Computational Techniques

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Module No. # 06

Lecture No. # 01

Differentiation and Integration

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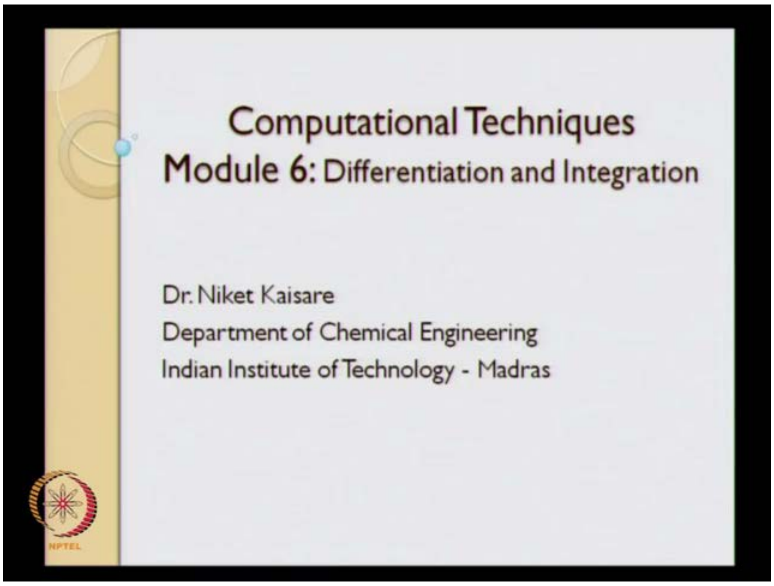

Hello and welcome to computational techniques web course. We are now in module 6; and module 6, we are going to discuss differentiation and integration - numerical differentiation and integration specifically.

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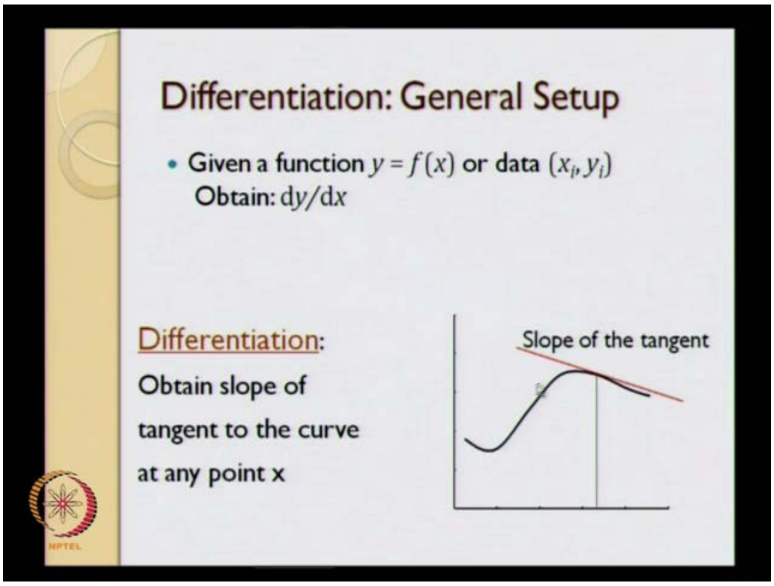

So, given a function y equal to f of x; sometimes we may not have function y equal to f of x, but just data points x i or y i or methods to just generate this data points (xi, y i).

So, no matter how we do that. Let us assume that we have some kind of a curve y equal to f of x, and we are interested in obtaining the differentiating and obtaining the value d y by d x what it means geometrically is the differentiation is nothing but obtaining slope of the tangents segment to the curve at the desired point.

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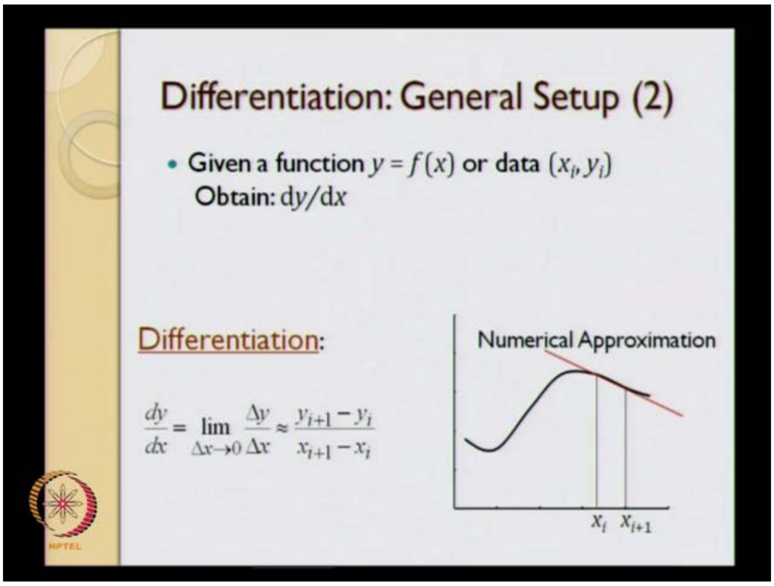

So, this is the curve f of x and the slope of the tangent at f of x is just the numerical derivative, but when if f of x is not available or if it is very difficult to differentiate this f of x analytically, we can resort to numerical techniques. And numerical techniques, this is the numerical approximation for the f of x. d y by d x definition is nothing but limit as delta x tends to 0 delta y divided by delta x, which we can approximately write as equal to y of i plus 1minus y i divided by x i plus 1 minus x i; this is delta x and the numerator is delta y.

