

**Computational Techniques.**  
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**Module No. # 06**

**Lecture No. # 02**

**Differentiation and Integration**

Welcome to lecture 2 of our module on differentiation numerical differentiation and integration. In the previous module, what we did was several numerical differentiation methods to compute  $f'$  and  $f''$  of  $x$ , wherein introduced we looked at a method called method of undetermined coefficients in order to find out how to obtain these numerical derivatives, and how to obtain the error function for those numerical derivatives. What we will do now and what we will start off with is will start off with of Microsoft excel.

So, that we can show numerically that some of the concepts that we have learnt in the previous lecture, **how** how the error decreases when we change our  $\Delta x$  the second part will show is how the 3 different methods the error changes as  $\Delta x$  or  $\Delta x^2$  that is what we will do next. And then, will see something interesting that it is not always that as  $\Delta x$  is reduced. will get the error to reduce monotonically, will see that at some point when  $\Delta x$  is reduced beyond the certain value the error does not really reduce but, it actually increases, and why that happens we **will see will see** that also in today's lecture.

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$\Delta x$	$x(i-1)$	$x(i+1)$	$x(i+2)$	$f(i-1)$	$f(i+1)$	$f(i+2)$	F (Cntr)	F (Fwd)	F (3-Pt)
0.1	1.9	2.1	2.2	0.74185	0.64194	0.58846	-0.4996	-0.5121	-0.5007
0.01	1.99	2.01	2.02	0.69813	0.68813	0.6831	-0.5	-0.5012	-0.5
0.001	1.999	2.001	2.002	0.69365	0.69265	0.69215	-0.5	-0.5001	-0.5
0.0001	1.9999	2.0001	2.0002	0.6932	0.6931	0.69305	-0.5	-0.5	-0.5
0.00001	1.99999	2.00001	2.00002	0.69315	0.69314	0.69314	-0.5	-0.5	-0.5
1E-06	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5
1E-07	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5
1E-08	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5
1E-09	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5
1E-10	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5
1E-11	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5

So, that is the overall plan for today's lecture. We will now go to Microsoft excel, What I have shown over here will take **this this** particular  $f$  of  $x$  minus 2 minus  $x$  plus  $\ln x$  and try to numerically derive  $f$  dash of  $x$  for this particular function 2 minus  $x$  plus  $\ln$  of  $x$ . Analytical solution for  $f$  dash of  $x$  is minus 1 plus 1 divided by  $x$  that is what we are going to get.

If we substitute any value of  $x$  i **in in** this particular in **this this** particular equation. What we will do is will choose our  $x$  I will choose that equal to 1 so, I will just increase the font size over here.

$x$  i is chosen to be equal to 1 will just formatted so, that looks better. When  $f$   $x$  i is equal to 1, when we substitute  $x$  equal to  $x$  i in this particular equation we get minus 1 plus 1 divided by  $x$  which is equal to 1.

So, minus 1 plus 1 which is 0.  $f$  dash at  $x$  equal to 1 is 0, for this particular equation. Any deviation from 0 we know that we do not have the correct the exact value.

What we will do is will try to solve this particular problem for various values of  $x$  delta  $x$ . We will take delta  $x$  equal to 1 0.1 so on and so forth. I will just drag it equal to this divided by 10 for various values of delta  $x$ , we have this  $x$  of  $i$  plus 1 is going to be.

We will have  $x$  of  $i + 1$  and  $x$  of  $i - 1$  as well. So,  $x$  of  $i - 1$  and take this and increase the font size to 18 for all of these. So,  $x$  of  $i - 1$  is going to be equal to  $x$  of  $i$  and I will put dollar signs over there because  $x$  of  $i$  is not going to change minus  $\Delta x$ . **this is this is** what will get actually I would not use  $\Delta x$  equal to 1.

Because  $\log$  of  $x$  is going to be equal to  $\log$  of  $x$  we will not get anything if we are going to use that equal to  $x$  equal to 0. **So** that is why I will I will just eliminate that particular value. This is going to be equal to  $x$  plus  $\Delta x$  and as before will put the dollars over here and this is going to be this guy  $x$   $i + 2$  is going to be  $x$   $i + 1$  plus  $\Delta x$ .

Take this and drag it below this problem over here and just unmerge the cells and I think this should be fine and we drag these cells over here. So, this these are the values of  $x$   $i - 1$   $x$   $i + 1$  and  $x$   $i + 2$  although these values look 1 **1 1** over here **it is it is** only because **we we** haven't given enough size **for for** those cells if we increase the size of the cells, let say to this size we will see that we actually get those values equal to something other than 1.

Now we will have  $f$  of  $i - 1$   $f$  of  $i - 2$   $f$  of  $i + 1$  and  $f$  of  $i + 2$  that those are also, something that will calculate so that is equal to  $2 - x$  plus  $\ln$  of  $x$ . so,  $f$   $i$  is going  $f$   $i - 1$  is going to be  $2 - x$  plus  $\ln$  of again this guy.

That is going to be eh  $f$   $i - 1$  and we will just **drag drag** it. So, will get  $f$   $i + 1$  and  $f$   $i + 2$  and then we will just drag and drop it over here.

These are the values of  $f$   $f$   $i - 1$   $f$   $i + 1$  and  $f$   $i + 2$ . Now over  $f$  dash by central and then will calculate  $f$  dash by forward and will also calculate our  $f$  dash by 3 point difference formulae and I will just resize some of these so, that we can view all the results simultaneously.

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$\Delta x$	$x(i-1)$	$x(i+1)$	$x(i+2)$	$f(i-1)$	$f(i+1)$	$f(i+2)$	F (Cntr)	F (Fwd)	F (3-Pt)
0.1	1.9	2.1	2.2	0.74185	0.64194	0.58846	-0.4996	-0.5121	-0.5007
0.01	1.99	2.01	2.02	0.69813	0.68813	0.6831	-0.5	-0.5012	-0.5
0.001	1.999	2.001	2.002	0.69365	0.69265	0.69215	-0.5	-0.5001	-0.5
0.0001	1.9999	2.0001	2.0002	0.6932	0.6931	0.69305	-0.5	-0.5	-0.5
0.00001	1.99999	2.00001	2.00002	0.69315	0.69314	0.69314	-0.5	-0.5	-0.5
1E-06	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5
1E-07	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5
1E-08	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5
1E-09	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5
1E-10	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5
1E-11	2	2	2	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5

So, central see f dash of central is going to be equal to  $f(x_i) - f(x_{i-1}) + f(x_{i+1}) - f(x_{i-1})$  divided by  $2 \times \Delta x$ . We have  $f(x_{i+1}) - f(x_{i-1})$  divided by twice  $\Delta x$  and this is going to be our f dash of central difference formula, keep in mind that our true f dash is equal to 0.

So so whatever f dash we get from the numerical value is the actual error also because, anything minus 0 is going to be equal to that particular value itself I will just drag and drop it below.

We have the the f dash using central difference formulae is  $3 \times 10^{-3}$ ,  $5 \times 10^{-5}$ ,  $7 \times 10^{-7}$ ,  $9 \times 10^{-9}$ ,  $3 \times 10^{-11}$  so on and so forth.

What we see initially is that decreasing the  $\Delta x$  by a factor of 10 we are improving f dash by a factor of 100. When  $\Delta x$  divided by 10 we choose we will get our f dash  $\times$  divided by 100. That is because as we had seen as we had derived earlier the central difference formula is accurate to  $\Delta x^2$ .

Let us see what happens with forward difference formula. For forward difference formula I will need  $f(x_i)$  so,  $f(x_i)$  is going to be equal to will calculate that so, that value is equal to  $2 - x_i + \ln(x_i)$ . So,  $f(x_i)$  is going to be equal to 1 as well I will just move this a little bit down so, that we are clear of what we had upward. This is our  $x_i$  this is our  $f(x_i)$  again beautified a little bit.

That is it is easier to see now our  $f'$  using the forward difference method is going to be equal to  $f_{i+1} - f_i$  divided by  $\Delta x$  and because  $f_i$  is not going to change the cell this green color cell has to **remain remain** the same when we drag and drag this contents of this cell I will put the dollar signs over there and I will just pull this downwards and this is what we are going to get.

What we get is  $f'$  is  $e$  the error for  $f'$  using the forward difference method is start of as a fairly high value over here the error is fairly high and as we decrease the overall  $\Delta x$  the error keeps decreasing and as we change the  $\Delta x$  the error decreases more or less linearly.

What that means is I decrease the  $\Delta x$  **by by** a factor of 10 and the error decreases by a factor of 10 i decrease it by another factor of 10 error decreases by another factor of ten so on and so forth.

What we see is we see a linear decrease in the overall error that is what we observe in this particular case and 3 point forward difference formula that we are going to use is equal to  $\frac{-3f_{i+2} + 4f_{i+1} - f_i}{2\Delta x}$  and I will put dollar signs over there plus 4 multiplied by  $f_{i+1}$  minus  $f_{i+2}$  the whole thing divided by twice  $\Delta x$ .

That is my equation over there and then I just drag it and again what I what I see is the error initially is 5 into ten to the power minus 3 then it become seven e minus 3 7 e minus 7 7 e minus 9 7 e minus 11 and then the error again increases let us try to do this for another value of  $x_i$  let us say  $x_i$  equal to two and for  $x_i$  equal to two this is going to be our  $f(x_i)$  and our true value of  $f'$  is minus 1 plus 0.5.

