Introductory Mathematical Methods for Biologists
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Lecture - 13
Numerical Calculation of Derivatives

Hi, welcome to this lecture on mathematical methods for biologists. So, far we have been studying about derivatives and how to use calculus in different context, and today we will so far we studied different formulas and how to use those tools compute and to calculate derivatives. Today we will discuss if you have data if you do an experiment what we will have as a data set we will have a table, you will have an x column and a y column; you have 2 or 6 or many columns. Given this how will we how can we calculate derivatives?

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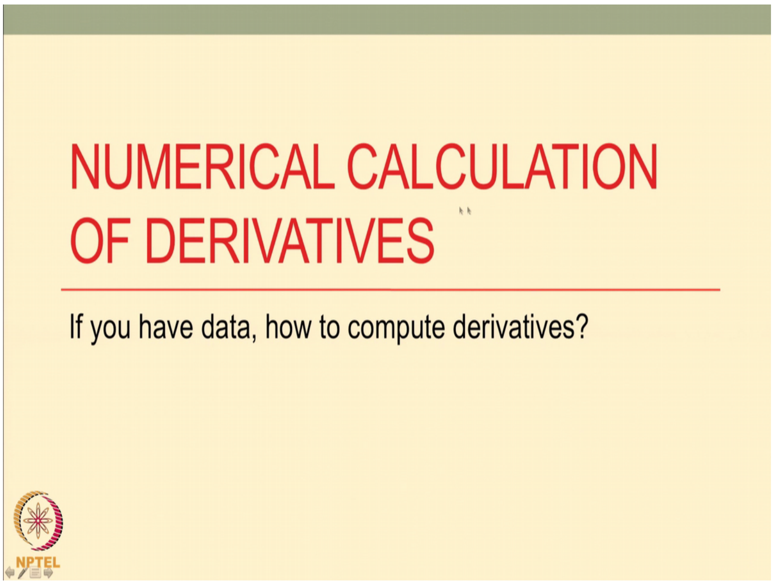

So, the title for today's lecture is numerical calculation of derivatives if you have data how to compute derivatives that is a question that we will answer if we have data from an experiment how do we compute derivatives from that data, that is a question that we will address today. So, to do that let us start with think about what we have.

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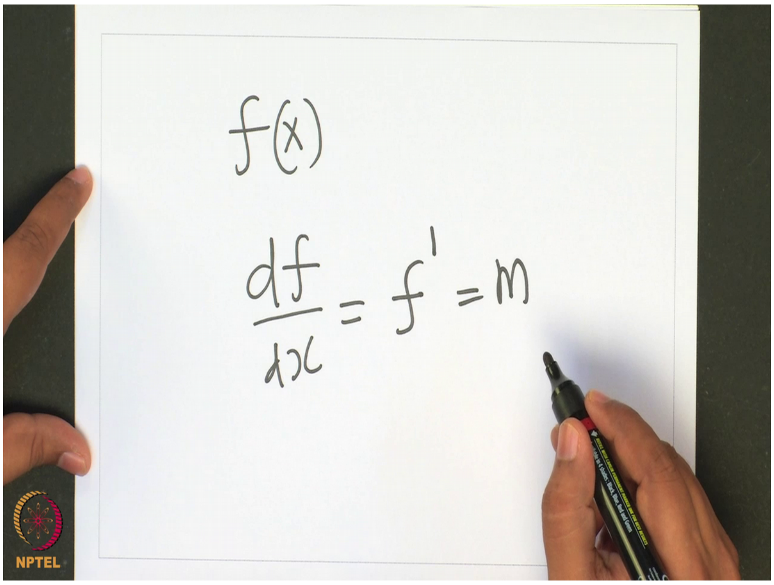

So, what does known here is you have some function f of x, and we said that this derivative is df by dx. So, typically this derivative we wrote m sometime people also write this f prime; f prime this means df by dx. So, 1 prime symbol here means one derivative, this is same as m we call it m which is the slope. So, this is the way we would compute this and the way we did to do this given a curve was the following that is we had any curve f of x.

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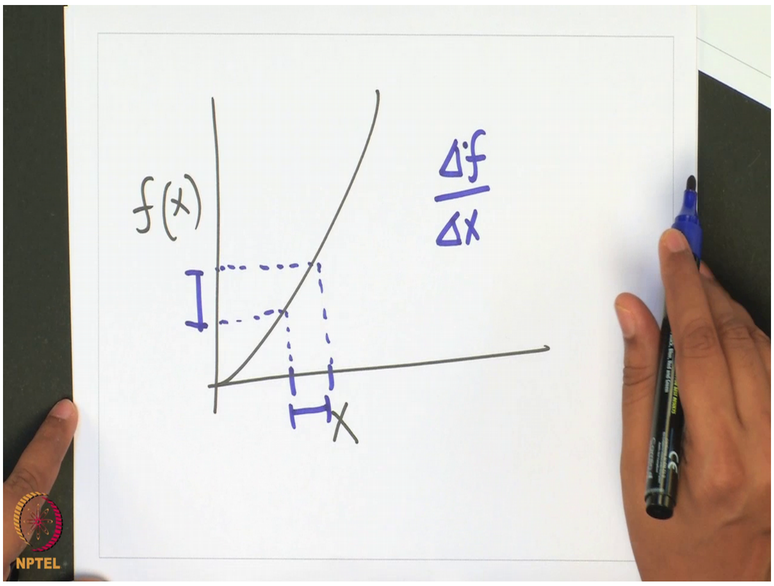

So, we had some curve x versus f of x and the way we did was that we took any 2 points, and calculate found out the corresponding the function value.

