Selected Topics in Decision Modeling
Prof. Biswajit Mahanty
Department of Industrial and Systems Engineering
Indian Institute of Technology, Kharagpur

Lecture - 25
Numerical Methods for Unconstrained NLP

So, for our course Selected Topics in Decision Modeling, today we are in our 25th lecture. So, if you recall we were discussing non-linear programming right. So, today we are going to discuss the Numerical Methods for Unconstrained NLP.

So, now the numerical methods for unconstrained NLP you know you have seen that there are several methods in which we actually solve non-linear programming problems. So, let us see where the numerical methods actually come in.

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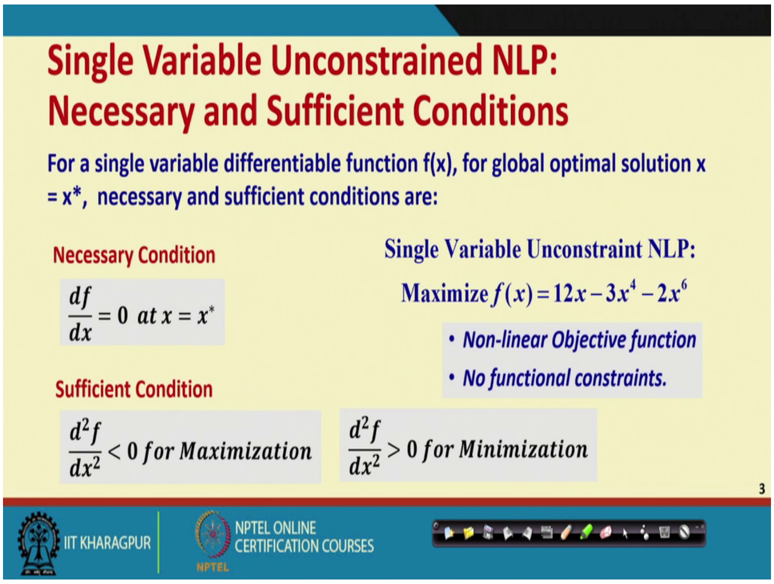

So, see if we have let us say single variable unconstrained non-linear programming problem, say we have a single variable differentiable function f x, and to find out the global optimal solution x equal to x star, we have the necessary and sufficient conditions.

So, you know the we take the first derivative put it equal to 0 at the given point that is the optimal point, but that alone is not sufficient no that is necessary condition. The additional constraint that we have to check for sufficiency, is whether the second derivative value is I it is less than 0 that is for maximization and greater than 0 for minimization. So, this is the simple thing that we have already seen.

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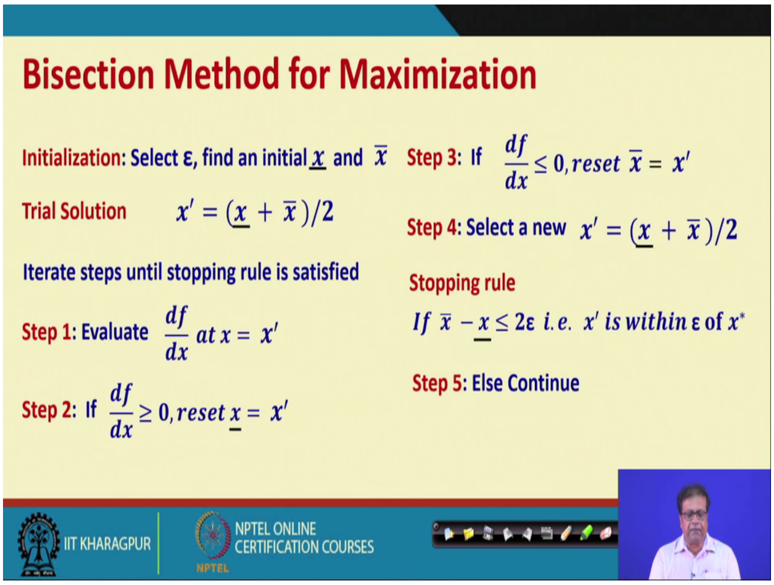

Then sometimes if the second derivative is difficult to obtain and also the first derivative is available, but you know not easy to solve, then we have a method called the bisection method and we have discussed it that method basically meant that we take 2 values x you know underline and x bar. And you know they should be between 2 extremes. So, that the extreme point lies in between that you have to ensure that these are the two extreme points one on one side and the other on the other side.

Then through the method of bisection and by evaluating the gradient and really noting whether the gradient is on one side or the other based on which we keep you know the averaging those two values and looking at which side it is on and then reducing the search space and finally, obtaining the extreme point. So, that was the bisection method.