So, as we bring x i plus 1 closer and closer to x i, we will start approaching - the numerical derivative - will start approaching the analytical or the actual derivative d y by d x. We cannot take x i plus 1 very close to x i, because the round of errors will start dominating. This particular method is just the first order method to find a numerical differentiation; we will use Taylor series expansion in order to get higher order and more accurate methods for numerical differentiation.

So that is the overall general set up and if we compare from the slope of the tangent, the actual tangent to this with the numerical approximation of the tangent. So, in this particular figure, when we look at that as you can compare the two red lines, the slope is different in those two cases.

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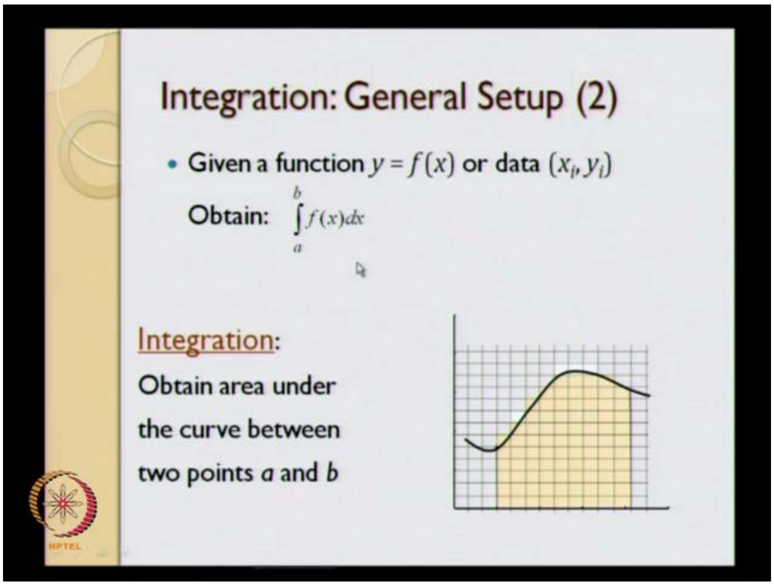

So, what is happening is that, numerical approximation is not going to be an exact representation of the differentiation, but it is going to be an approximate representation of the differentiation. Let us now talk about integration; in integration, again we are given the function y equal to f of x or some data x i, y i between the values a and b, and we are interested in finding out the integral from a to b of f x d x.

Integration is nothing but obtaining the area. This is the same curve, integration is obtaining the area under that curve between points x equal to a to point x equal to b. This shaded area that we see over here is the integral from a to b f x d x.

And geometrically what it means is, we will draw the various grid points as shown over here and integration is nothing but the summation of the total number of rectangles that we have over here. Clearly, if we take smaller and smaller gaps in this particular gridding, that means, if we grid this in a much more finer mesh, we will get more accurate value of the integral when we do this numerical integration. And those concepts are something that we will we will try to understand when we do numerical integrations sorry we will when we do numerical integration using various methods for integration.

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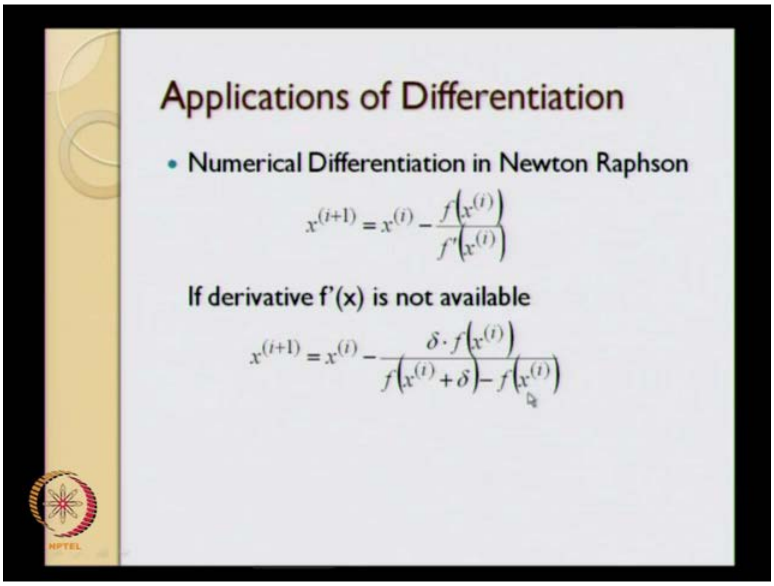

Now, the next question, of course that comes to mind is where is differentiation-numerical differentiation - and numerical integration going to be used. And the application of numerical differentiation is one application is in Newton Raphson's method, what if f of x is obtained such that it is very difficult to find f dash of x? In in such cases, in Newton Raphson's method, we will use numerical differentiation. If f dash is not available, we can then use a numerical value of f dash, remember the numerical differentiation of f dash was x i plus 1 minus x i.