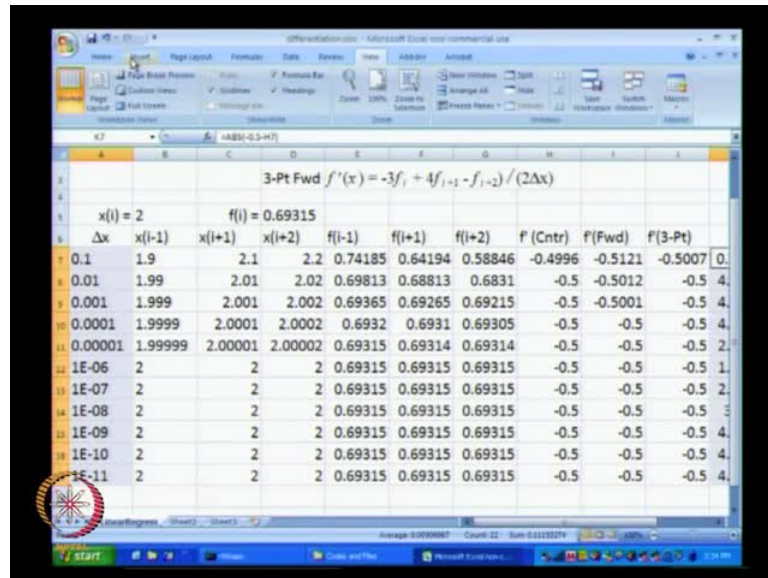
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	f(i-1)	f(i+1)	f(i+2)	F(Cntr)	F(Fwd)	F(3-Pt)	ERRORS
7	0.74185	0.64194	0.58846	-0.4996	-0.5121	-0.5007	0.0121
8	0.69813	0.68813	0.6831	-0.5	-0.5012	-0.5	4.2E-06
9	0.69365	0.69265	0.69215	-0.5	-0.5001	-0.5	4.2E-08
10	0.6932	0.6931	0.69305	-0.5	-0.5	-0.5	4.2E-10
11	0.69315	0.69314	0.69314	-0.5	-0.5	-0.5	2.3E-12
12	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5	1.4E-11
13	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5	2.6E-10
14	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5	3E-09
15	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5	4.1E-08
16	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5	4.1E-08
17	0.69315	0.69315	0.69315	-0.5	-0.5	-0.5	4.1E-08

So, that true value is minus 0.5 so let us now look at the errors in in these in these values so the next three cases are going to be errors in values, so I will just format this size. Our true value that we know is minus 0.05. So, absolute of minus 0.5 minus of the value that we obtained over here. So that is going to be our error and then will just drag it over here and likewise will just drag it in this direction.

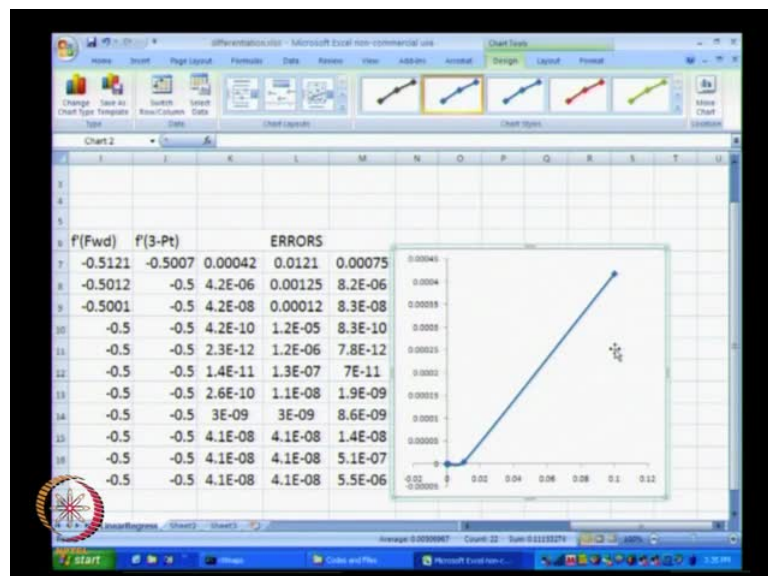
What we see over here is have for the central difference formula the error starts at 4 e minus 4 4 e minus 6 4 e minus 8 4 e minus 10 4 e minus 12 and then it is starts increasing the error starts increasing. For the forward difference formula the error is 1 e minus 2 1 e minus 3 1 e minus 4 1 e minus 5 and so on. And then after a certain point it it it increases and same thing that we see for the 3 point forward difference formula also.

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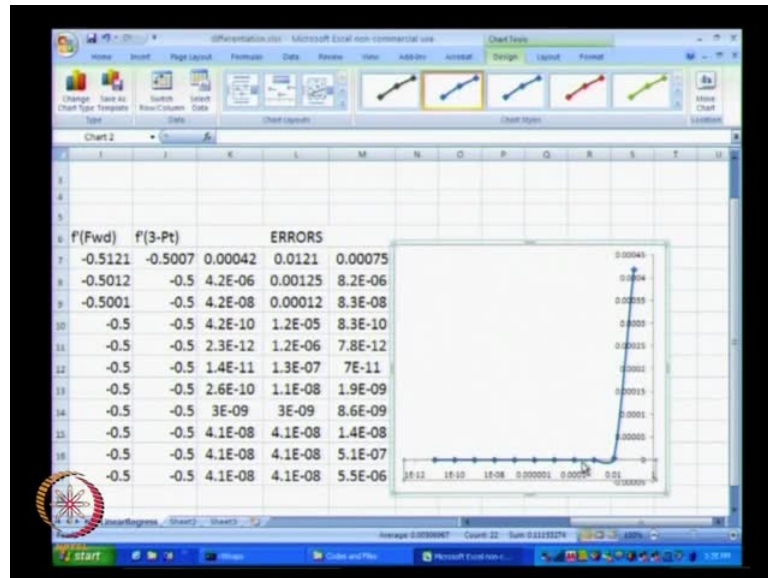


What will now do is we will plot our errors against delta x. So I will just go out of the full screen mode so can I so that i can include the the plots. So what I will do is I will select this delta x and I will select this error and then I will go on to insert, and I will insert a scatter plot.

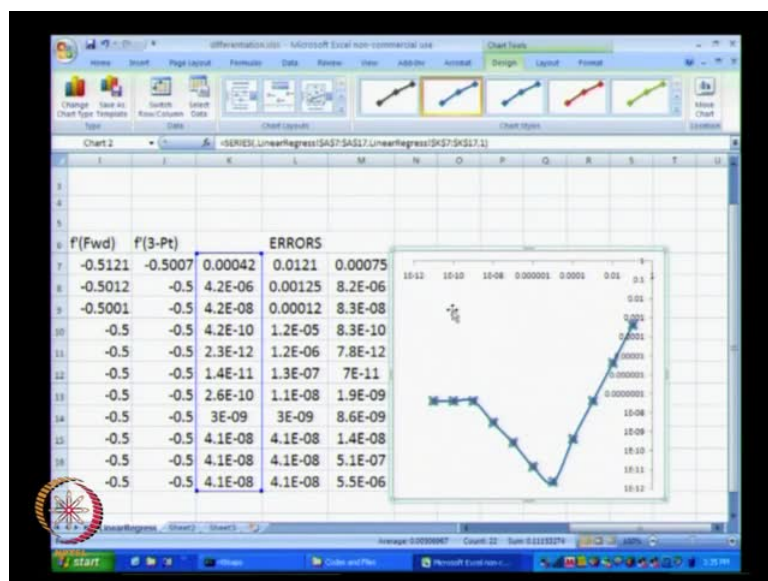
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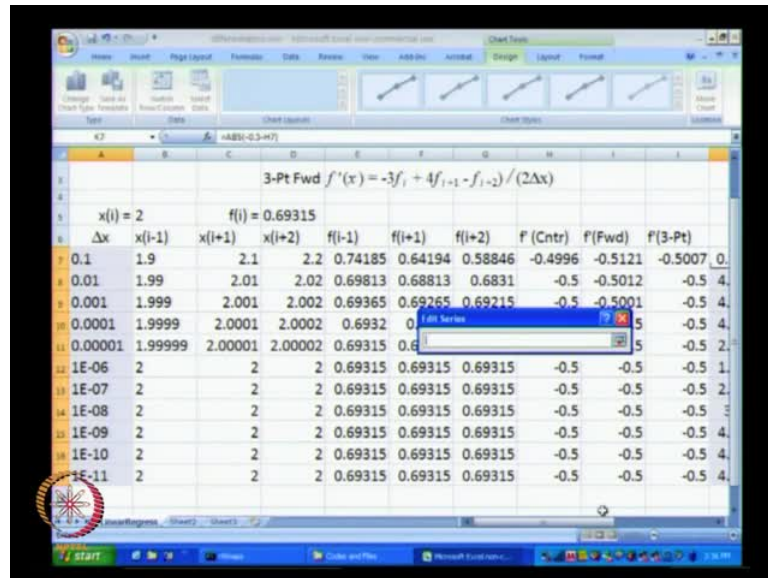
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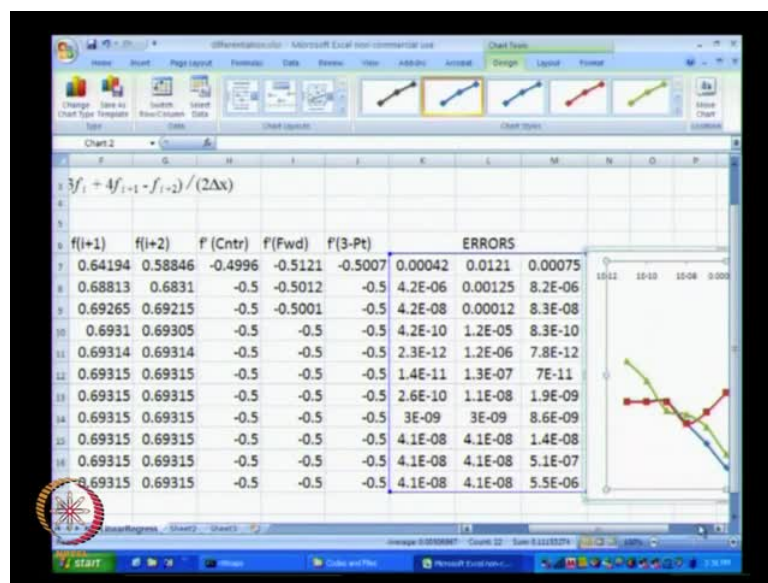
This is the plot that I have inserted over here. I will delete the legend and what we want to do is plotted on the logarithmic scale both or the x axis as well as for the y axis, format axis select the logarithmic scale.



