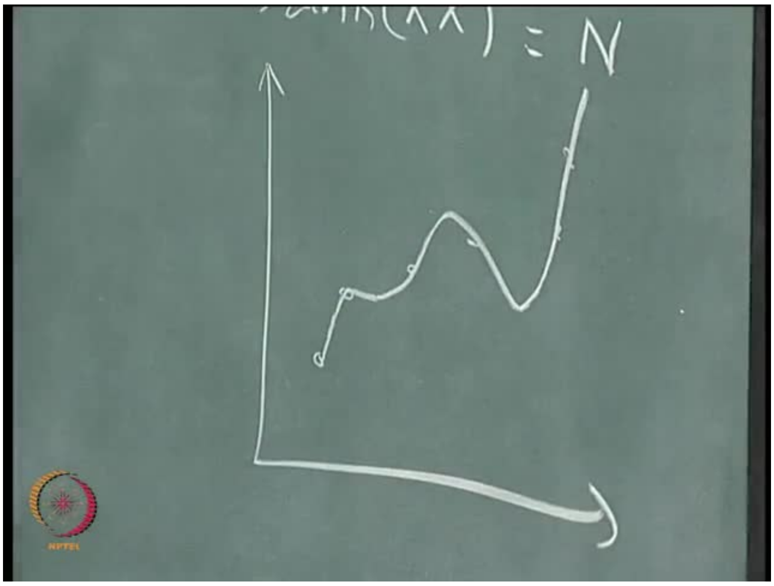

So, we fit and N minus one th order polynomial to N data points, using the equation of this sort phi was we obtain was equal to X inverse times Y. Then we went on to Microsoft excel and in Microsoft excel, we found out that this particular function indeed gives us a curve that passes through all the data points; the curve that went through the various data points, that we obtain look somewhat like this, I am just drawing that as cartoon.

So, this is what we observed when we used Microsoft excel. And finally we covered Lagrange interpolating polynomials, where f of x was given as summation of the data y i multiplied by the polynomial P I, where polynomial P i had a form of this type. So, that is really what we have covered in today's lecture.

The next lecture would be the last lecture, in this module and in that lecture, I will cover what is known as Newton's interpolating polynomial.

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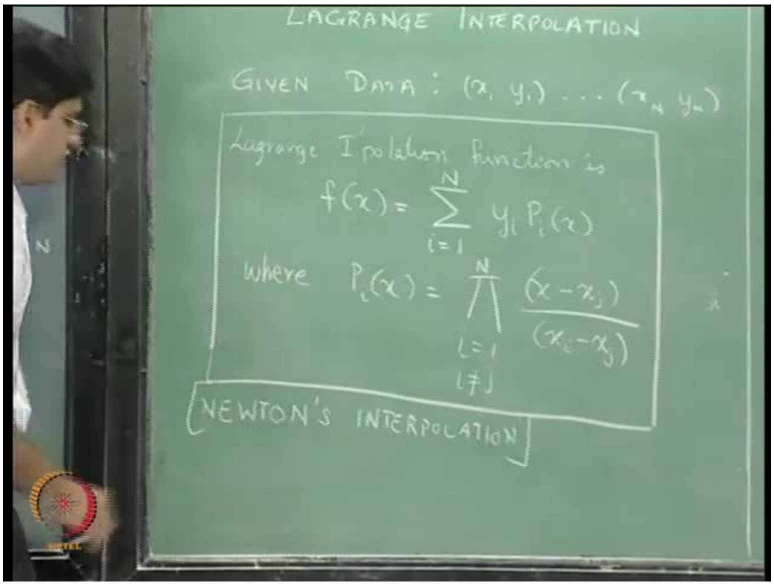

And specifically we will cover Newton's forward difference, Newton's backward difference and Newton's divided difference formula and after at the end of that, I will just summarize what we have done in regression and interpolation that is what we will do in the next lecture. Thank you.