We will write x i plus 1 is nothing but x i plus delta. So, this is going to be f of x i plus delta minus f of x i divided by x i plus delta minus x i. So, the denominator for f dash is nothing but delta, because f dash is itself is in the denominator that delta becomes a numerator in this Newton Raphson's scheme.

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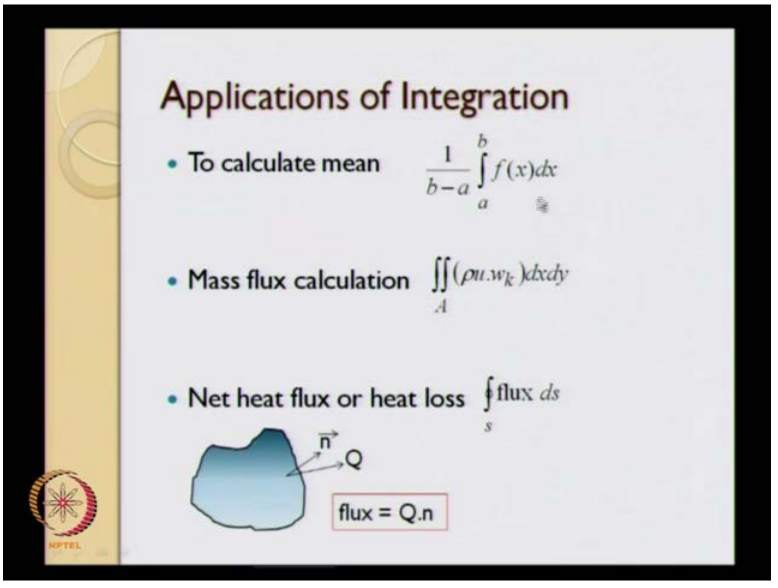

So, the Newton Raphson's scheme, when the analytical derivative f dash of x is not available becomes x i minus delta of f divided by f of x minus x plus delta minus f of x that is the value that we will get for the Newton Raphson's method. Couple of examples of numerical integration, is in order to calculate the mean; in the mean that we obtain was nothing but summation of x divided by the number of data points. But if we want to calculate the mean of an independent variable related to the dependent variable at the mean of the dependent variable f of x related to the independent variable x, the mean is calculated using an integral of this sort, 1 divide by b minus a integral from a to b f of x d x. So, this is one place where integration will be required. Another example, where integration is required is the mass flux calculation.

So, let us say we have a tube through which some kind of reactors of some kind of fluid is flowing. In that particular case, the mass flux of any species in the fluid is going to be represented as the area integral with respect to x and y coordinates of the overall flow flux, which is row multiplied by u multiplied by w k, w k is nothing but the mass fraction of this species k in in this particular system.

Another example is to calculate the net heat loss through happening through this particular surface. And the net heat loss through the surface is the surface integral of flux multiplied by the surface the differential surface d s will integrated over entire surface s. So that is going to be the flux that exists from any infinite area in this overall body. This is how we will calculate the flux.

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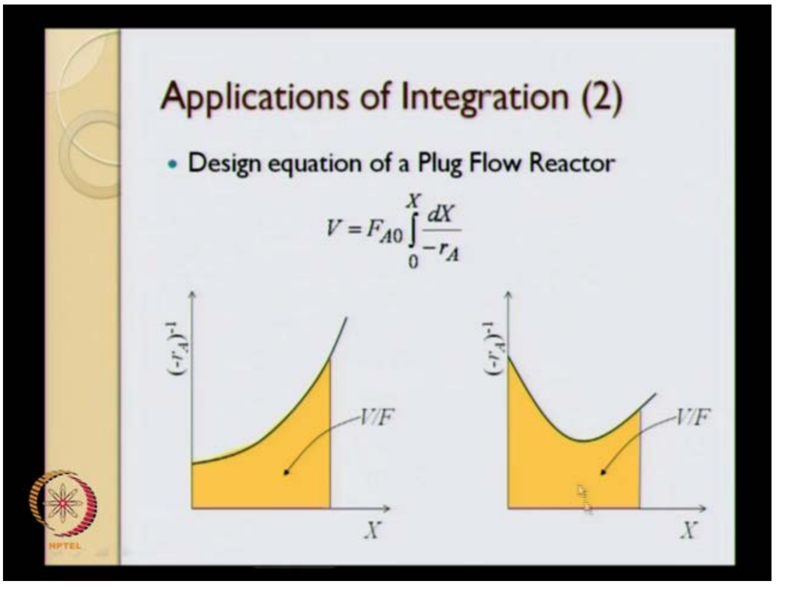

Another example of integration is the design equation of plug flow reactor. So, if you have done your reaction engineering course already, you will recognize this design equation for plug flow reactor and you will also be able to recognize this Levenspiel plots in order to find out the volume of the p f r and volume of c s t r's that we are going to use.

And this particular case what we do is, we plot 1 divided by r A as the y axis and conversion X on the x axis and this is the curve that we get. The area under the curve is nothing but the volume of the c s t r that that is going to be required v by f for that c s t r.

So, this is the curve we get for a first order reaction kinetics for example, and this is the curve that we will get for biological reactors.