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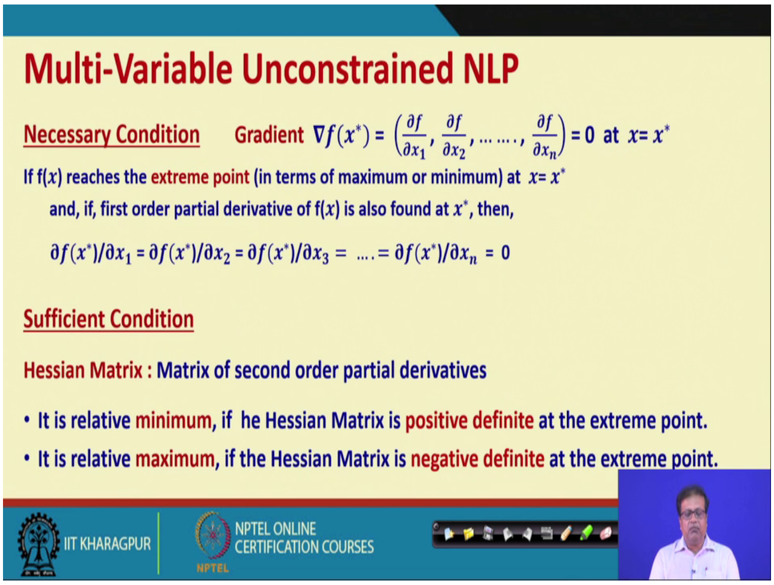

But moment we had multivariable then you know it is not easy to obtain the first or second differential, that time we had two more concepts we have introduced that was the concept of gradient and the concept of Hessian matrix.

The concept of gradient is actually these are all first order partial derivatives, we equate them to 0 at the x star, which is our maximum or minimum that is an extreme point. But then additional the sufficient condition is that, the second order partial derivative that is the Hessian matrix, you know that matrix should be positive definite for the relative minimum and negative definite for relative maximum is it alright.

So, when will take that Hessian matrix and we find the eigen values, they will actually determine the you know the positive definiteness or the negative definiteness of the matrix.

So, this far we have already seen.

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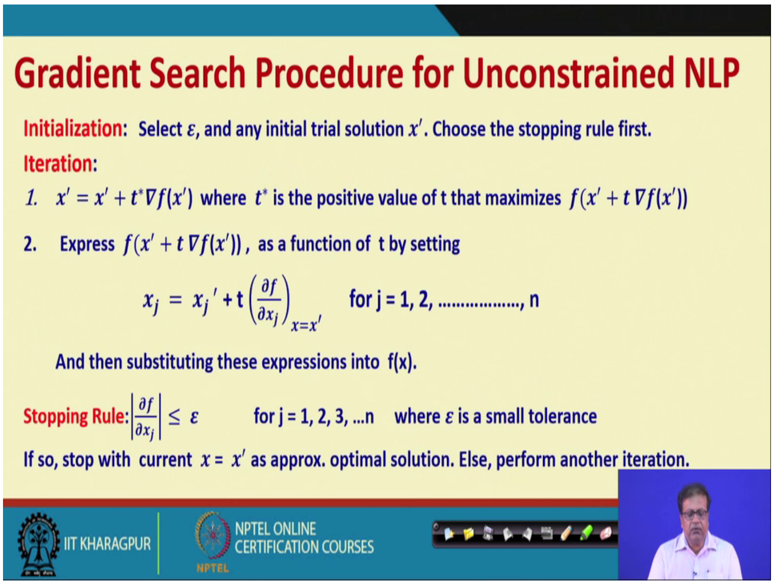

Now, there was another very important method that was the gradient search procedure, they are the real advantage is that we really do not need the second that is the Hessian matrix to be computed. So, if we know the concavity or convexity of the you know the function as the case may be, concavity for maximization then you know we take the iterative step that, x dash equal to x dash plus t star the gradient of the function at the given point. And you know keep finding that starting from a point x, I mean trial solution x dash you know move towards the gradient.

The essential idea is that if we are having a maximization problem, then as you move on the gradient should go up right; with increasing gradient that means, the increasing function value move towards the extreme point and keep modifying your trial solution till you reach almost at the extreme point. So, that was the gradient search procedure is all right.

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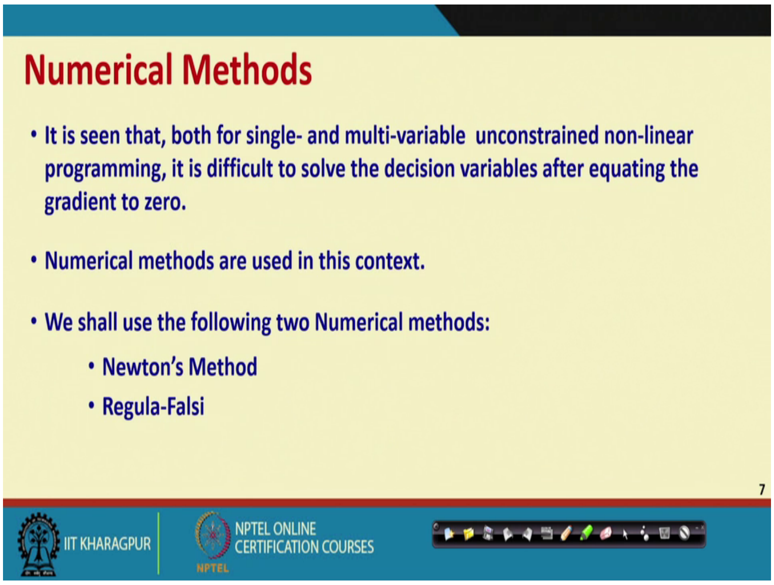

Now, sometimes we have what is known as the numerical methods also. So, supposing we equate the f dash x that is the first order derivative to 0, but then it may not be easy to solve that particular resulting equation because it may be having higher order terms right. So, what we can do? We can make use of numerical methods. So, in these particular lecture we are going to discuss two such methods; the Newton's method and the Regula-Falsi right.

Once again why do we need this numerical methods, this numerical methods are required to solve unconstrained non-linear programming problems, particularly when we equate the gradient to zero, but then the resulting equation is of higher order and you know we need to it is difficult to solve directly. So, let us see the procedure.