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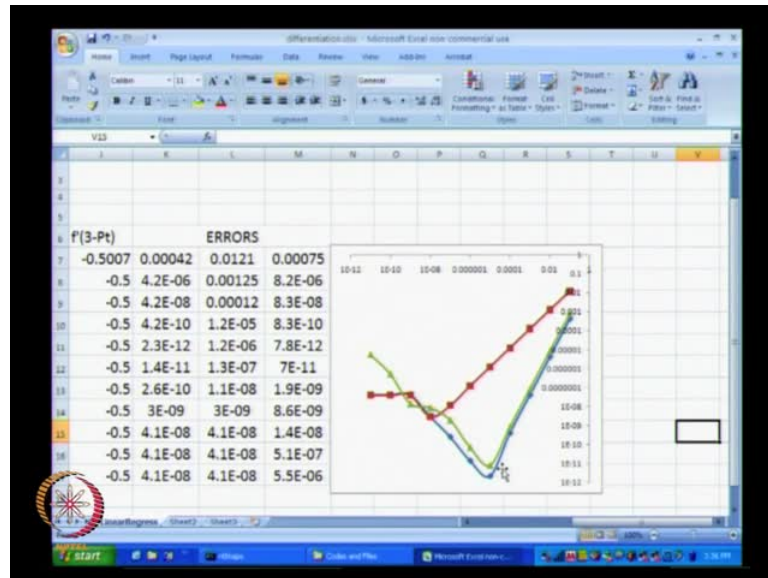


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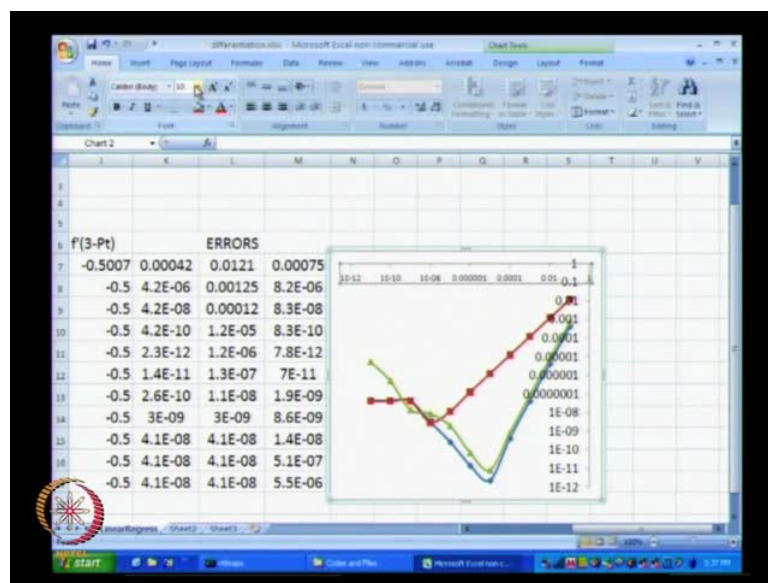


So this is this is the overall plot that we get for the central central difference formula. Likewise now we will do the plot for the forward difference formula and we will add another series. The x values remain the same and the y values we will choose them over here and will add the errors for the third third guy as well and the x values again remain the same and the y values that we are going to choose are the errors in a 3 point formula.

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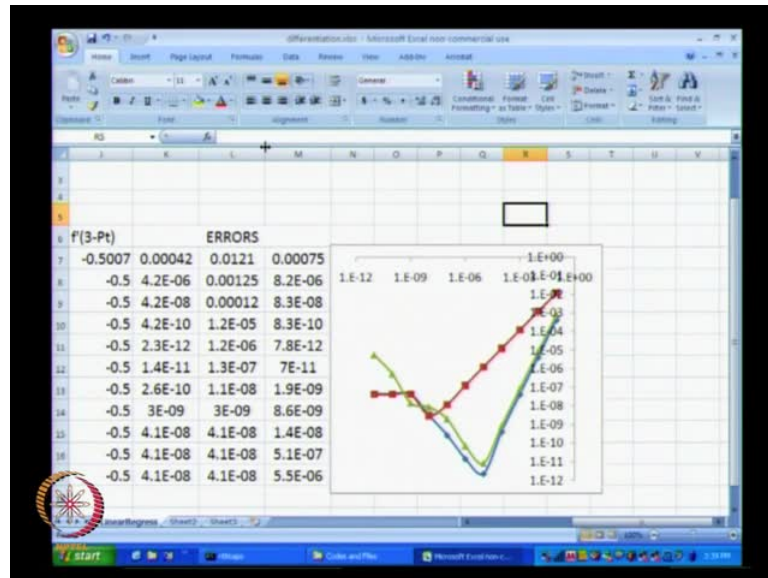


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The blue line over here corresponds to **the so** in y axis. We have the errors and in the x axis we have the delta axis 14. I will just again go ahead and format the number I will use that as a scientific notation and likewise I will change this also to a scientific notation.

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This is the overall errors that we get the red line indicating the errors for the forward difference formula, the blue line indicating the error for the central difference formula and the green line indicating the errors for the 3 point forward difference formula. As we see is that the errors in the central difference formula are lower than the errors in the forward difference formula.

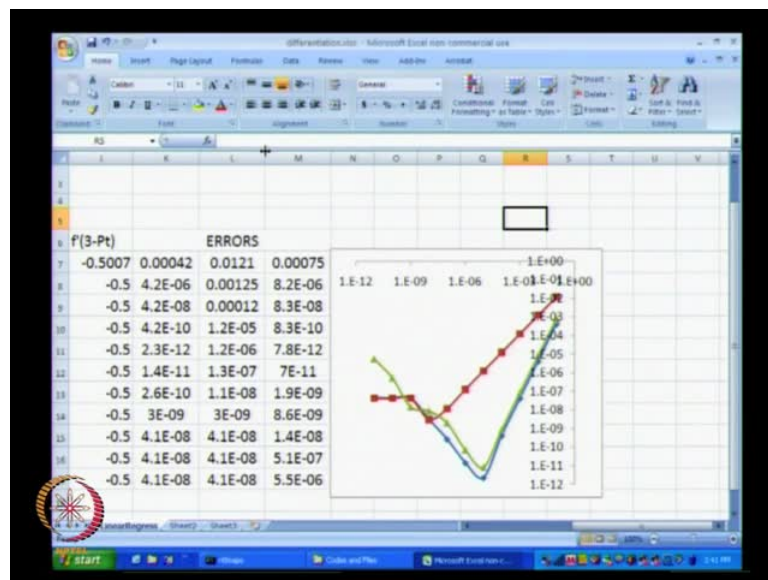
However in both the cases in the forward as well as the central difference formula. As we decrease **the the** value of our delta x. So, there is an increase in the errors that we see after a **particular particular** point of time and this is because of the truncation and round of errors what happens initially is that the truncation errors are keep decreasing and round of errors are low enough. After a certain point the round of errors start getting larger than the truncation error.

Keep in mind what is happening over here. what we observe over here is that for the central difference formula the optimum value of delta x that we get is approximately 10 to the power minus 5 or 10 to the power minus 6 something in that ball park range where, as for the forward difference formula **the the** value for best delta x happens to be over here which is approximately 10 to the power minus 8.

**So** the overall take home message was one the errors. The overall take home message that we get from what the excel results is that number one is that, the errors are in the

central difference formula are typically tend to be lower than the errors in the forward difference formula. The second observation that we made is that the second the central difference formula the the value of delta x that gives the best value for the the errors turns out to be approximately of 10 to the power minus 5 or may be 10 to the power minus 6, where as in case of the forward difference formula the best delta x occurs at around 10 to the power minus 10. Will see why why that that is in in in a short in a short file from now. And the final thing the that we that we observed is for pretty much the entire range of conditions, the central difference formula attended to be more accurate than the forward difference formula.