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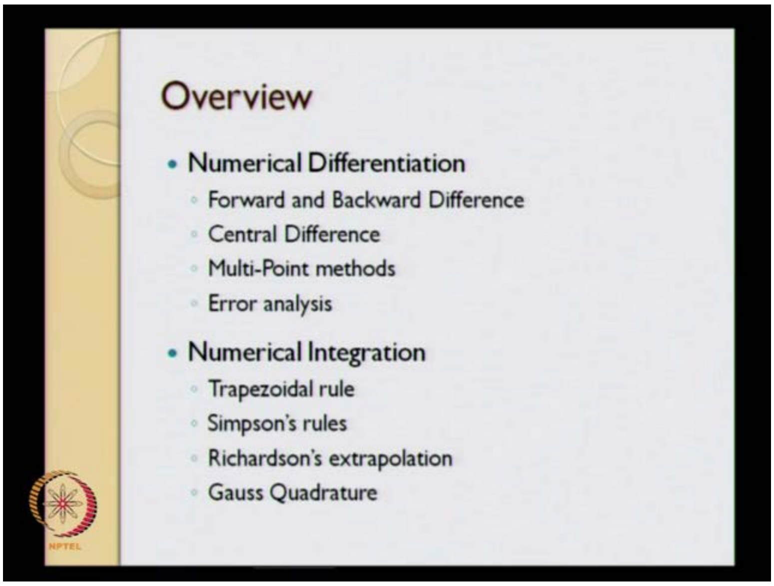

So, what are we going to cover in this module? The overview that we are going to cover in this module - we will first cover numerical differentiation perhaps in about one and half to two lectures, and then we will cover numerical integration, which will be covered perhaps in the above three and half four lectures. In numerical differentiation, we will look at forward, backward and central difference schemes, and then we will look at multi point method, and then we will do the error analysis. As i had mentioned in the passing previously, what we find is that we take x i plus 1 closer and closer to x i in numerical differentiation scheme, we find the error reducing.

But we cannot bring x i plus 1 too close to x i, because then although the truncation error reduces, the round of error is going to increase, that is what we will cover overall in the numerical differentiation. In numerical integration, we will cover various methods to do numerical integrations, specifically the trapezoidal rule, Simpson's one third and three eights rule, then we will talk about Newton's extrapolation how we can use sorry Richardson's extrapolation how we can use Richardson's extrapolation to improve Simpson's one third, three eight's rule or trapezoidal rule, and finally, we will talk about Gauss quadrature method. The first two methods come under the more general title of Newton cotes formulae, whereas Gauss quadrature method is kind of an open method.

We will talk of all these methods in the numerical differentiation and integration that will cover in the current module.

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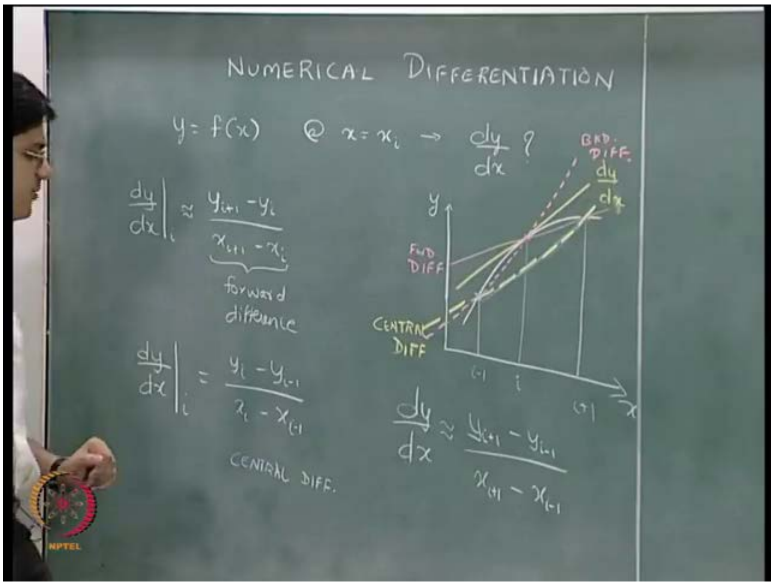

Start off with numerical differentiation over here. We have, So, at any point x i, we want to find d y by d x. Say y equal to sum function f of x at x equal to sum x i, we want to compute d y by d x that is the question that we are trying to ask ourselves. d y by d x is nothing but the slope of the curve f x versus x at value x i.

So, let us make the curve in this form; let us consider this as point i; let us consider this as point i plus 1 and let this be point i minus 1. So, we are interested in finding out the slope of this particular curve. The slope of this curve is the slope of the tangent to this curve, at point i. So, I will just draw the tangent segment over here; so the yellow represents the true derivative d y by d x. We are plotting x versus y; x as the abscissa, y as the ordinate.

So, at x equal to x i, we can write d y by d x, at i as approximately equal to y i plus 1 minus y i divided by x i plus 1 minus x i. This is the forward difference form and this can be represented as a line - the slope of the line - joining the points x i y i with the point x i plus 1 y i plus 1.

So, the red line that I am showing over here is the forward difference approximation and alternatively, we can write d y by d x at i as y of i minus y of i minus 1 divided by x i minus x i minus 1. Just the way we have written it in this form, we can write it alternatively in this form. This becomes our central difference formula and the central difference formula, in this particular case is going to be nothing but the line joining x i minus 1, y i minus 1 to x i y i.