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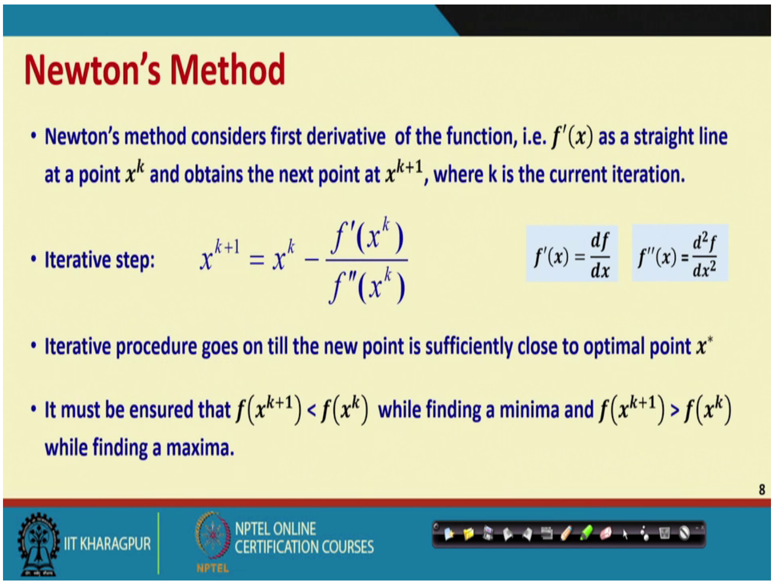

So, really the procedure is like this that, we consider the first derivative of the function that is f dash x f dash x as a straight line, at a given point x k and then obtain the next point at x k plus 1 where k is the current iteration. So, what we need to do? We need to find out the first derivative and we need to find out the second derivative at that point this is all right. So, we take a trial point x dash k, and then find out the first derivative and the second derivative and you know these two are helping us to iterate from a given point to the next point.

So, that is that is the Newton method and then we have x k plus 1 value you know and x k plus 1 equal to x k minus f dash k x k by f double dash x dash k where f dash x is our first derivative and f double dash x is the second derivative right. So, that is the first process iterative procedure and what we should ensure? We really should ensure that the function value is really decreasing, if we are finding a minima and function value is increasing if you are find a maxima.

So, it may so, happen that you know if it is not happening obviously, the process has come to a point where it is not helping anymore right. So, that is the Newton's method.

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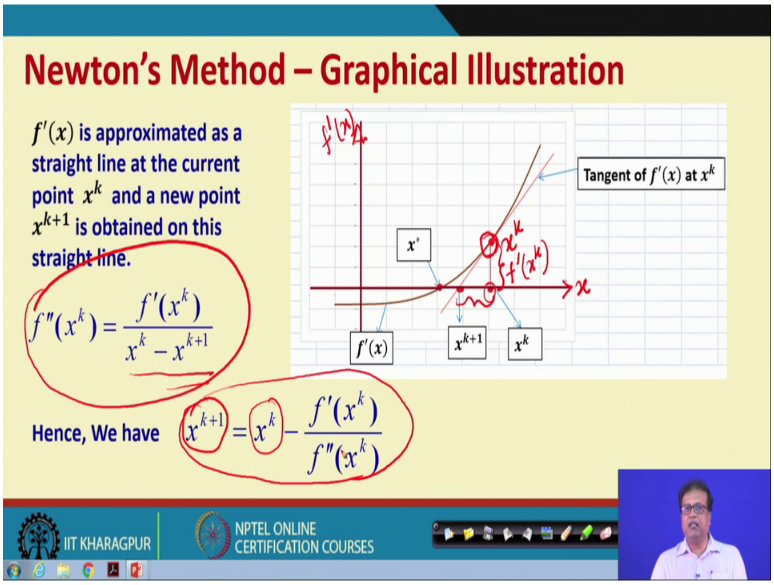

Now, let us see an example or before that let us look at the how exactly it is happening. So, supposing we plot a f dash x. So, you know this side is x and this side is the function. So, see this side is our x and this side is our function, that is f dash x right. So, let us say this is our plot now assuming just arbitrarily so, that let us say this is where our x star that is the optimal point lies.

So, what happens you know if I take a given point say what is this point? This point is our x k that is our trial point. So, actually this is our x k value at this point because this side is x. So, this is our x k value.

Now, if I take the gradient you know tangent of this f dash x and then take the slope that is nothing, but f double dash x k is it not? Because that is the second derivative because this line is first derivative f dash x, and if we take it slope at a given point x k ah; obviously, that should be our second derivative. So, that is the equation written here that is f double dash x k is f dash x k my x k minus x k plus 1 you know.

So, this is our new point x k plus 1. So, this side is you know what is this value x k minus x k plus 1 and this side is our f dash, because this is f dash value at this point this much is our f dash x k value that is the functional value. So, this is can be the way by which we can define the f double dash x k.

So, a little manipulation you know you can find out that x k plus 1 because x k minus x k plus 1, take it that side is f dash x k by a double dash x k and then just rearrange the terms and then we get the new iteration value is the old iteration value minus first derivative by second derivative at that point is it alright.

So, I hope you understood the method how exactly this Newton's method really works. So, if you have understood the method, then let us go ahead and solve problem and then see how exactly it works.