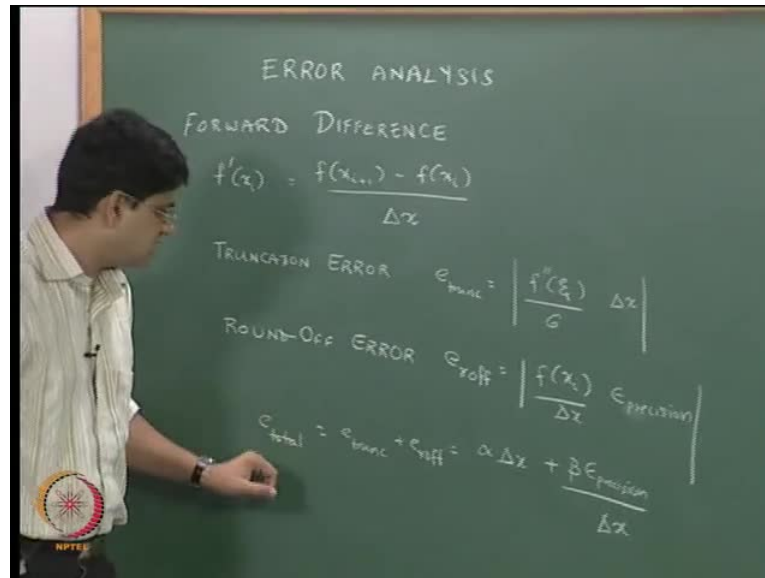
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So, now I will go on to the board and try to explain why we get some of the observations.

So let us now use the board in order to derive some error analysis results for numerical differentiation.

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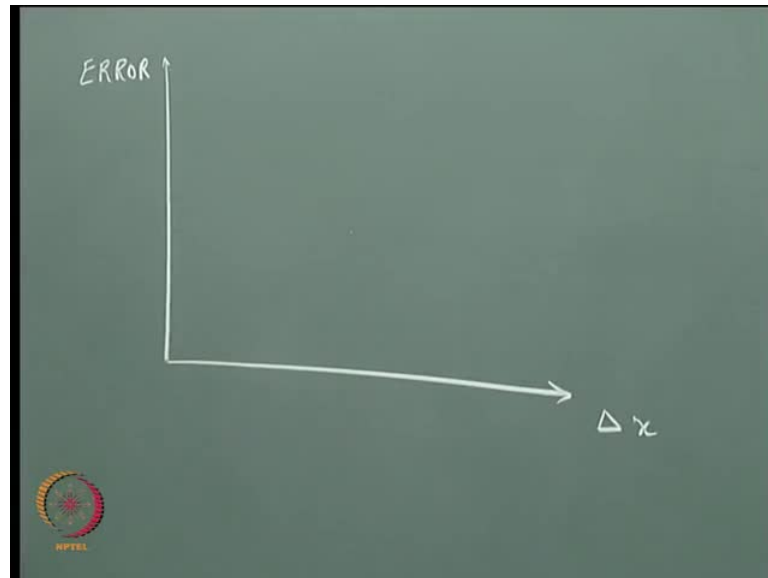


For forward difference  $f'$  of  $x_i$  was equal to  $f$  of  $x_{i+1}$  minus  $f$  of  $x_i$  divided by  $\Delta x$ , and the truncation error was of the order of  $\Delta x$ . **So** it was proportional to  $\Delta x$ . I will use some kind of a constant multiplied by  $\Delta x$  that particular constant was  $f''$  of  $\xi$  divided by 6 multiplied by  $\Delta x$ , and we do not worry whether the error is positive or negative.

We are going to put absolute values of this. In addition to truncation error there is also the round of error associated **with with** the overall problem but, the actual round of error is going to be determined by the absolute value of  $f$  multiplied by the. As a result of this we will get round off errors is going to be proportional to  $f$  of  $x_i$  divided by  $\Delta x$  multiplied by epsilon machine precision. So, that is going to be our truncation error this is this fellow is going to be our round off error. **So** our total error  $e_{total}$  is going to be just  $e_{trunc}$  plus  $e_{roff}$  which we are going to write let us call this  $f''$  of  $\xi$  divided by 6 absolute value of that as  $\alpha$ .

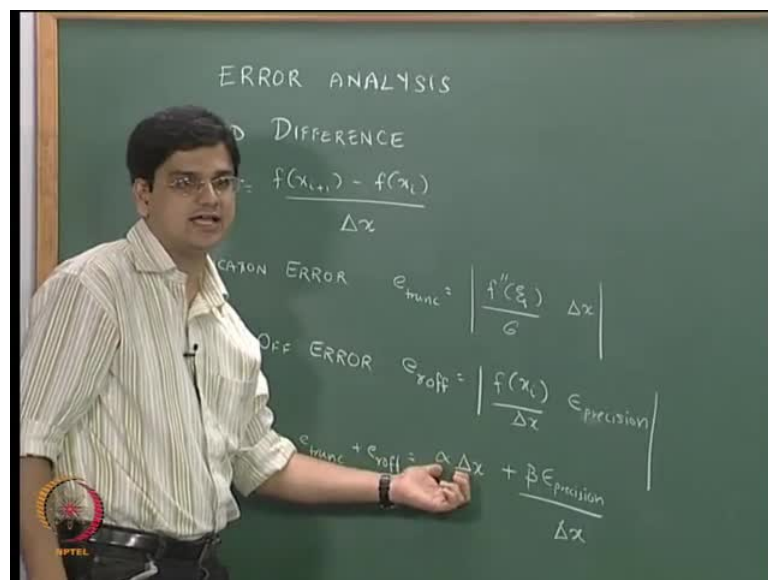
Let us so that we will write that as  $\alpha$  multiplied by  $\Delta x$  and let us let  $f$  of  $x_i$  let us call that equal to  $\beta$  the absolute value of  $f$  of  $x_i$  we will call that as  $\beta$ . **So** we will have  $\beta$  epsilon precision divided by  $\Delta x$  **so** that is our total error. Now we want to find out the value of  $\Delta x$  at which the total error becomes minimum.

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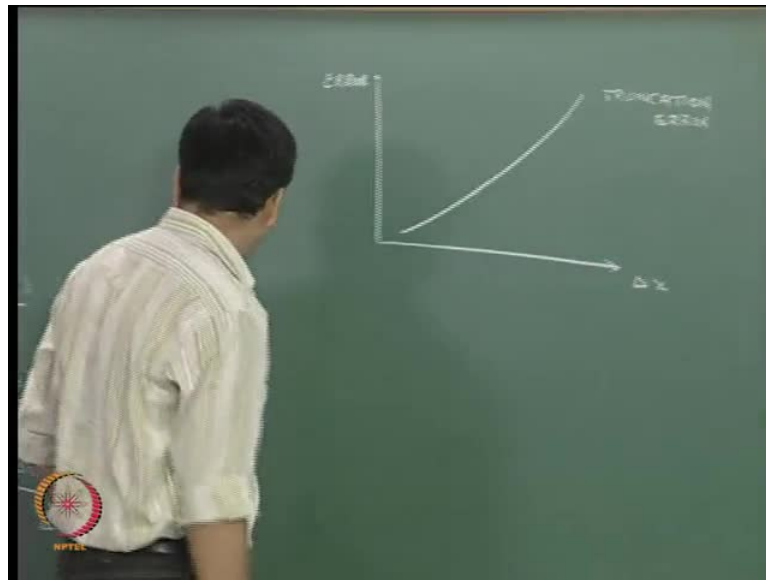


If now if we were going to plot the truncation and round off errors. **So** will start with a large enough value of delta x and we will start reducing the value of delta x.

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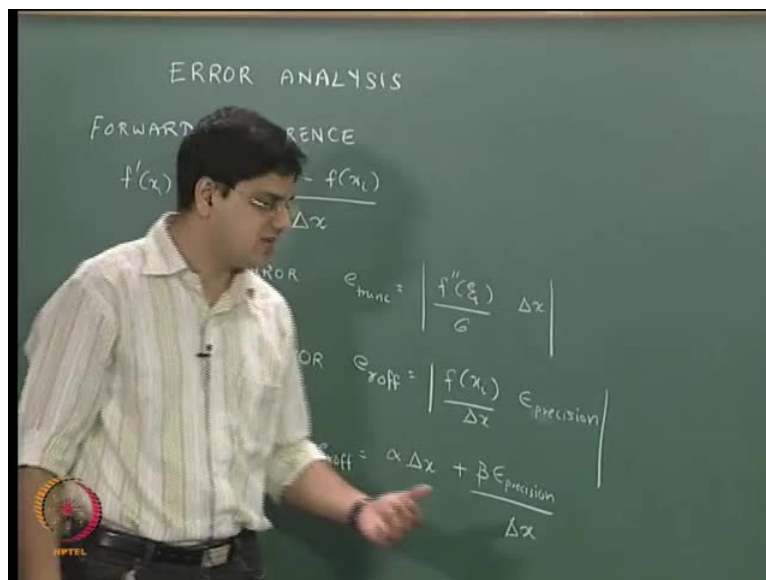


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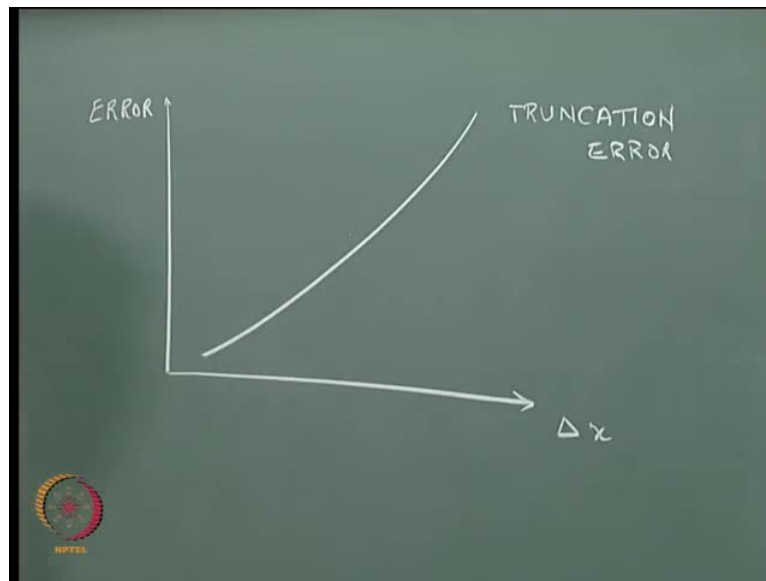


The truncation error is proportional to delta x. **So** as delta x decreases the proportional the truncation error will keep decreasing, **so** the truncation error will decrease something like this.