So, I will have this; join with a dotted line and this I will call as backward difference. And the third possibility, again the third possibility that you would had considered previously is what is known as the central differences. And in the central differences, we will have d y by d x written approximately equal to y i plus 1 minus y i minus 1 divided by x i plus 1 minus x i minus 1. What that is, is nothing but the slope of the curve that joins the point x i minus 1 y i minus 1 with the point x i plus 1 y i plus 1. So, its slope of this particular dotted line, I have not drawn it too well; so I will just join it with another yellow dotted line over here and this is the central difference.

So, the yellows solid line is the true d y by d x, the true derivatives of the function y equal to f of x with respect to x, at point i; the red solid line is the forward difference approximation. We can clearly see over here that the forward difference approximation of the d y by d x is, there is a fair amount of error associated with it; likewise, there is a backward difference approximation shown by this particular dash line, there is a fair amount of error even in the backward difference approximation for this particular system. Slope of the dash line in the central difference approximation turns out to be much closer to the slope d y by d x compared to either of those two red line segments that I have shown.

So that is the whole idea behind using some of the forward and backward and central differences in order to get the numerical derivatives of the approximations of the numerical derivatives in given a function either given a functional form f of x or there has to be some mechanism to generate the values of y, given the values of x using some kind of a function y equal to f of x.

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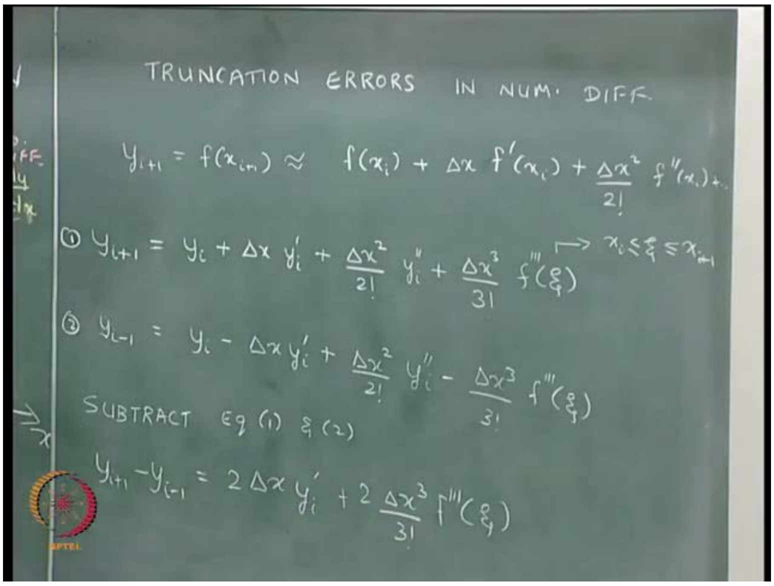

So, let us analyze what are the various truncation errors associated with these numerical derivatives. Truncation errors in numerical differentiation y of i plus 1 is nothing but f of x of i plus 1. So, f of x of i plus 1, we will write that approximately equal to we will take a Taylor series expansion around x i. So that is approximately equal to f of x i plus x i minus x i minus 1, we will write that as delta x f dash of x i plus delta x squared by 2 factorial f double dash of x i plus dot dot dot that is what our y i plus 1 is going going to be.

So, likewise, we can write y i minus 1 also. So, I will I will just write y i plus 1 again in the short hand notation, y i plus 1 is equal to y i plus delta x multiplied by y dash i plus delta x squared by two factorial multiplied by y double dash i plus delta x cube by 3 factorial multiplied by, in this particular case we will write f triple dash of zeta, where zeta is sum point lying between x i and x i plus 1; we get this using the mean value theorem; we are able to obtain this.

Likewise, we will be able to write as y i minus 1 as y i minus delta x times y dash i plus delta x squared by 2 factorial y double dash i minus delta x cubed by 3 factorial f triple dash of zeta. Now, what we will do is subtract these two equations; if we subtract these two equations, we will get y i plus 1 minus y i minus 1 is going to be equal to y i and y i will get cancelled; we will get x delta x plus delta x multiplied by y dash.

So, it is going to be 2 times delta x multiplied by y i dash. These terms are again going to get cancelled and this will be plus 2 times delta x cube by 3 factorial multiplied by f triple dash of zeta.

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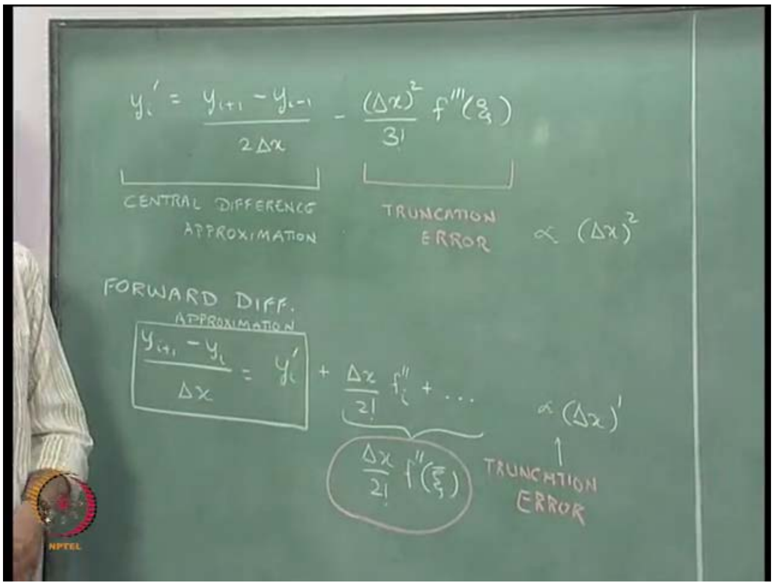