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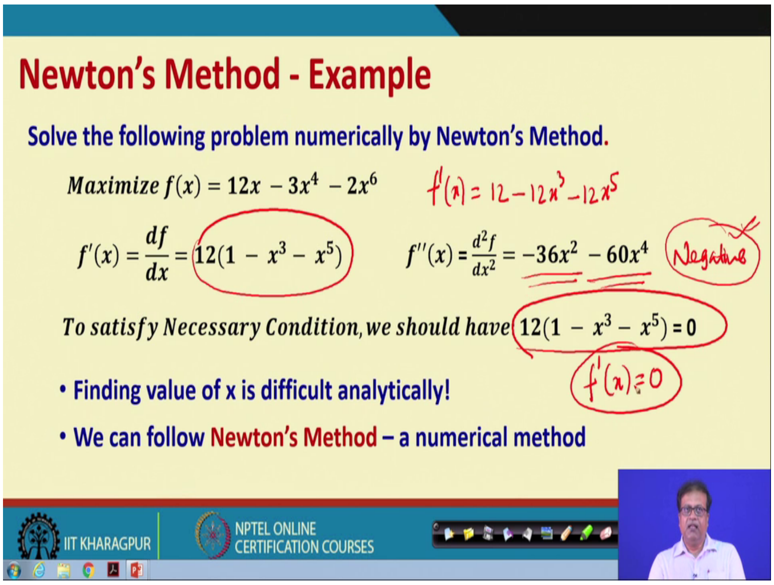

So, here is our problem that solve numerically the optimal point, suppose we have maximize f x 12 x minus 3 x to the power 4 minus 2 x to the power 6. So, at a given point if I take the derivatives, that is the first and the second derivative what will be our first derivative? The first derivative will be you know equal to f dash x if you take then 12 x it should be 12 minus 3 x to the power 4.

So, 12 x 2 cube, 2 x 6 minus 12 x to the power 5 is it alright. So, the same thing is written here, 12 into 1 minus x cube minus x 5. So, if this is our first derivative what will be our second derivative? Look here minus 12 x cube so, minus 36 x square and minus 60 x to the power 4 alright. So, that is how we have found the first derivative and the second derivative.

Now, to satisfy the necessary condition, we have to put f dash x equal to 0 right so, that should be our extreme point. Now in the question is that this particular value is not easy to find out, what should be the value of x at this point because we have put it equal to 0. So, finding the value of x is difficult analytically.

So, that is where we are trying to find out through Newton's method the numerical method. Not only that we have to ensure see one thing is ensured already that the this one is a negative quantity. Can you see that? That whatever be the value of x x the x square and x to the power 4, they are positive so, since we have minus 36 x square minus 60 x to the power 4. So, these has to be a negative quantity.

So, since the second derivative is negative, that actually ensures the concavity of the curve; that means, we have an extreme point which is a maxima alright. So, that we have already ensured. So, after we have ensured that, now the question is that what is the value of x if I put f dash x equal to 0 that is our real challenge now.

Now, let us see how it actually happens.

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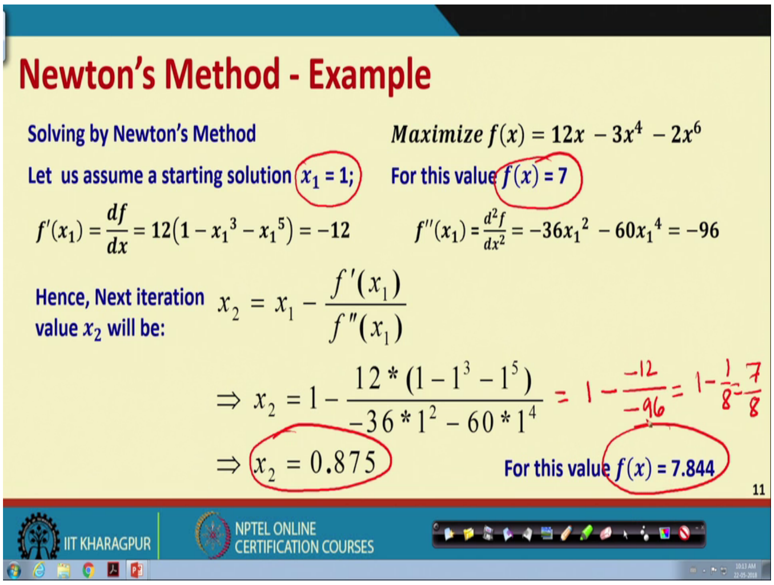

So, what we do we find the first derivative at this point which is 12 into 1 minus x 1 cube, minus x 1 to the power 5. So, it comes to minus 12 right and what is f double dash x 1? So, it will be minus 96 for a given point. See we started an arbitrary point x 1 equal to 1 right. So, suppose we arbitrarily start at a given point, now for that particular point the f x value is a went the question is why do we start with 1? Because first of all we see that by putting 1 we at least get a positive value and if we by looking at the nature of the function, if I would have put 2 ah; obviously, the value would have been negative. So, we have to have a good starting point that is an important thing to begin with.

Now, we find the first derivative and we find the second derivative and then we can iterate and find out the next value of x 2, which comes to 1 minus you know the f dash x by f double dash x. So, that is equal to 1 minus minus 12 by minus 96. So, 1 minus 1 by 8 equal to 7 by 8 right. So, that is what you get and which is 0.875.

So, this is our next iteration look here if you put 0.875, then our f x value comes to 7.844 right slightly better value is obtained. So, from a value of f x equal to 7, we have now come to 7.844. So, that leads us for our next iteration.