And we said that this minus this divided by this minus this, that is we say delta y or delta f here by delta x. So, this is our delta x and this is the delta f or delta y. So, this distance minus the divided by this distance and if you do this for a small enough delta x you will get nice perfect transitory derivatives. So, this is what we did so far to compute the derivatives.

Now, what we have is a data. So, let us think about; what do we get if we have data. So, let us say what we have it is a curve from a data sets.

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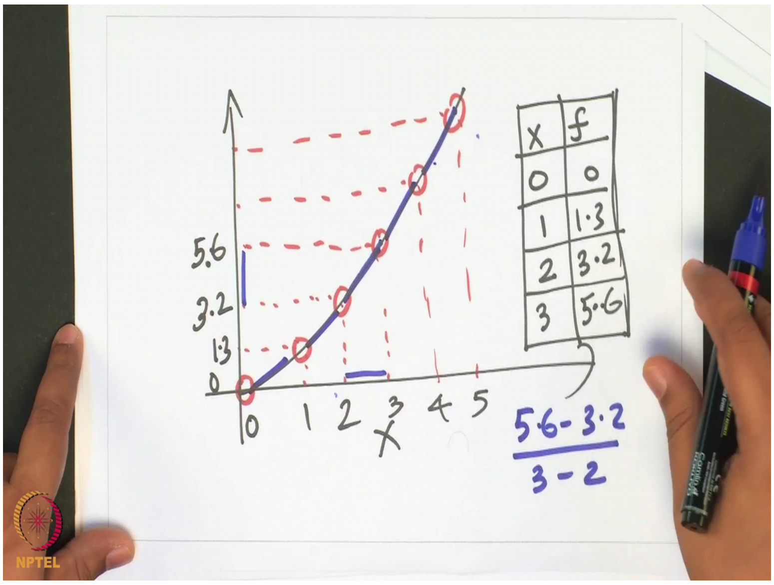

So, we have instead of this curve what we have is data given to us. So, these are some data points you do not have this full curve we only have this data. So, for 0 it is 0 for this there is a value for this, there is a value. So, this is what we have for each point this is the data that we get experimentally.

So, experimentally what we have is essentially a table x, which is this axis and whatever we measured in the y axis could be concentration, it could be whatever. So, some f and then we have data point 0, 0, 1, 1, 1.3, 2, 3.2, 3, 5.6 some data like this. So, this is we have what we have 0, 1, 2, 3, 4, 5. So, for each value correspondingly we have some y value. So, this 4 0 0 4 2 4 1 let us we write this as 1.3 for 2 let us write this as 3.2, for 3 let us write this as 5.6 and so on and so forth this is for example, I am writing this. Now if you want to calculate the derivative the slope at any point here let us this slope if you want to calculate.

If this values are close enough we can accurately calculate the slope which is this difference divided by this difference. So, 5.6 minus 3.2 divided by 3 minus 2. So, this is this would give us the data, this would give us the slope for this particular. So, each point each segment we can calculate slope. So, this is we can this is the way to numerically calculate the slope, if you think about and if you want to generalize this what we will have from an experiment is some table which is x and f of x, what we have will have x 1, x 2, x 3, x 4 x 5 and so on and so forth.

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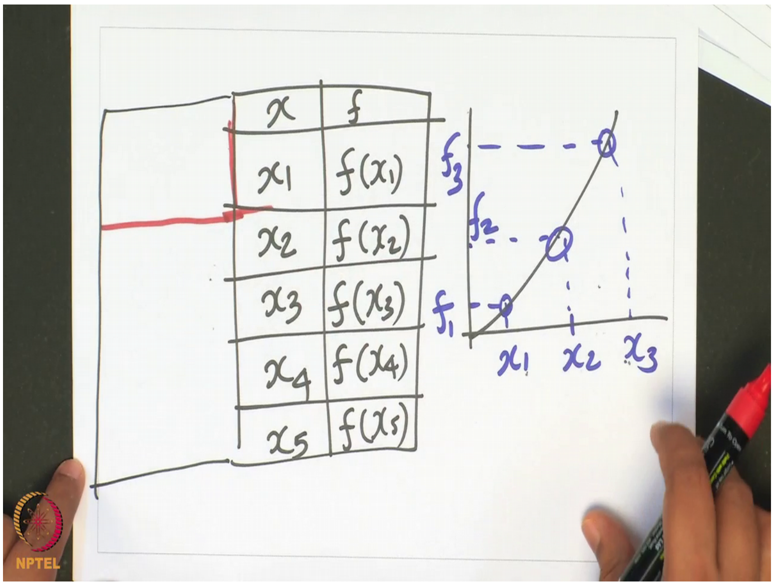

Correspondingly for x 1 there is some f corresponding to x 1 there is some f corresponding to x 2, there is a f corresponding to x 3, there is an f corresponding to x 4 there is an f corresponding to x 5 right this is what a typical curve would curve graph would look like. So, typical experimental data, if you just draw this rate data, this is let us say this is the first point this is our x 1 this is f corresponding to x 1. Let me call it f 1 for simplicity this is the x 2 and there is some f corresponding to x 2 and similarly there is x 3 and there is an f corresponding to there is an f corresponding to x 3. So, the format for corresponding to every point for x there is a corresponding y value, that is the value that they are measuring then this is what you would have. So, given this this is a slope here so, we can calculate the slope here.