We divide throughout by 2 delta x and we take this particular term on to the left hand side, rearranging we will we will get the final result, that is, y i dash is going to be equal to y i plus 1 minus y i minus 1 divided by 2 delta x, we have divided throughout; we have taken this 2 delta x and divided throughout. So, this 2 and this 2 will get cancelled, instead of delta x cubed, we will have delta x squared, and because we have taken this term to the other side, it will get a negative sign.

So, we will have this as minus delta x squared by 3 factorial f triple dash of zeta; this part is the central difference approximation and this represents the truncation error. And in the central difference approximation, the truncation error is proportional to delta x squared. So, that means, if you make the delta x one tenth, the truncation error is going to reduce by one hundredth; if you double the delta x, you are going to make the make the error - truncation error - in d y by d x 4 times greater.

So that is what this this particular thing means. So, in conclusion y i dash, that is the first derivative of y i using the central difference approximation is, y i plus 1 minus y i divided by root wise delta x and the truncation error in the central difference is of the order of delta x squared.

Now, let us look at the forward difference approximation. In forward difference approximation, let us go back to what we had written over here. What we will do is, we will take y i on to the left hand side and divide throughout by delta x.

When we do that, what we will get is y i plus 1 minus y i divided by delta x is going to be equal to y i dash plus delta x by 2 factorial f double dash of i plus bunch of other terms. This is the leading term over here. based on another mean Again applying mean value theorem, this term will become delta x divided by 2 factorial f double dash of sum value sum other values zeta; we will just call it zeta bar, because this zeta is different may be different from this particular zeta.

So, in this particular case, this becomes our forward difference approximation and this represents the truncation error; and truncation error in forward difference approximation is proportional to delta x to the power 1 or its proportional to delta x.

And going back to the geometrical interpretation that we had of Newton's forward difference and backward difference and central difference formulae, this is what we had seen with forward, backward and central difference. Forward backward and central difference and what we had stated at that time is from this particular cartoon, it looks as if central difference approximation does a better job of approximating the actual derivative numerically compared to the forward difference and the backward difference.

The derivation that we have obtained using the Taylor series approximation over here verifies that particular geometric intuition or the geometric claim that we had made in the in the previous part of this lecture that, truncation error reduces as delta x squared for central difference, where as it reduces as delta x to the power 1 for the forward difference approximation. So, at this stage we will end the module 1 sorry lecture 1 of module 6. What we have covered so far is forward and central difference approximation for the first derivative of any function f of x. What we will cover in the next lecture is to look at the higher derivatives, that is, f double dash, f triple dash of x so on and so forth, as well as higher order accurate formulae. We will use another different method called method of undetermined coefficients in order to determine the higher order formulae also and finally, we will finish off with talking about truncation versus round of errors.

So, what we have seen so far is how to get the first derivative of that is d y by d x given some kind of function f of x either a function f of x are discrete value of f of f x at certain given points of of x. We have looked at how we will get the first differential with that. Now, let us look at how to get the second derivative from this.

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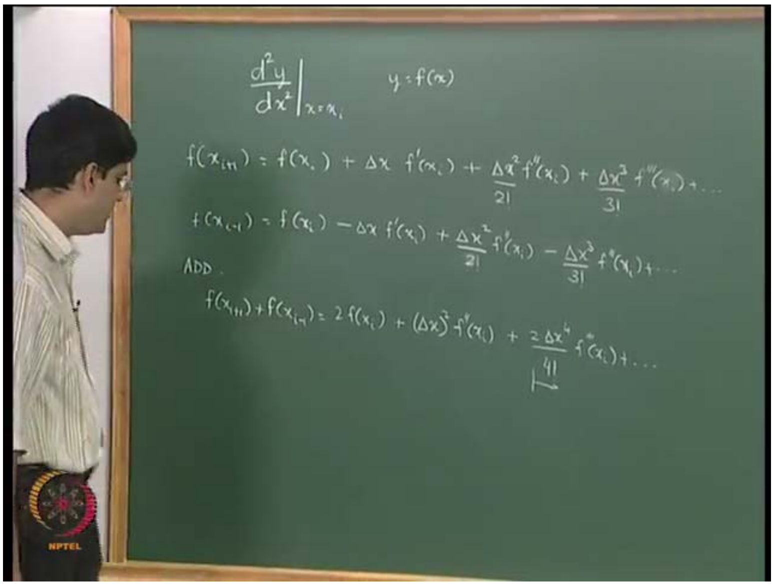

So, what we want to get actually is d squared y by d x squared at x equal to x i. So, this what we are interested in getting, where y equal to f of x, so that is the overall function that we have. As we have done before, what I will do is, I will write down the same expressions all over again is f of x i plus 1 is f of x i plus delta x times f dash of x i plus delta x squared times f double dash of x i plus delta x cube time f triple dash of zeta and I forgot, divided by 2 factorial and divided by 3 factorial over here.