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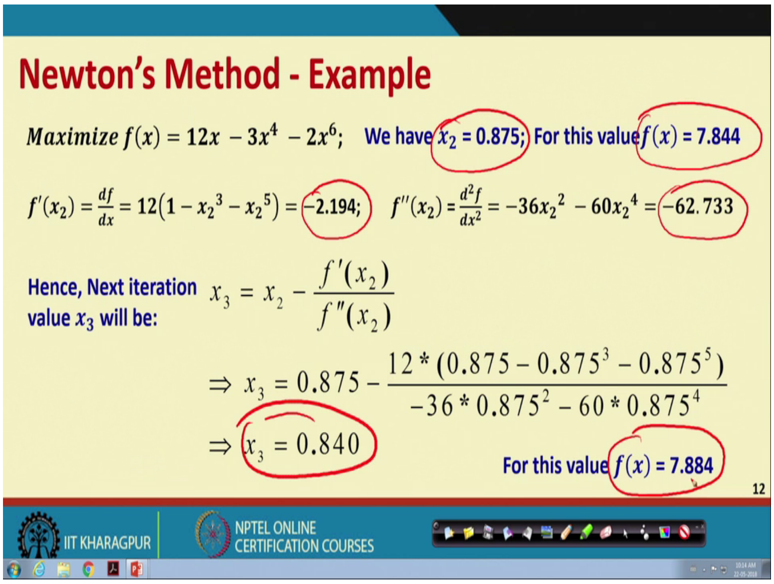

So, again we move ahead now, this time we have taken our next value x 2 is 0.875 if you recall our functional value was 7.844. So, again if we actually obtain at this point the first derivative and the second derivative, the first derivative comes to minus 2.194 and second derivative comes to minus 62.733 by putting the x 2 value.

So, again by the similar computation, x 3 comes to 0.840 right. So, that is our next iteration value and what is the functional value here? That becomes 7.884 right. So, from 7.844 we have improved it further to 7.884.

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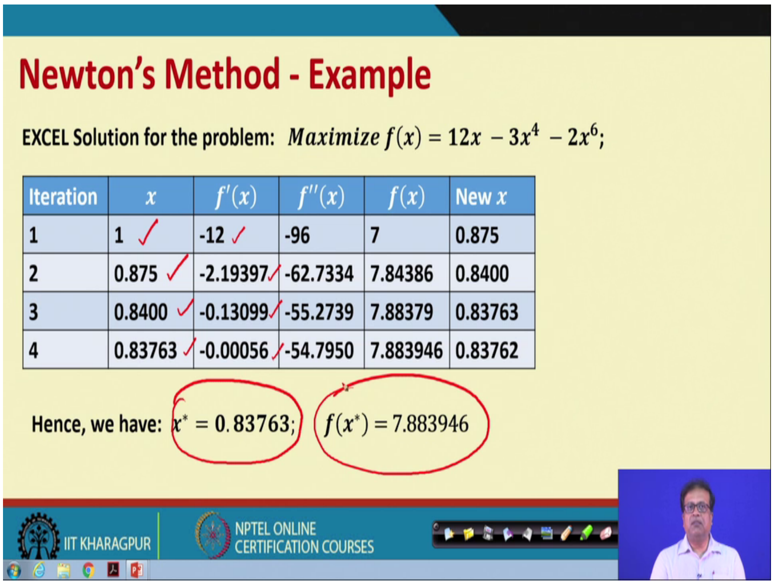

Let us move further at the next iteration, now we have used what is known as the an excel sheet and what we did we actually put those values and you know use that same iteratively similar calculations. So, we just copied number of times, the x obtained from the first becomes the x for the second and x for the second becomes x for the third, for the third whatever comes out at the end goes for fourth like this like this. So, that is how it progresses.

So, initially we start with a value of 1, then 0.875 then 0.84 up to this point we have seen and then further if you go, we get 0.83764 and subsequent look at the f dash x value. So, you know it starts from minus 12 to minus 2.19 something, minus 0 point 1 3 and finally, minus 0. 000. So, you see with subsequent iteration the first derivative is nearing as 0 value is alright.

So, you know it x is also slowly merging to a given value. So, may be after these many iterations probably we can say that for this value that is 0.83763 you know probably is a good approximation for the fx value of 7.83946, then iterate further, but we have to see whether we are really improving is alright. So, that is the Newton's method.

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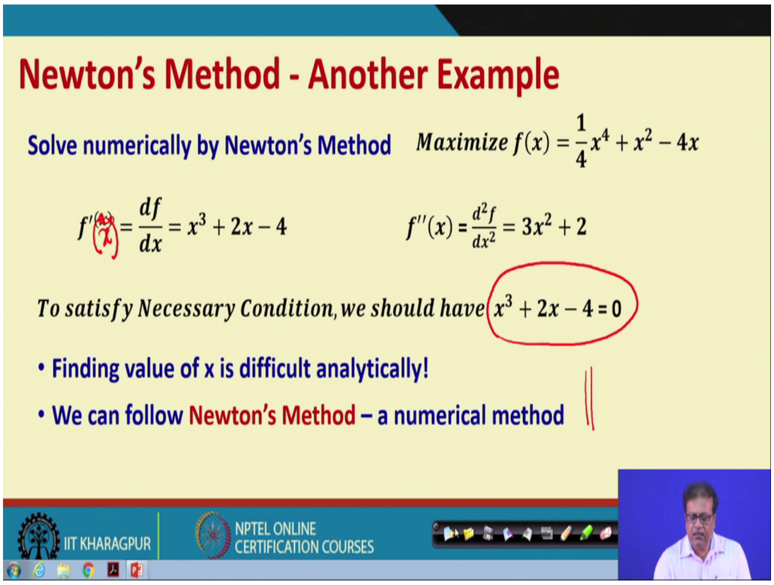

So, to have a review of what exactly we have done let us take another problem and quickly see supposing we have to solve numerical by Newton's method maximize fx equal to 1 by 4 x to the power 4 plus x square minus 4 x, again take the first derivative and the second derivative. So, the first derivative f dash x equal to you know df d x is x cube plus 2 x minus 4, and the second derivative become 3 x square plus 2.