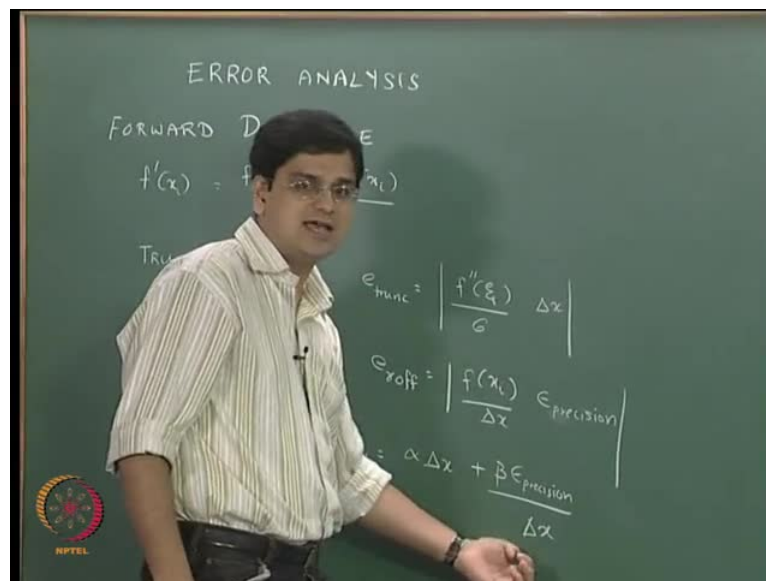
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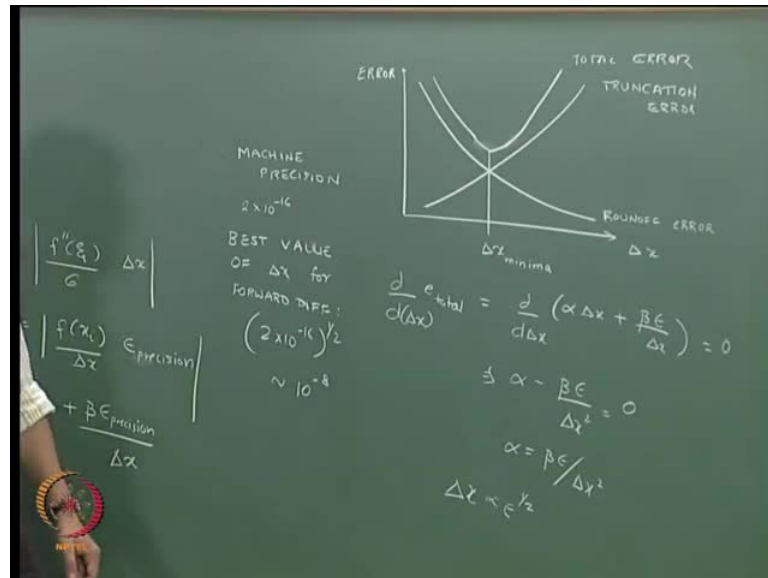
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The round off error on the other hand increases as the **delta delta** x decreases or it decreases as delta x increases. **So** for example if we are going to start with a very low value of delta x  $\epsilon$  will be a fairly large round off error **in in in** delta x, and as the delta x keeps increasing the round of error is going to decrease simply because delta x is in the denominator.



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This is how perhaps the round of error is going to look like. **So** if we sum these two guys up the total error will look somewhat like this with the minima happening at a particular value of delta x will call that as delta x minima or delta x where there is the minimum total error in the numerical derivative.

This is what we are going to get. And clearly the delta x that is going to minimize the total error is going to be given by d by d delta x of E total which is going to be equal to d by d delta x of alpha delta x plus beta epsilon by delta x equal to 0, which is going to be equal to alpha minus beta epsilon by delta x squared equal to 0 or will write alpha equal to beta epsilon by delta x squared, and which will yield us delta x that gives the minimum value of the error is going to be proportional to epsilon to the power half.

Now our machine precision for a double precision **machine the machine** precision that is, double precision is what Microsoft excel uses is of the order of 2 multiplied by 10 to the power minus 16.

So, the best value of delta x for forward difference is 2 to the power 10 to the power minus 16 to the power half and that is half of the order of 10 to the power minus 8 and if you recall what we observed a few minutes earlier we actually observed that the error when we started off with x equal delta x equal to 0.1 and we started decreasing that delta x, we found that the error happened the minimum error happened at around 10 to the

power minus 8. So, this is what we observed with the forward difference formula when we solved it in excel. Now we will do this entire derivation again for the central difference formulae, let me remind you the result that we got from excel using the central difference formula the  $\Delta x$  minima for central difference formulae. If you remember was of the order of  $10^{-5}$  to  $10^{-6}$  approximately in that range is what we had obtained in Microsoft excel.

Let us try to derive use the same idea in order to derive for this central difference formula. The central difference formula was  $f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1}))}{2\Delta x}$  which is equal to or the truncation error the round off error in this particular case is equal to some  $\alpha$  multiplied by  $\Delta x$  divided by  $\Delta x$ .

Where  $\alpha$  in this particular case is going to be absolute value of  $f'(x_{i+1})$  divided by 2 that is what the round of error is going to be proportional to the truncation error. If we recall the truncation error in the central difference formulae that central difference formulae was the second order accurate in  $\Delta x$ .

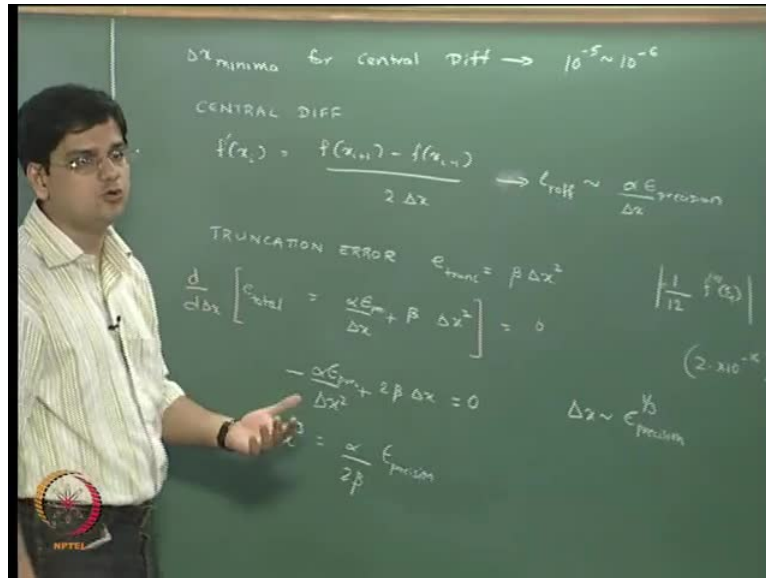
So the truncation error we can say is  $\beta \Delta x^2$ . This  $\beta$  was  $\frac{1}{12} f^{(4)}(\xi)$ . So this  $\beta$  was or the absolute what we take the absolute value.

It was  $\frac{1}{12} f^{(4)}(\xi)$  that is that was what the value of  $\beta$  we had we had obtained through the derivation. As a result  $e_{total}$  is going to be  $\frac{\alpha}{\Delta x} + \beta \Delta x^2$ , and to find out the value of  $\Delta x$  for which we get the error to be minimum what we are going to do is we are going to differentiate this particular equation this particular guy  $d$  by  $d \Delta x$  and equated to 0. And the result is going to be fairly straight forward we are going to get  $-\frac{\alpha}{\Delta x^2} + 2\beta \Delta x = 0$  or we will essentially get we take  $\alpha \Delta x^3$  squared on to the this side we have  $\Delta x^3$ .

What we should have over here is round of error is proportional to  $\alpha \epsilon$  precision by  $\Delta x$ . So we miss that so, what will get here is  $\frac{\alpha}{2} \epsilon$  times precision or our  $\Delta x$  is going to be proportional to  $\epsilon^{1/3}$  ok.