So, this is the overall expression that we get on expanding f of x i plus 1. Likewise, we will expand f of x i minus 1 and that is going to be f of x i minus delta x times f dash of x i plus delta x squared by 3 factorial 2 factorial f double dash of x i plus sorry minus delta x cube by 3 factorial f triple dash of x i plus dot dot dot, in fact i will change this to f triple dash of x i plus dot dot dot. Now, i will add these two equations.

So, when I add these two equations, we will get f of x i plus 1 plus f of x i minus 1 is going to be equal to twice f of x i this term and this term will get cancelled; this term will be retained. So, its 2 times delta x square multiplied by f double dash divided by 2.

So, we will have plus delta x squared f double dash of x i this term and this term will get cancelled, the leading term that will remain is going to be 2 times delta x to the power 4 divided by 4 factorial f 4 dashes of x i plus dot dot dot.

So, this is the leading error term that we have. And for this part of the equation, we will apply the overall mean value theorem and we will convert from x i to zeta, where zeta is going to be any point that lies between x i minus 1 and x i plus 1. So, we will what we will do is, we will take this 2 twice f of x i on to so all the terms, rather except delta square f double dash, all other terms will take on to the left hand side and divide throughout by delta x squared.

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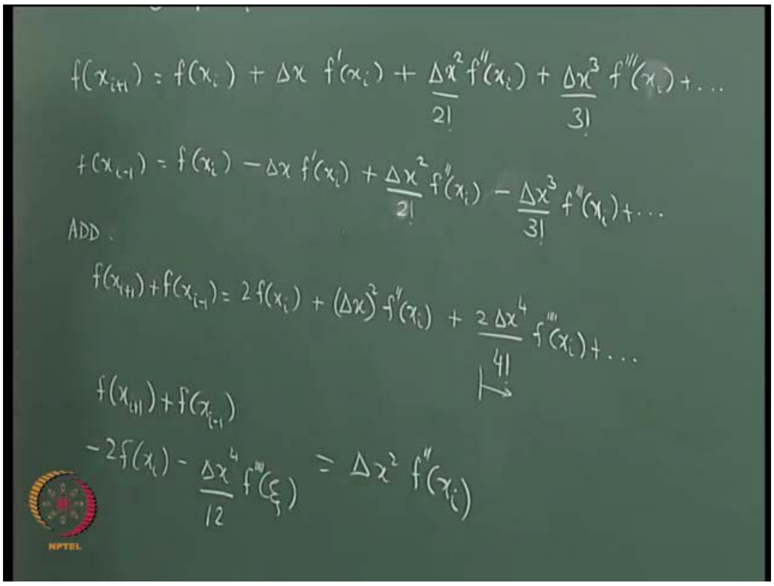

So, when we do that, we will have f of x i plus 1 plus f of x i minus 1 minus 2 times f of x i minus, so 4 factorial is going to be 4 multiplied by 3 multiplied by 2 multiplied by 1 that guy divided by 2 is going to be 4 multiplied by 3, which is essentially 12.

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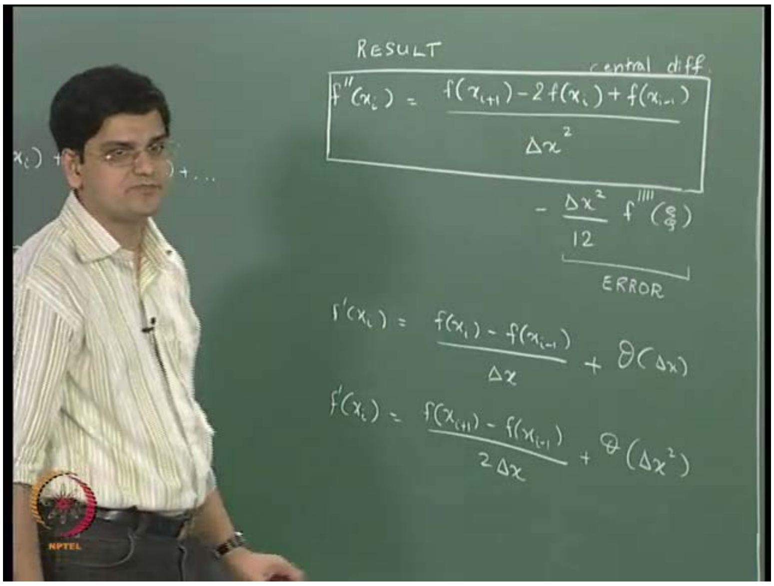

So, minus delta x to the power 4 by 12 f 1 2 3 4 of zeta is going to be equal to delta x square f double dash of x i. And we divide delta x square throughout and we will get our final result is f double dash of x i is going to be equal to f of x i plus 1 minus twice f of x i plus f of x i minus 1 divided by delta x squared.