So, that was the first and the second derivative and after obtaining that, you know the necessary condition the first derivative should be equal to 0 that is the necessary condition. So, again it is difficult to solve it. So, we follow what is known as a numerical method. So, what is that numerical method?

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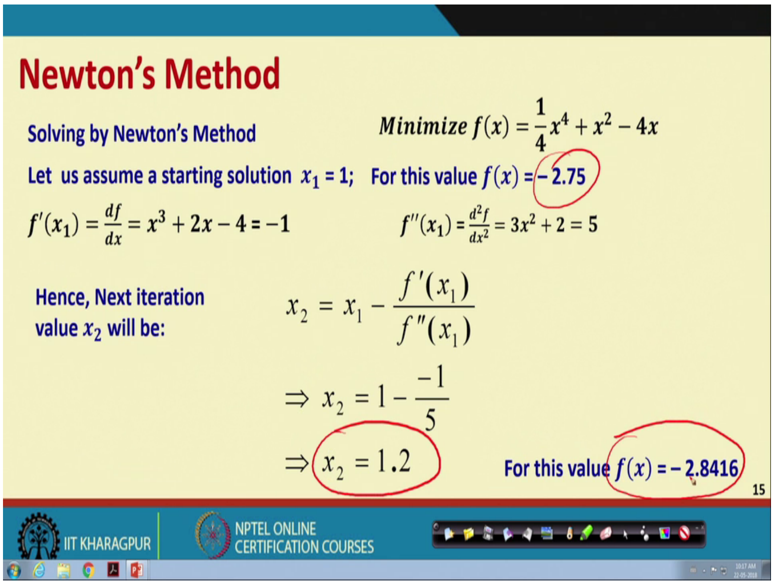

Once again let us see that by Newton's method in the first iteration, what we do we evaluate the f dash x let say again we start with a value from 1 and fx is minus 2.75 and here you know this was the minimization function. So, we find that the new value of x 2 comes out to be 1.2 right and functional value from minus 2.75 goes down to minus 2.8416 alright that is the first iteration.

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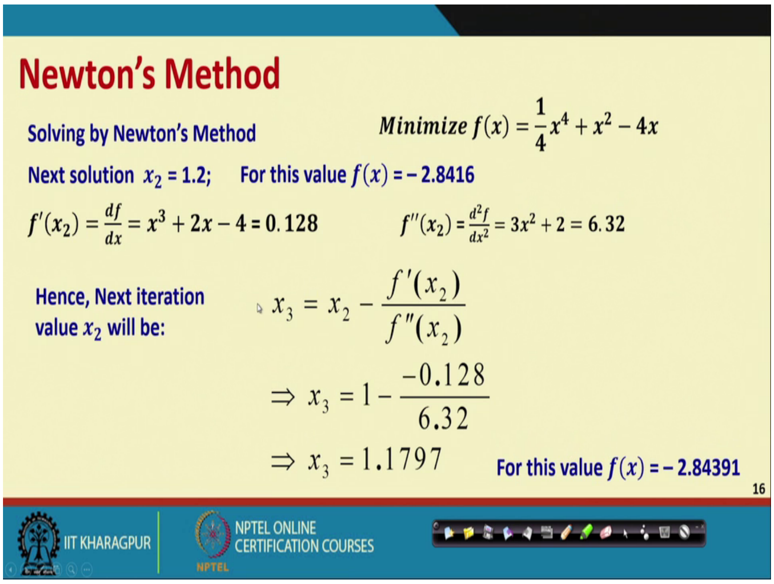

Then subsequently using this value we move to the second iteration and again we compute the first derivative and the second derivative and when you take the ratio, then we get 1.1797. And the functional value move up move down from minus 2.8416 to minus 2.84391ok.

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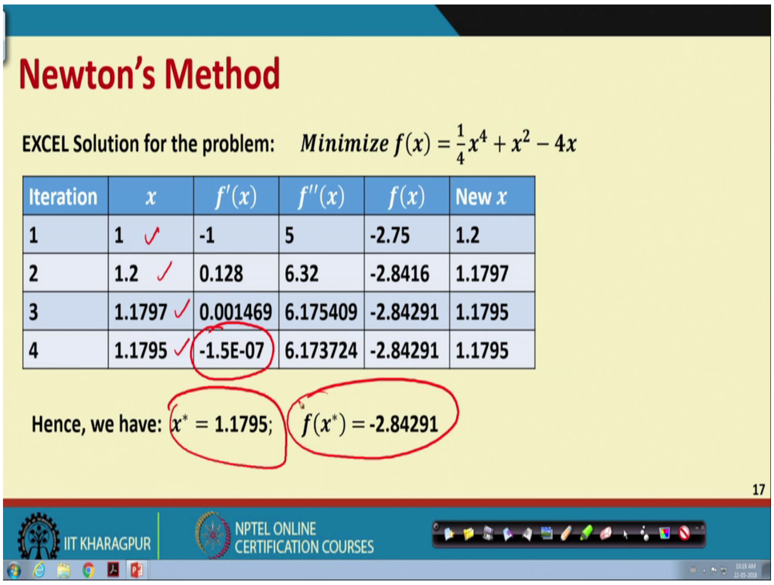

So, that is the second and again using excel we have tabulated the value moves from 1 to you know 1 to 1.2 1.1797 and 1.1795 is alright.