So, let us let me write on this side the slope, for these 2 data together given sorry given x 1 and x 2 together. So, let me similar things will be right again. So, what was what were what are we having.

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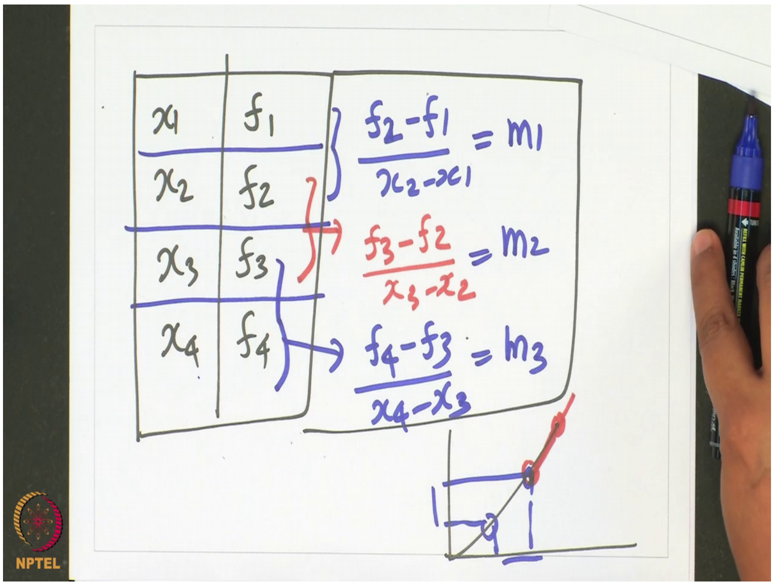

We are having x 1 correspondingly f 1, f of x 1, if you want x 2 corresponding the f 2, x 3 f 3 x 4 f 4 and so on and so forth. So, then I can calculate the derivative here. So, given these 2 data x 1, x 2, f 1, f 2, I can write f 2 minus f 1 divided by x 2 minus x 1 is the slope between these 2 points. So, if I were to plot this as a graph and if I have these 2 points and I can calculate the slope this divided by this. Similarly I can calculate the slope between these 2 slope corresponding to this.

I can write f 3 minus f 2 divided by x 3 minus x 2. This is the slope between the next 2 points if you have this point at this point the slope between this is this and similarly I can slope find the slope between f 3 and f 4. So, I can find 3 slope values corresponding to this for here. So, f 4 minus f 3 divided by x 4 minus x 3. So, given 4 data points I get 3 slope values let me call this m 1, this is m 2 and this is m 3. So, I can get 3 slope values corresponding to 4 data points that I have. If I have 4 data points like this x 1 f 1 these are 2 values that I would get from experiment. So, I have 4 data points from this 4 data points I can calculate 3 slope values any 2 you take in the neighbouring once you can calculate a slope.

So, as we know the first derivative is basically the difference, so the standard formula the first derivative as we know it is also called the forward difference formula.

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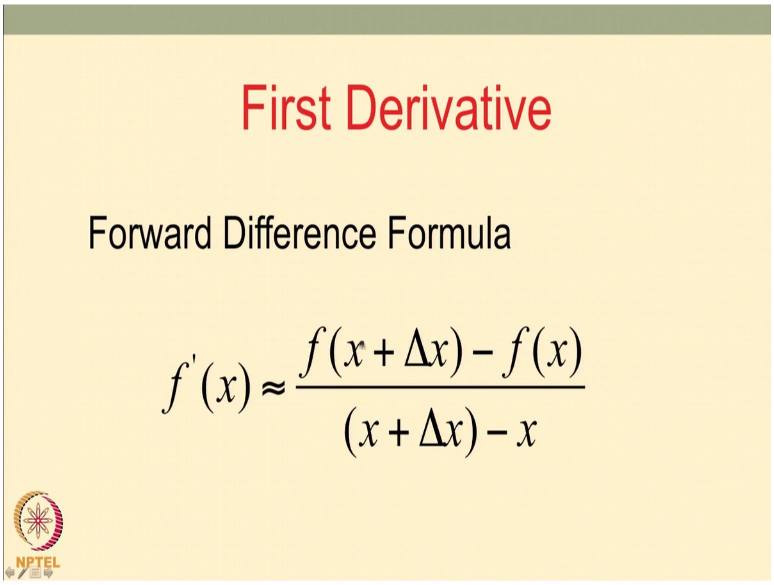

If you know f function at x plus delta x and function at x, the f plus x plus delta f of x plus delta x minus f of x divided by x plus delta x minus x is the f prime of x. This symbol here is prime. So, f prime of x is the first derivative, and this is this will you give you approximately the first derivative this is the numerical way of calculating this. But if you look at it here, if you look at this if you look at in this I could actually calculate the derivative taking these 2 or these 2. So, as far as this point x 2 is concerned, if you want to calculate the point I take derivative near x 2, I put a either use f 2 and f 1 or f 2 and f 3 what am I trying to say what am I trying to say is the following, that if we want to calculate derivative at a particular point. So, let us say you have this graph.