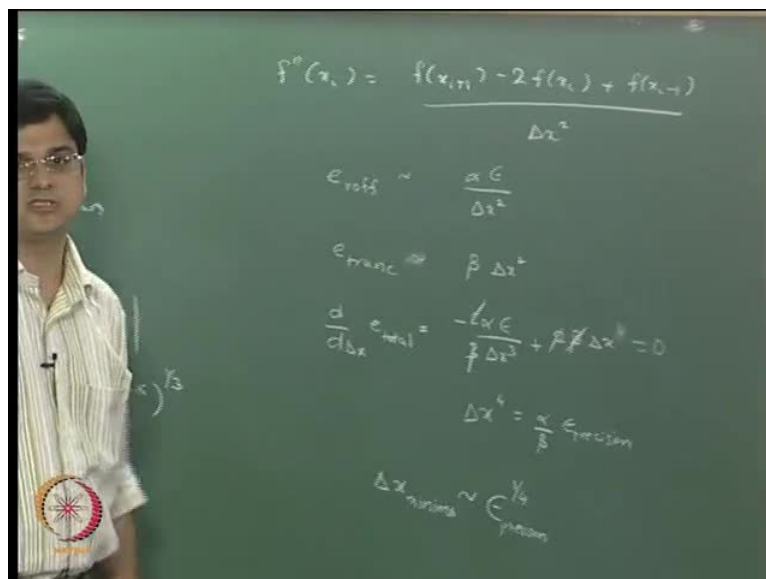
And epsilon precision as we said was  $2 \times 10^{-16}$  to the power minus 1 by 3 is approximately in the range of  $10^{-5}$  to  $10^{-6}$  ok.

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This is the result this is the reason why we get the central difference formula the delta x should be chosen to be cube root of the machine precision ok.

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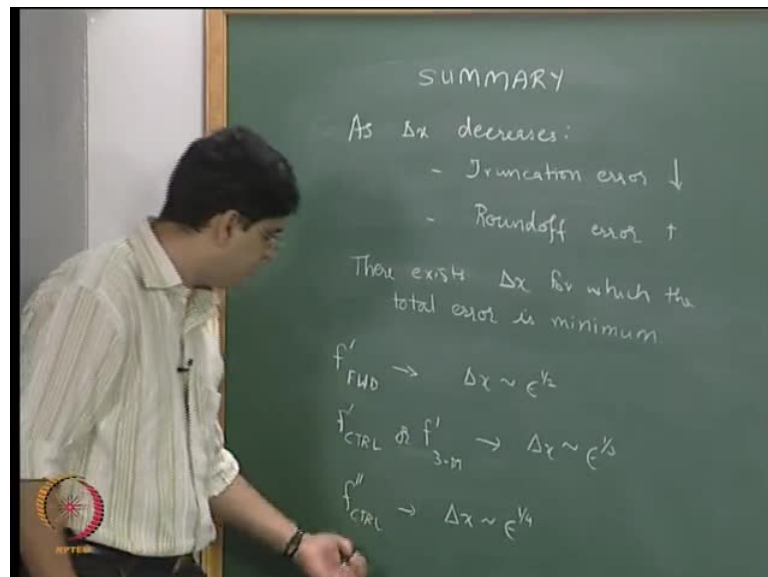
That is really what I wanted to cover for the error analysis in the same manner we can do error analysis for the central difference formula to get the second derivative. The second derivative is  $f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1}))}{\Delta x^2}$ .

The round off error is of the order of  $\alpha \epsilon$  divided by  $\Delta x^2$  and the truncation error is proportional to  $\beta \Delta x^2$ . The central difference formula for  $f''$  is second order accurate. So the total error is going to be equal to  $\alpha \epsilon / \Delta x^2 + \beta \Delta x^2$ .

We arrange  $\alpha \epsilon / \Delta x^2 + \beta \Delta x^2$  and we divide by  $\Delta x^4$  and we get  $\alpha \epsilon / \Delta x^4 + \beta \Delta x^2$ . The minimum error is going to be proportional to  $\epsilon^{1/3}$ .

This is what will get with respect to the error analysis. So, let me now summarize what we did in a error analysis and let us come up with what are really the ways to use numerical differentiation.

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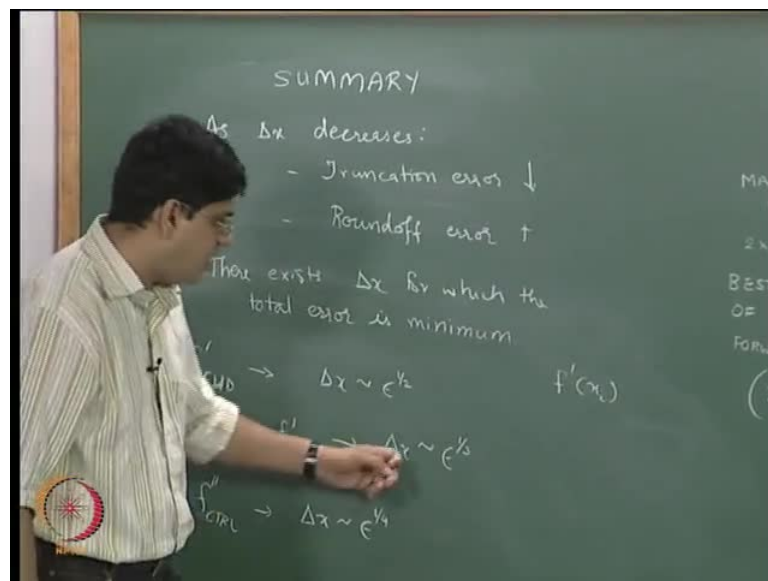


As  $\Delta x$  decreases truncation error decreases and round off error increases. So, there exists  $\Delta x$  for which the total error is minimum. So for forward difference for the forward difference formulae our  $\Delta x$  has to be proportional to  $\epsilon^{1/2}$ .

half for  $f'$  using central difference or  $f'$  using 3 point forward difference  $\Delta x$  is proportional to  $\epsilon$  to the power  $1/3$  and to use  $f''$  using central difference formula  $\Delta x$  is going to be proportional to  $\epsilon$  to the power  $1/4$  ok.

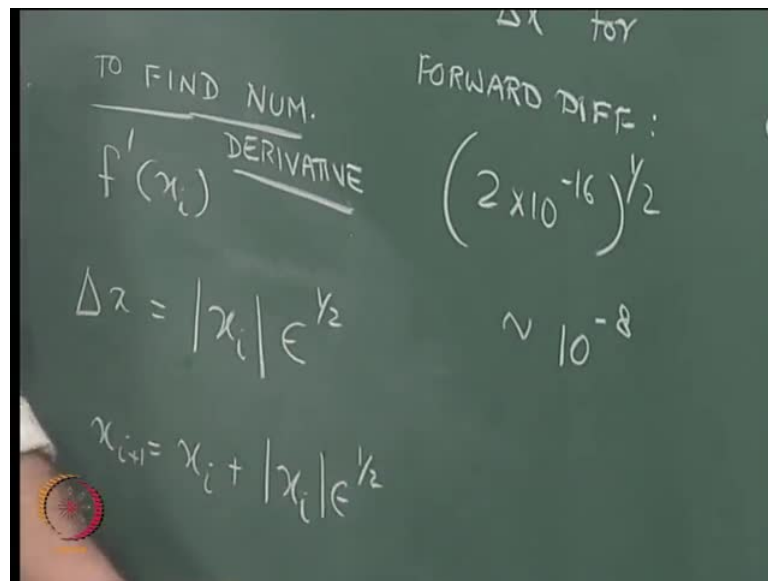
I am just stopping over here mainly because  $f'$  using forward difference,  $f'$  using central or 3 point different and  $f''$  using the central difference formulae are likely the most common numerical differentiations that a typical chemical engineer in count us.

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I would not go into anything anything beyond that now question is how do we choose the actual  $\Delta x$  even when we are going to implement. And the way we choose the actual  $\Delta x$  is let us say we want to find out  $f'$  of  $x_i$ . Keep in mind all these are in relative terms its they are relative with respect to the absolute values of  $\epsilon$  of the of the current system that we are we are looking at.

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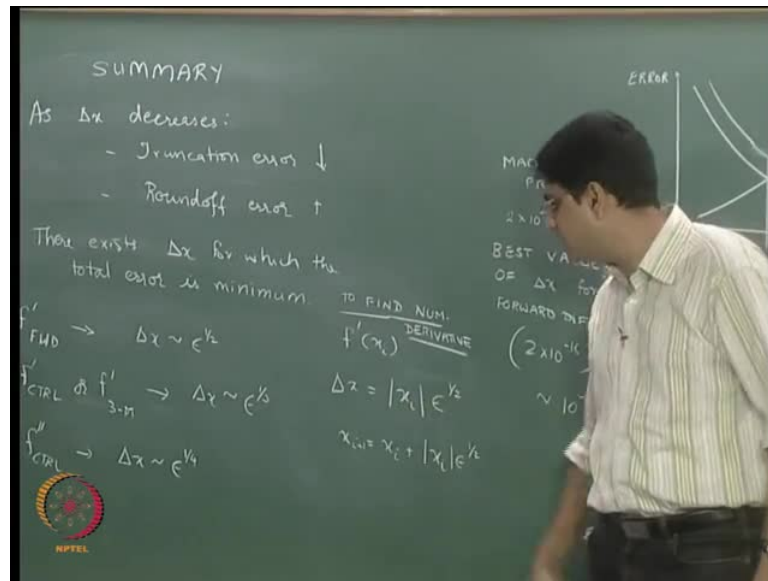


If we want to find the numerical derivative of  $f'$ . If we select let say we have selected the forward difference scheme than our delta  $x$  is going to be equal to the absolute value of  $x_i$  multiplied by epsilon to the power half. Do not just use epsilon to the power half, it is the absolute value of  $x_i$  multiplied by epsilon to the power half.