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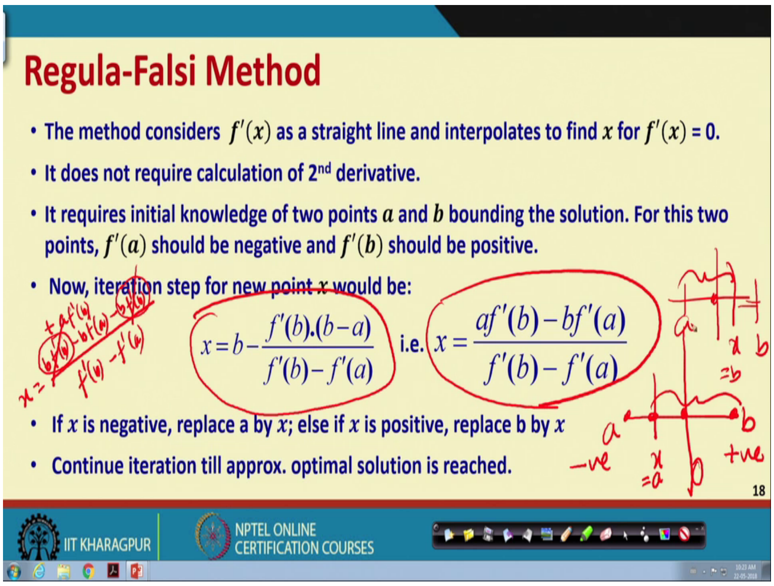

So, at that level look at the f dash value is almost 0 right nearly almost 0. So, that is how we find our optimal solution that is x star equal to 1.1797 and fx equal to fx star equal to minus 2.84291 is alright. So, this is a kind of method through which we can find out the functional value you know the extreme value by the method of iteration.

Now, see the other method which is known as the Regula-Falsi method. So, again this is another method where the g dash x the first derivative is considered as a straight line is alright as a straight line and the interpolation is made use of to find the value of x at for f dash x equal to 0.

The advantages with there is no need to calculate the second derivative right, but then we need to have 2 starting point a and b, such that the f dash a is negative and f dash b should be positive. So, see there is a function f dash x for a value of a, the value is negative for value of b f dash x is positive. So obviously, f dash equal to 0 should be somewhere in between so, that we can interpolate between them.

So, this is the interpolation equation that we have that x equal to b minus f dash b, b minus a f dash b minus f dash a right. So, if you do a little bit of manipulation you know it will be like this, x equal to f dash b minus f dash a and on top what you have? B into f dash b that is the first term minus b into f dash a that is the second term and then if you again see here then first term is b into f dash b and the second term is you know I am writing it here plus a into f dash b alright.

So, look here these b f dash b and b f dash b they cut each other. So, what is remaining? a into f dash b minus b into f dash a, by f dash b minus f dash a. So, if I put it here that is how we get that from the interpolation equation we have been able to find an expression that is x equal to a f dash b, minus b f dash a by f dash b minus f dash a. So, is nothing you just calculate this you will get here is alright.

So, now the question is that resulting x does the iterative value, you compute and then see whether it is negative or positive. If it is a negative value then replace the x a by x because a is the negative. So, a should be now replaced by x. So, it is like this. So, suppose there is a line, suppose this value is 0 this is a and this is b, a is negative b is positive alright. Now, what happens suppose we get x here so, if we get x here npw x will become a. So, this will become a. So, this is our new a, but on the contrary suppose this is a and this is b and we get x here, and x will be our new b this is alright.

So, now the iteration should be here or in this case it should be here. So, like these you know with every subsequent iteration, you are nearing the point that is the 0 point which you are trying to find out. So, that is the iterative method in the Regula-Falsi fine. So, now, that we know what it is let us see an example.

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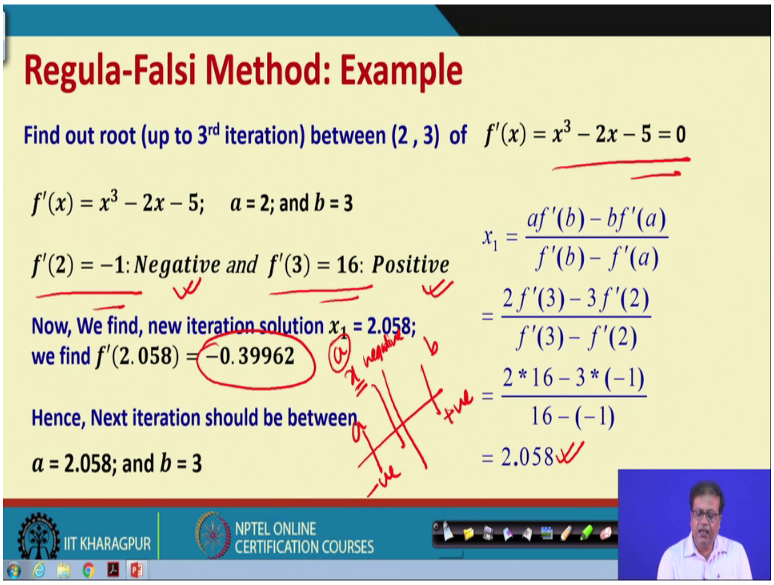