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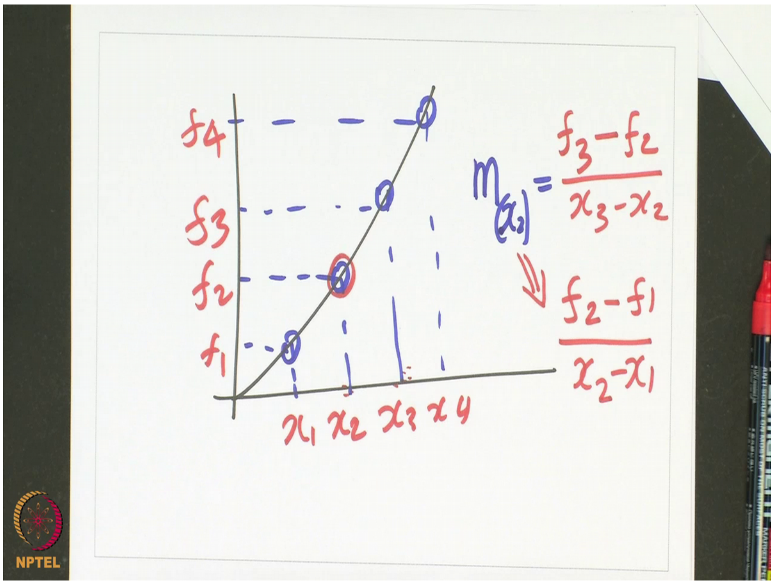

And you want to calculate derivative then we have function, and the corresponding x and y values you have. If we want to calculate the derivative near this point, I can either calculate derivative using this data that is x 1, x 2, x 3, x 4. So, I can use there is a f 1, f 2 f 3, f 4, I can use f 3 or x 3 or this. So, one of it is called a forward difference if I use x and x plus delta x, if I take this and this that is called a forward difference formula. So, that is why here f of x plus delta x minus f of x by x plus delta x minus x. So, this is.

So, if we consistently use always the forward this is the most popular one I would see where we consistently take the higher one and the lower one, the f of x plus delta x minus f of x divided by delta x, you could also take the backward one that is I could just write. So, what I want the slope, the slope at near 2 right near x 2 the slope near x 2 I could write as I said f 3 minus f 2 divided by x 3 minus x 2 or you could also write f 2 minus f 1 divided by x 2 minus x 1. If we consistently calculate everywhere if let us say if we were to use this, then this is the next one; this is the next one consistently if we use you would get the similar answer everywhere.

So, either use this or use this consistently. So, the other formula is called the backward difference formula, which is f of x minus f of x minus delta x divided by x minus x minus delta x. So, this is also we could use. So, this is also formula if you want to calculate the derivative at x, either you could take f of x and subtract f of x minus delta x the previous point and find the difference or.

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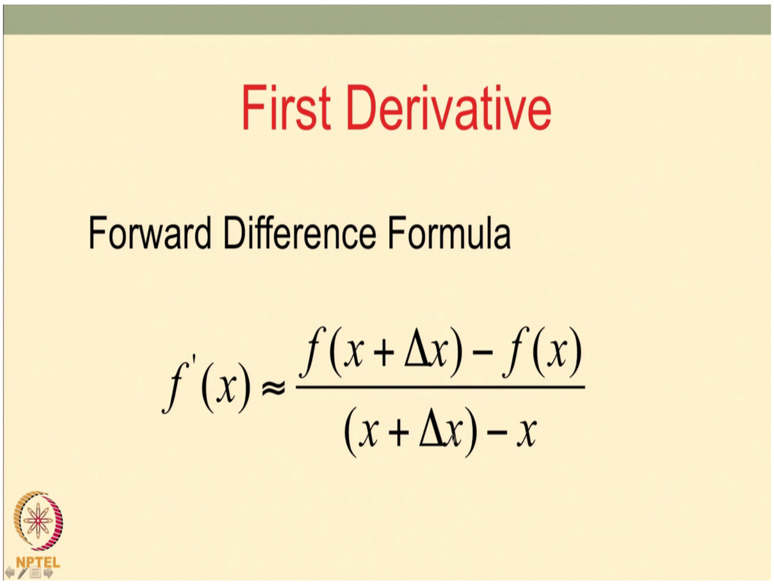

You could take the next one and subtract the value from the next point f of x, plus delta x and minus f of x and calculate this difference.

So, this is another way, but there is a there might be a casual situation where you have a lot of data points imagine that you have lot of data points very close by.

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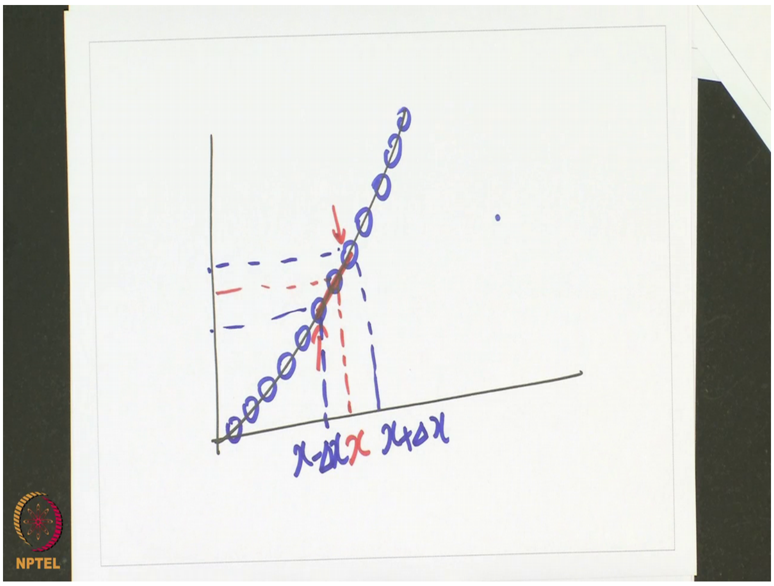

So, let us say you have lot of data points very close be, and you want to calculate the derivative at this particular point. So, you want to calculate derivative for this particular point x.