**So**  $x_{i+1}$  is going to be equal to  $x_i$  plus this guy for  $x_i$  plus 1. So,  $x_i$  plus 1 is going to be equal to  $x_i$  plus  $x_i$  epsilon to the power half. **So** if  $x_i$  is positive then  $x_i$  plus is going to be equal to  $1 \times x_i$  multiplied by  $1 + \epsilon$  to the power half **ok**.

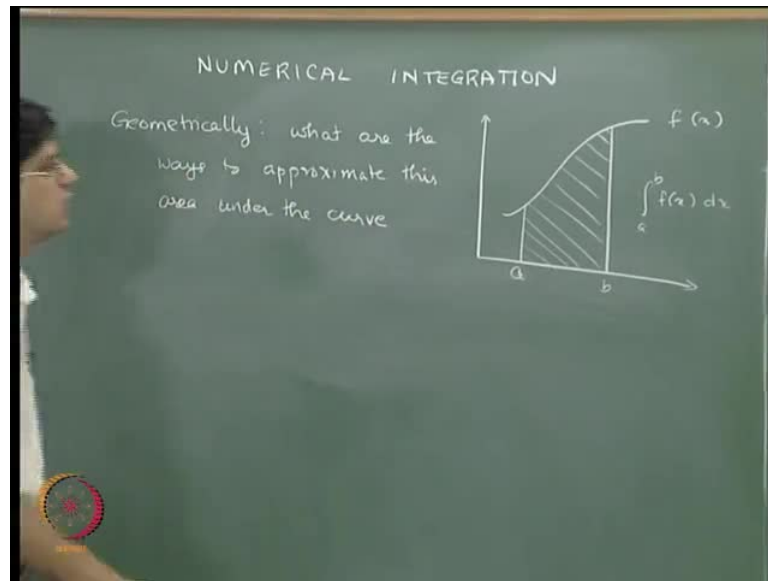
**So** that is the choice that you need to take **with with** respect to what delta  $x$  you will choose for forgetting the numerical derivative and if you want to get the numerical derivative  $f'$  using central difference formula it is going to be absolute value of  $x_i$  multiplied by epsilon to the power one third because, this is what we get over here. **So** this is how we are going to practically implement the overall use of numerical differentiation. So, to summarize what we have done in numerical differentiation what we started off with was **we we** just said that geometrically numerical differentiation means finding the slope  $f'$  of a particular curve and then we saw the forward central and backward difference methods and the geometric interpretation of using them.

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Next we use the Taylor series expansion in order to derive the forward and central difference formula for  $f'(x)$  and the central difference formula for  $f''(x)$ , then we went on to a method called the method of undetermined coefficients in order to get the derivation for  $f'(x)$  and  $f''(x)$ . So that is what we covered with respect to deriving this overall formulae after that we covered the error analysis of the truncation error we saw of that the error in  $f'(x)$  was proportional to  $\Delta x$  for the forward difference formula. What was proportional to  $\Delta x$  squared in the central difference formula proportional to  $\Delta x$  squared in a 3 point forward difference formula, then we saw that as  $\Delta x$  is changed round off error increases as  $\Delta x$  decreases the truncation error decreases as  $\Delta x$  decreases. And there is a particular value of  $\Delta x$  at which the error is minimum and then we finally, derived the condition for which  $\Delta x$  is minimum and we finished off by giving practical hints as to what  $\Delta x$  that we need to choose, such that this particular error in finding out the numerical derivative is minimized.

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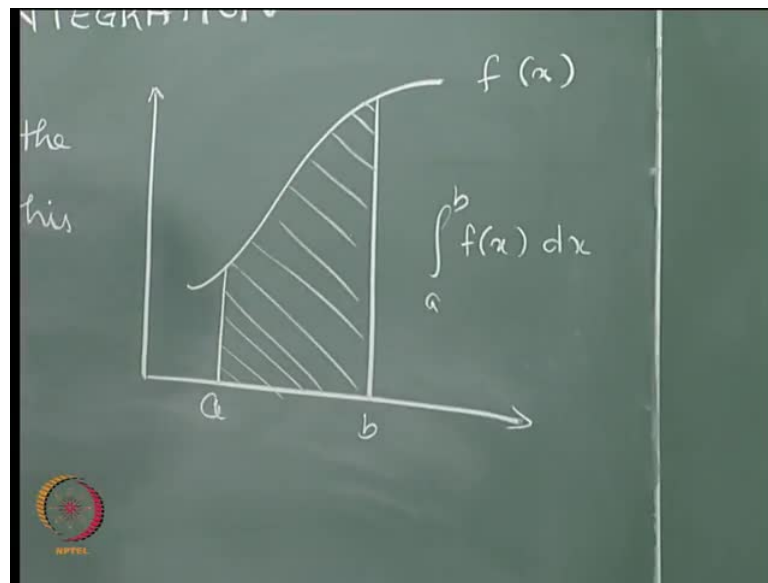


That is essentially what I intended to cover in numerical differentiation. Now will go to the second part of this particular module and that is numerical integration. Now we go on to numerical integration as we had said earlier numerical integration is nothing but, finding the area under a curve. So in fact not just numerical integration in general is finding the area under a curve ok.

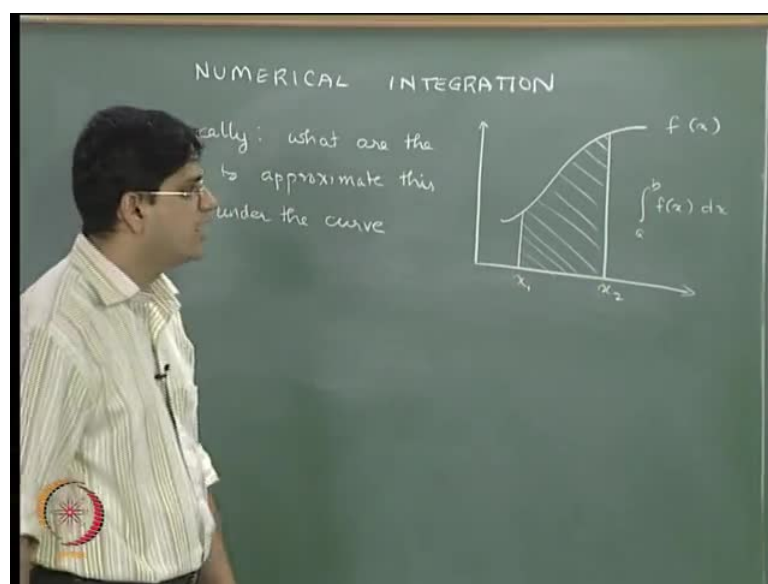
Let us say we have some curve  $f$  of  $x$  and we want to find the integral of  $f$  of  $x$   $dx$ . So this integral of  $f$  of  $x$   $dx$  is nothing but, this particular area under the curve. So geometrically what are the various ways to approximate that area.



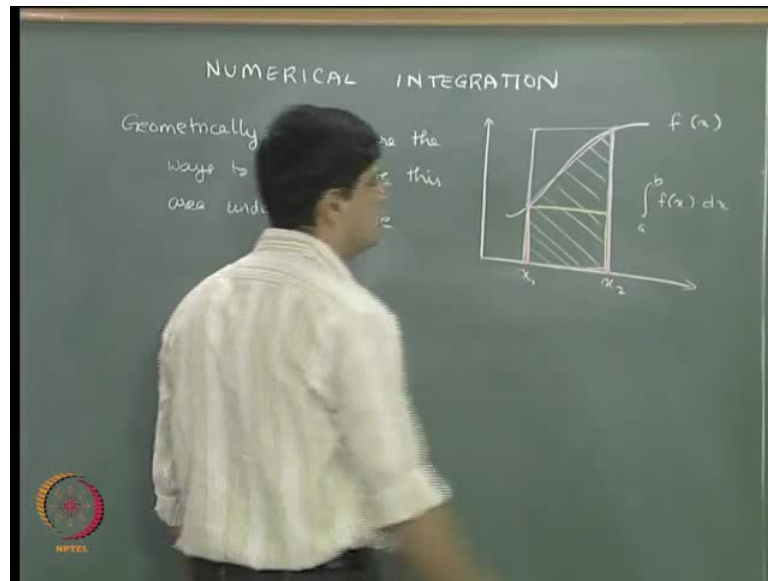
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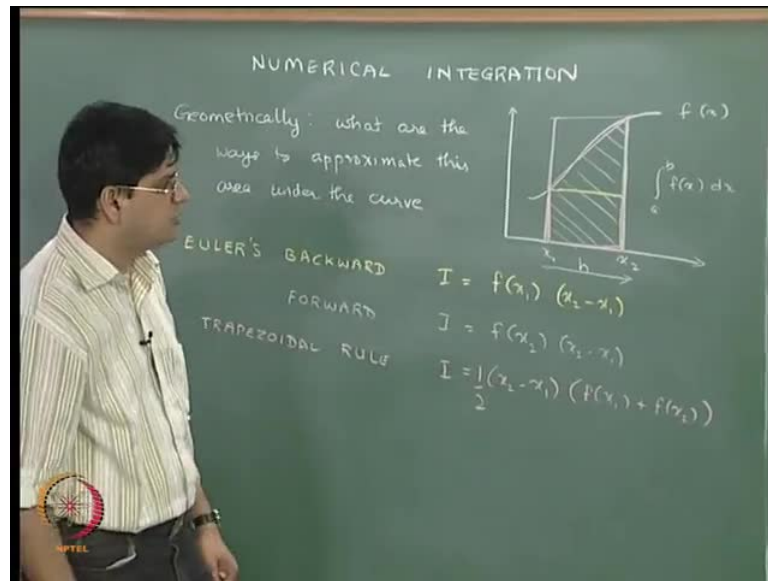