So, let us take an example that f dash x equal to x cube minus 2 x minus 5 equal to 0 we take 2 points 2 and 3 arbitrarily knowing that, if I put 2 we get 2 to the power 3 is 8, minus 4, minus 5. So, we know f dash 2 equal to minus 1 and if I put 3, then x 3 to the power 3 is 27 minus 6, minus 5. So, we get f dash 3 equal to 16. So, 1 is negative and the other is positive. So, we have one value on negative another value on the positive side and then we iterate what is the iteration state? X 1 is a f dash b b f dash a by f dash b minus f dash a.

So, we already found f dash 2 and f dash 3. So, 2 into this minus 3 into this and please note that the function itself is f dash x. So, we there is no need to differentiation because that was the function itself right. So, we find equal to 2.058 and the new value for the function f dash 2.058 is a negative number. So, since you know as I say in the scale this side is somewhere in between.

So, this is negative, this is positive, this is a, this is b. So, we get an ex which is negative so; that means, now this should be our new a fine that should be our new a. So, what is our new a going to be? It should be 2.058 right. So, then we should iterate between 2.058 and 3 right.

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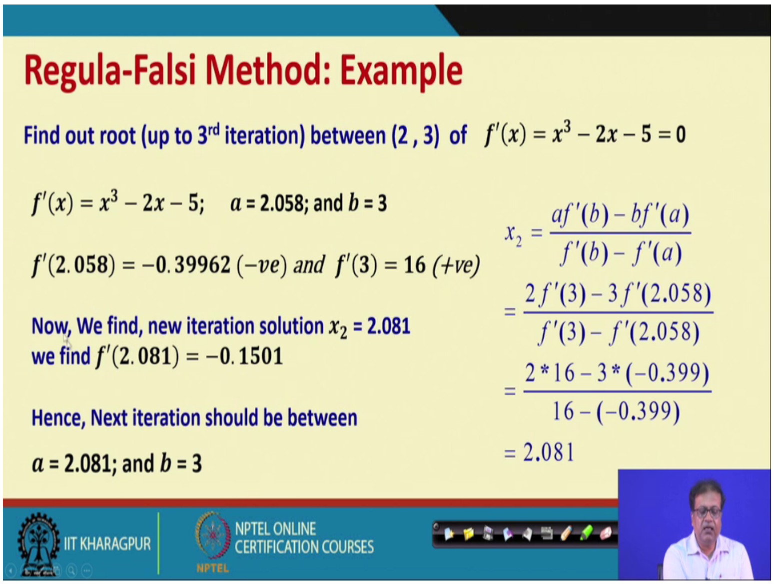

So, again we do that. So, again same thing we find f dash 2.058 which is again negative and f dash 3 is positive. So, we find again through that at the next iteration we find x 2 value is 2.081 and when you put that we find a another negative value. So, that should be our new a is it alright.

So, once again we followed this is nothing, but the second iteration and at the second iteration by following similar procedure, we found a is 2.081 and b equal to 3.

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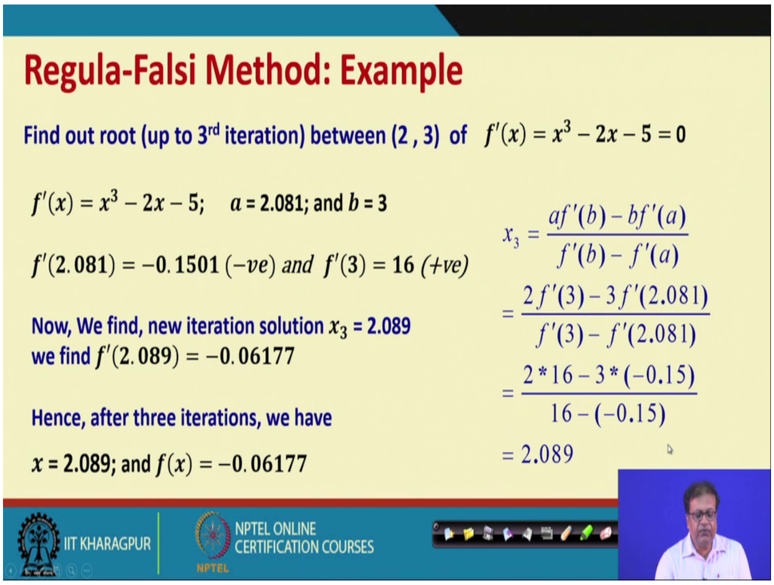

Let us move further at the next iteration, again we put 2.081 we find minus 0.1501 and that equal to 16 and again the computation shows 2.089. So, the new value is minus 0 0.06177. So, that is what we get after 3 iterations the x equal to 2.089 and f dash x equal to minus 0.06177 is it alright.

So, that is how the Regula-Falsi method calculates the f dash x equal to 0 it is all and finds the optimal point is it alright. So, we have seen the numerical methods for unconstrained optimization in this particular lecture right.

Thank you very much.