It is also fine to calculate this slope let us take this point and take this point, and this slope can be also said to be the slope at x. This is an equivalent way of saying all of these are correct these are depending on what way you want, you could use any of this formula. So, there is also called a. So, there is a forward difference formula, there is a backward difference formula, there is also a central difference formula which is using these 2 points right.

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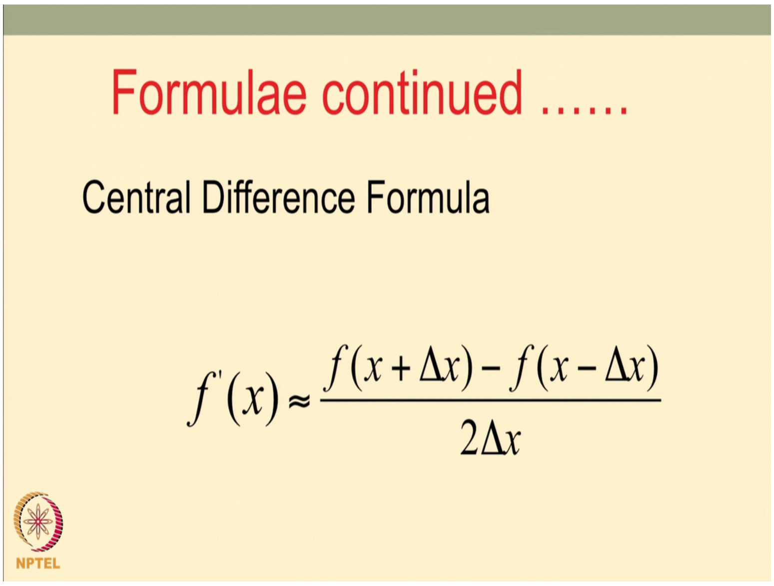

So, this is this point I could call it x plus delta x, this is x minus delta x. So, if I use these 2 points and the corresponding f values, the formula would look like this f at x plus delta x minus f at x minus delta x divided by 2 delta x.

So, this is you take 2 points, which is one point slightly above this or next to it and one point slightly below this or just behind it, and find those difference and that would be a e also a valid interesting formula for right formula for computing the for the derivative first derivative. So, f have prime of x. So, remember this prime means derivative f prime of x is equal to f at x plus delta x minus f at x, divided by 2 delta x. Another way of thinking about this is the following that to imagine that you have this data.

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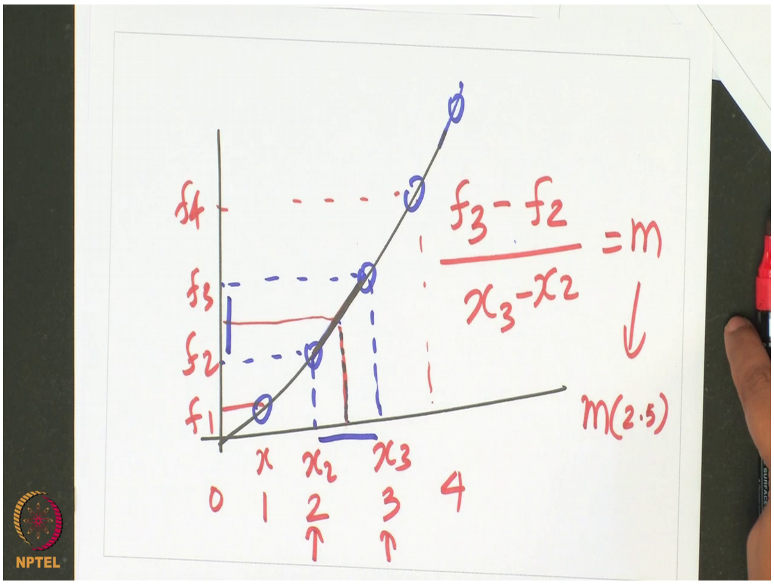

So, we had this data points here, here, here, here. Now let us take these 2 points correspondingly we have now let us call this. So, let us let me call this x 1, this is x 2, this is x 3 correspondingly you have here f 1, f 2, f 3 and of course, f 4 and f 4 here.

Now, if we calculate the slope here that is if I calculate the slope here which is f 3 minus f 2 divided by x 3 minus x 2 this is the slope, but this is a slope corresponding to what x value. So, one could claim that this is a slope I found I took these 2 and I took this. So, I would say I could say that this is this slope m, but m is for what x value. I could say that this m is for this x value. So, if I take this x value which is between x 2 and x 3 right if I take this x value corresponding to some number between x 2 and x 3. So, let me let us write here 0, 1, 2, 3, 4 and correspondingly we have. So, this if I just take value 2 and 3 and use this formula I could say that this m is a slope at 2.5 when x at x equal 2.4 in between value.

So, you could say that by doing this I got the slope at 2.5, this is the equivalent way of saying at the in some for at some x value in between x 2 and x 3. So, this is another way of saying it, once we consistently do this any of this would give us correct answer this central difference formula is very interesting because.