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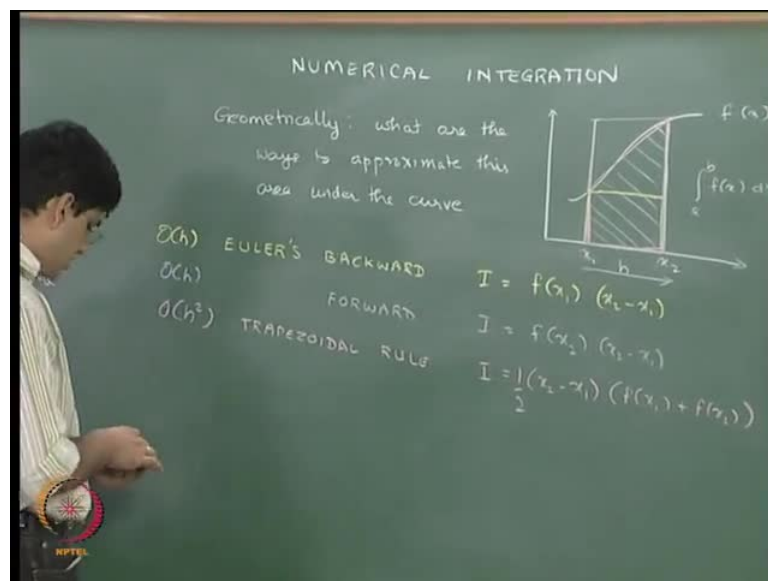


So **the** geometrically the various ways to approximate the area under the curve is basically this particular interval we can split into many intervals since, the splitting up usually is going to be our choice we will split up into many various equally spaced intervals, and then find area under the small part of the curve for each of these intervals. **So** let us say that the entire region I have split into various intervals and the smallest interval is now represented as this particular curve. **So what what** I have done is for this curve of looked at the smallest interval and then I have zoomed in that particular smallest interval and let me call this the smallest interval rather than going from a to b **let** **let** me call this going from say  $x_1$  to  $x_2$ . And now I want to find out the integral going from  $x_1$  to  $x_2$  of  $f(x) dx$ . **So**, what I will do is I will find out integral from  $x_1$  to  $x_2$  of  $f(x) dx$   $x_2$  to  $x_3$   $x_3$  to  $x_4$  **and and** so on starting with  $x_1$  equal to a and ending at  $x_n$  equal to b. So, that is the strategy that I will do now we zoom in into one particular interval and try to see what are the **different different** ways. And different areas that one can possibly think of is you connect this particular horizontal line and the area under this yellow line is going to be one possible way of approximating that area under the curve. The other possible way of approximating the area under the curve is take this particular line and complete the rectangle over here so, that is the purple area. **So** the first area is the yellow rectangle, the second area is the purple rectangle and the third area is you connect this point with this point with a straight line, and the third is the area under the trapezoid **ok**.

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Based on this we have 3 different numerical approximation. The yellow numerical approximation is going to be Euler's backward method in which the integral I will ride back will equal to f of x 1 multiplied by x 2 minus x 1. The length of this segment is x 2 minus x 1 the length of this segment is f of x 1 so, the integral I is going to be nothing but, f of x 1 multiplied by x 2 minus x 1.

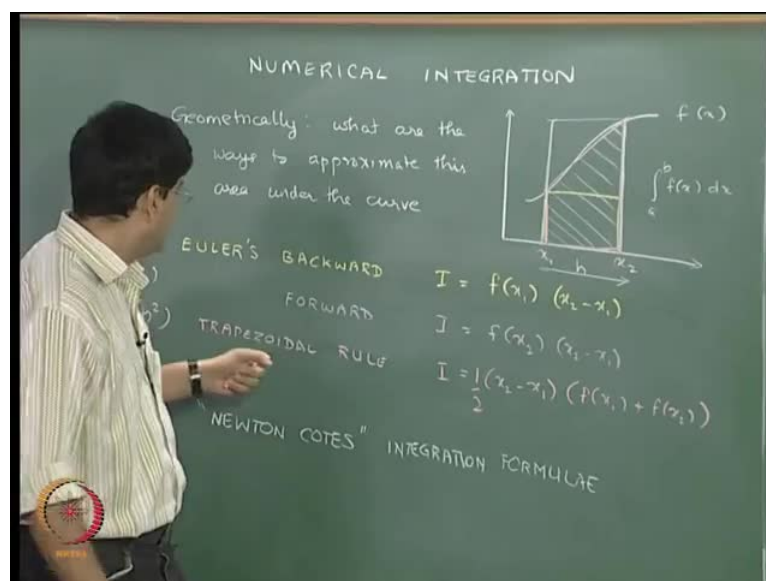
Euler's forward method is going to be I equal to f of x 2 multiplied by x 2 minus x 1. **So** this is f of x 2 and the this particular area for this particular this rectangle is f of x 2

multiplied by  $x_2 - x_1$  that is the Euler's forward method. And the third method that we talked about is called the trapezoidal rule. And in trapezoidal rule I is going to be equal to the area under the trapezoid. The area under the trapezoid is if you remember from our basic geometry is nothing but, this length multiplied by this length plus this length divided by 2.

Ok so the trapezoidal way is going to be that is the breadth multiplied by  $1 + \frac{1}{2}$  divided by 2. That is the area under a trapezoid will substitute those values over here breadth is nothing but,  $x_2 - x_1$  and we have this term half multiplied by  $f(x_1) + f(x_2)$ . Right its half multiplied by breadth multiplied by the first length plus the second length and that is going to be the trapezoid rule ok.

So based on the geometric interpretation we have the Euler's backward method Euler's forward method and the trapezoidal rules. These are the 3 different ways these 2 methods are first order accurate in  $\Delta x$ , if we call this difference as  $\Delta x$  or let us call this is in using an a simpler notation  $h$  if we call this particular difference as  $h$  the Euler's backward difference method is order  $h$  accurate. The forward difference method is also order  $h$  accurate the trapezoidal rule is order of  $h^2$  accurate ok.

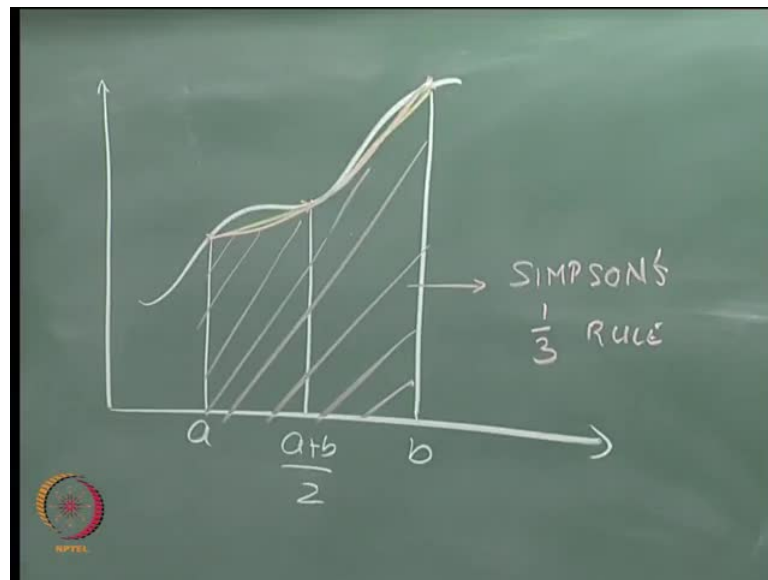
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So what we are actually going to do in the next lecture onwards is going to derive this trapezoidal rule. We will actually derive so this is using the geometric method that we

have derived derived trapezoidal rule were, we will derived trapezoidal rule once again using 3 different methods. In in the next lecture and then we will go on to higher order formulae these particular formulae are clubbed under the name Newton cotes integration formulae.

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Ok in the forward and backward Euler's in the Euler's method we use the function value only at one point and create a rectangle in case of trapezoidal rule we use the function value at 2 points and create a trapezoid. We have higher order Newton cotes formulae where we will use 3 points 4 points and so on and so forth. In order to create up a more accurate method. And so essentially what we are going to see in the next lecture is this is, let us say we have an arbitrary curve of this sort and we want to find an integral between a to b, one possible thing is to take this.

Particular midpoint which is  $\frac{a+b}{2}$ . And of course,, one thing we can do is we can construct a trapezoid between the first two points and another trapezoid between the next two points and get the area under the curve. Other alternative is to connect these 3 points with a second order polynomial curve and that is second order polynomial curve is probably going to look like this and so the area under the red curve can be obtained as a better approximation of the of of the true area and this particular red curve will be known as Simpson's one third rule ok.

If instead of 3 points we are we are going to draw in third order curve to the four four data points will get Simpson's three eighth rule and so on and so forth. We can go to higher order rules as well usually, we do not go beyond the Simpson's three eighth rule and we will see why why that particular thing happens or that that particular thing is what we do in in the next lecture. And after that we are going to cover the overall derivations and the error analysis of all this all this these methods. So that is going to be our strategy for for the next lecture while covering the numerical integration formulae. Thank you and I will see you in the lecture 3.