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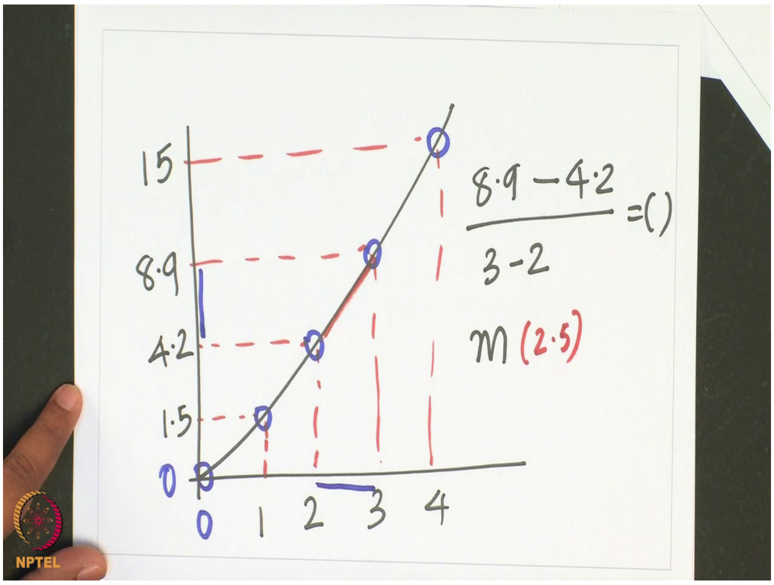

It could be really useful and it could be more accurate some cases little bit, but. So, let us calculate think about it once more. So, you have this value 0 here, 0 here, then let us say corresponding to this.

Let us write down some values. So, let us say there are values are 0 1 2 3 and 4 and here correspondingly you had 1.5 and 4.2 and 8.9 and 15. Let us say these are the corresponding y values that I got or the f values I got. Now if I calculate the slope between 2 and 3. So, I could take this delta x and I could take this. So, if I do this, I could write this slope as 8.9 minus 4.2 divided by 3 minus 2. So, this would give us some give us some value this is a slope corresponding to.

I could say this is a slope, this is a slope is corresponding to 2.5 now what I could get. So, for this data 1 2 3 4 5. So, imagine that I have this data which is corresponding to 1 2 3 4 5 and you have correspondingly.

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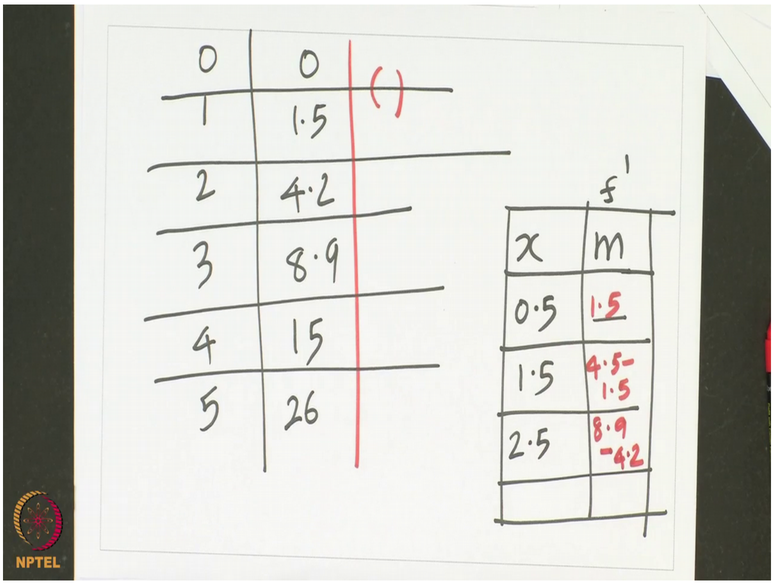

So, let us say 0. So, they have 0, 1.5, 4.2, 8.9, 15, 26 or some values like this, you could calculate the corresponding slope between these 2 values. So, you could take these 2 values and write the slope between this. So, 1minus 0 divided by 1.5 minus 0. So, you could write the slope here and say that the slope is between 0 and 5. So, slope at 0.5. So, I could take another table here.

I could make another table here which is x versus m or f prime or f prime is currently f prime. So, here you have 0 and 1. So, between 0 and 1, I could take 0.5 and can I find the slope which is this minus this. So, this I could write the slope then I could write 1.5 and 1.5 is between 1 and 2. So, I could write 4.2 minus 1.5 divided by 2 minus 1 right. So, you could write 4.5 minus 1.5, 2 minus 1 is 1 here I could write 1.5. So, this is correspondingly here 1.5 minus 0. Similarly I can calculate the slope at 2.5, the slope at 2.5 is 8.9 minus 4.2 divided by 3 minus 2. So, 8.9 minus 4.2 divided by 3 minus 2. So, the point I am trying to make is that the central difference formula, we could we could calculate a slope.

By central difference formula and say that this corresponds to the slope, which is at a value between those 2 x values that we took. So, we take if you want to calculate the slope at x, you could take the value at x plus dx take the value at take the function at x plus dx, take the function at x minus dx find the difference divided by 2 times delta x.

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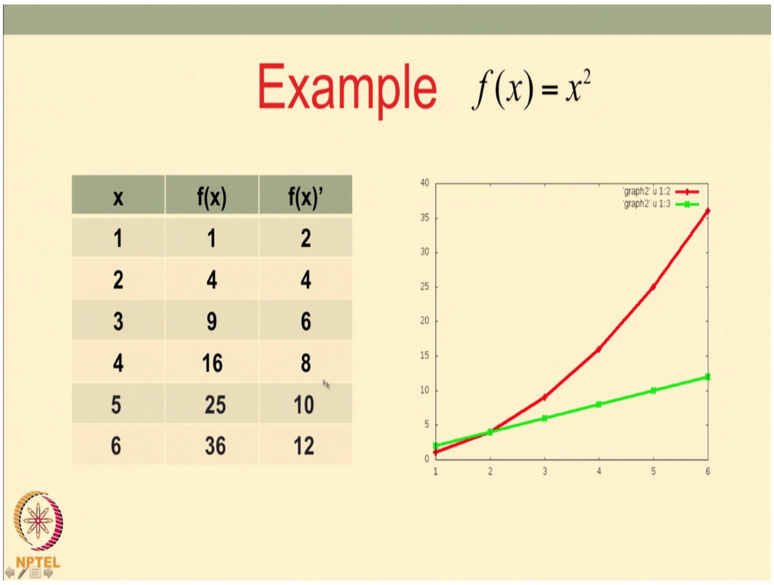

So, this is what is a numerically done here. So, you have 1 2 3 4 5 6. So, correspondingly you have x square which is 1, 4, 9, 16, 25, 36 and these are the data points you have a x and x square and we have the f prime of x which is this difference, 4 minus 1 divided by 2 minus 1 and so on and so, this is computed using forward difference methods.

So, look at this how this is computed this is computed using forward difference method and we could get corresponding the derivative formula. Now the question is we have this first derivative; how do we compute the second derivative? So, we could also we need to also compute the second derivative. So, let us think about this quickly.

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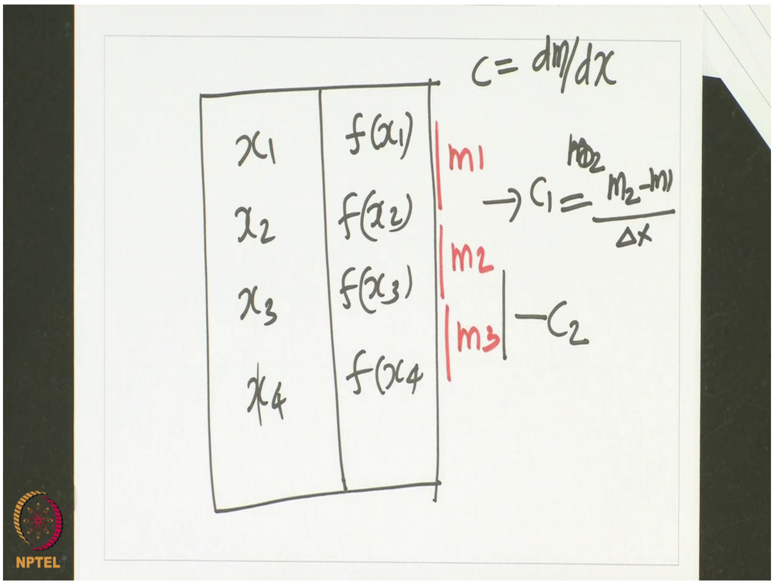

So, what we have is x 1 f of x 1, x 2, f of x 2, x 3, f of x 3, x 4, f of x 4 and so on and so forth. From these 2 I can calculate m 1, from these 2 I congratulate m 2, from these 3 I can calculate m 3. So, I have 3 derivatives and correspondingly I will have an x value. So, I could take it x 1 or x 1 between this values.

But consistently if you want to calculate second derivative, you could also calculate c one which is the secondary. So, consider these 2 as your functions. So, as you know the second derivative c is dm by dx; this is what the second derivative is. So, take these 2 values and corresponding x values right. So, you could take m 2. So, you could write c 1 as m 2 minus m 1 divided by the corresponding x values for this right delta x for this. So, if you do this properly m 2 itself, remember m 2 itself as a delta x m 2 is f of x plus delta x minus f of x divided by delta x. So, we have another delta x here similarly between these 2 I can calculate c 2. So, given 4 data points I have 3 first derivatives, and 2 second derivative c 1 and c 2.

So, these 2 values I can take and calculate c 1 these 2 items I can calculate the difference between these 2 which will be a derivative of m and that will be corresponding to the second derivative. So, if you write this just remember m itself as m itself can be written as f of x plus delta x minus f of x divided by delta x, and there is a divided by delta x again here. So, if I do this I will get a delta x square.

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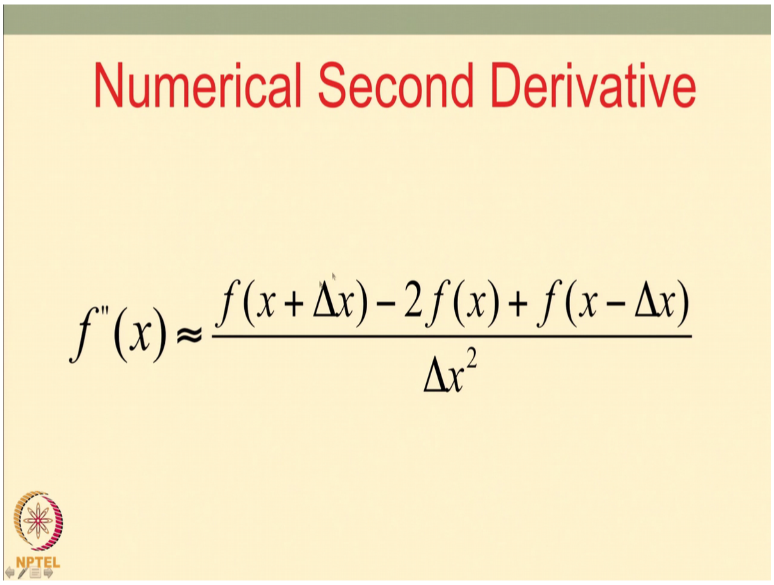

So, the numerically second derivative can be written as f of x plus delta x minus 2 times f of x plus f of x minus delta x by delta x square. So, if I do this; if I know the values of f at different points. So, we what am I what is it known to me? I have what I am what is known to me is just this f values, if I just know this f values.

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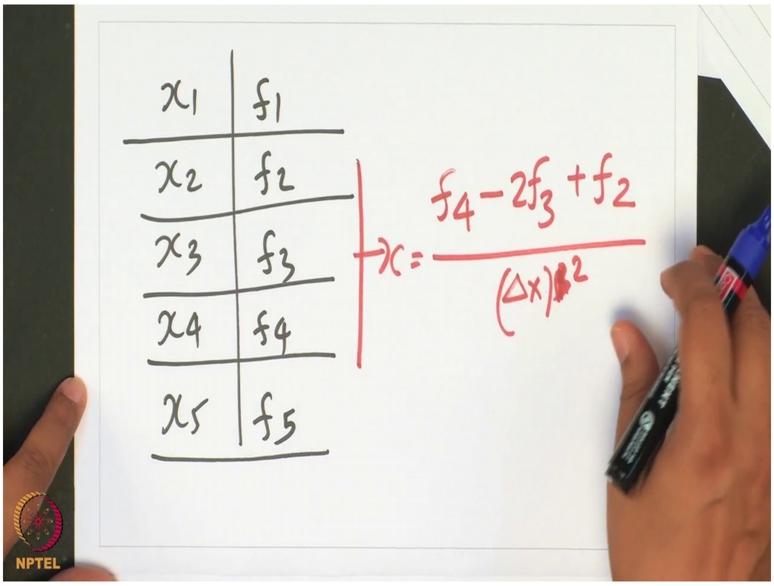

So, let us say I know this x 1, x 2, x 3, x 4, x 5 and so on and so forth and corresponding I have f 1, f 2, f 3, f 4, f 5 this formula says that use f at x plus delta x. So, if I just wanted to calculate if I any 3 points you take you can calculate a second derivative. So, let us take these 3 points, I can calculate the second derivative between these 3 points and the second derivative formula if you look at here, this is f at x plus delta x minus 2 times f of x minus f at x minus delta x. So, you have to know f of x, you have to know f at x plus delta x you have to know f at x minus delta x. So, these 3 things you have to know. So, here the assumption is that the x 1 minus x 2 (Refer Time: 28:39) delta xs are same.

If you assume all of this delta x are same what you could do you could write this as f 4 minus 2 f 3 plus f 2 divided by delta x square, which is the difference between delta x is x 3 minus x 4, x 3 minus x 2 minus x 1 or. So, upon sorry x square delta x square. So, this is this would give you see the second derivative corresponding to this value let us just see corresponding to the value x 3. So, corresponding to this value x 3 if you want to calculate second derivative take a point about this take a point below this, and use this formula here that would give us the second derivative.

So, this is f double prime of x. So, double prime means 2 derivatives second derivatives which is also we wrote as c of x. So, this is the way to calculate second derivatives numerically, given these 3 data points given 3 data points we can calculate second derivatives. Here if you take any 3 data points we can calculate the second derivatives. So, the finally, to summarize I could write this in a different way I could write.

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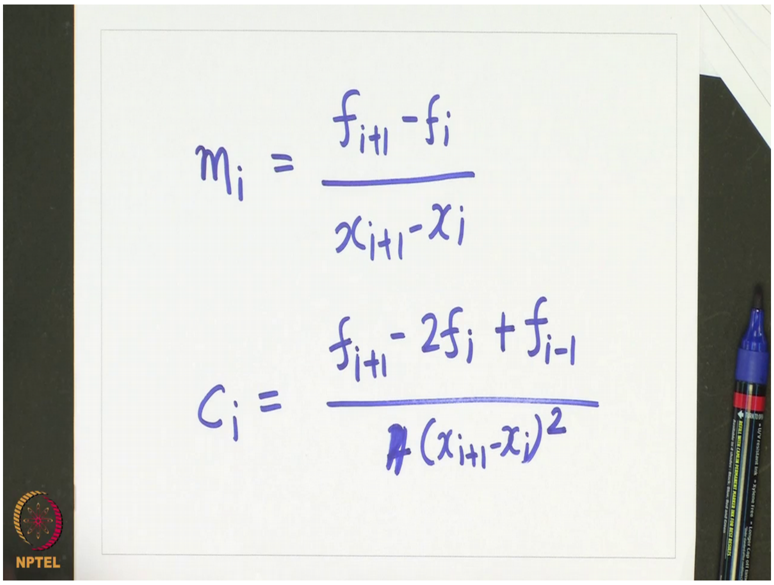

Slope at a location i at f at i plus 1 minus f at i divided by x i plus 1 minus x i this is one another way of writing general formula for slope, similarly for curvature second derivative which is C i we could write this formula which is f at C i is f at i plus 1 minus 2 f i minus sorry plus f i minus 1 divided by 2 x i plus 1 minus sorry this not 2 here x i plus 1 minus x i whole square assuming that all x i and x i plus 1 are same for the difference between all x values, if you take it as same we would take assume this as the formula for the second derivatives.

So, I urge you to read a little bit more and compute known about computing first derivative and second derivative given the data set, we can compute first derivative second derivative using this formula, with this we will stop this lecture where we computed first derivative and second derivatives numerically. See you in the next class.