So, if you look at this particular expression its f of x i plus 1 plus f of x i minus 1 minus twice f of x i divided by delta x squared, and this is the residual term, which would be delta x squared by 12 multiplied by f 4 dash of zeta. So, minus delta x squared by twelve f 1 2 3 4 of zeta; so this is the central difference formula and this is the error in the numerical derivative.

So, what we have seen so far is that for the central difference formula either whether we are going to use the central difference formula for finding f double dash or we are going to use the central difference formula for finding f dash, we observe that the error is proportional to delta x squared. So, as we reduce our delta x to smaller and smaller values, the error- the truncation error- in fact reduces as the delta x reduces.

And in the forward difference method or the backward difference method for getting f dash that reduction is directly proportional to delta x, whereas in the central difference method its proportional to delta x squared. As a result of this, the central difference methods are going to be more accurate than the forward or the backward difference methods.

So, in order to summarize the other f dash x values that we have gotten f dash of x i was equal to f of x i minus f of x i minus 1 divided by delta x plus error was of the order of delta. x f dash of x i that we wrote as the central difference formula was f of x i plus 1 minus f of x i minus 1 divided by twice delta x plus order of delta x squared and like this, we had also we could also write the forward difference method, where f dash of x i was equal to f of x i plus 1 minus f of x i divided by delta x.

So, these are the derivations based on the Taylor series expansion. What I will do next is, do one more derivation again of the same formula. The purpose of doing this derivation is to introduce a new method called method of undetermined coefficients. We will use this method, because this method is more general and you can apply to get higher order formulae more accurate formulae so on and so forth ok.

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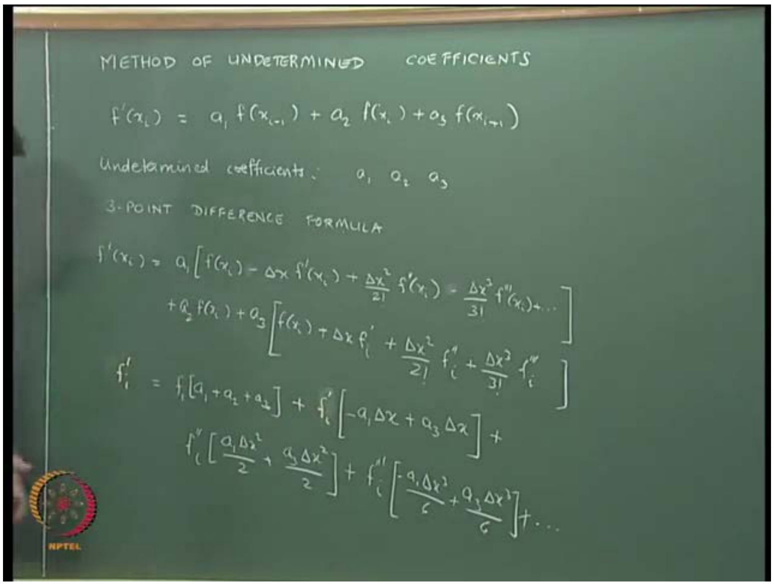

So, this method is called method of undetermined coefficients. So, we will go back to what we had written as our Taylor series expansions. We had written our Taylor series expansions for f x i plus 1; we had written our Taylor series expansion of our f x i minus 1, and then we could pick and choose which data points do we want to use in order to get the first differential or the second differential or higher order differentials of f.

So, I will demonstrate that method, again we will try to find f dash of x. So, I will write our f dash of x as sum a 1 multiplied by f of x i minus 1 plus a 2 multiplied by f of x i plus a 3 multiplied by f of x i plus 1.

So, our undetermined coefficients are a 1, a 2 and a 3. What we are trying to do is, we are trying to get a three point difference formula for differs derivative f dash of x at x equal to x i. So, we are trying to get a three point difference formula, why three point difference formula, because we are going to use point x i minus 1 x i and x i plus 1 in order to get to derive that particular formula.

So, what is the three point difference formula for f dash of x i? Three point different formulas for f dash of x i is nothing but the central difference. So, what we expect is really our a 1 over here; if we compare it to this particular equation what we expect our a 1 to be is minus 1 by 2 delta x.

We expect our a 2 to be equal to 0 and we expect our a 3 over here to be equal to 1 plus 1 divided by 2 delta x. So, we have three undetermined coefficients; so we require three equations - three linearly independent equations - in order to obtain unique values of a 1 a 2 and a 3.

So, we will substitute the Taylor series expansion over here and Taylor series expansion over here and the Taylor series expansion over here. So, we can write down f dash of x i is going to be equal to a 1 times f of x i minus 1, which is f of x i plus delta x i am sorry not plus, it should be minus delta times f dash of x i plus delta x square by 2 factorial f double dash of x i plus delta x cube by 3 or sorry again minus delta x cube by 3 factorial f triple dash of x i plus dot dot dot plus a 2 times f of x i plus a 3 times f of x i plus delta x f dash, I will just use short hand f dash of i plus delta x squared by 2 factorial f double dash of i plus delta x cube by 3 factorial f triple dash of i.

Now, we will collect the terms in f dash, f double dash, f triple dash and so on so forth. So, what we will get is f of x i multiplied by a 1 plus a 2 plus a 3. So, f i multiplied by a 1 plus a 2 plus a 3 plus f dash of x i multiplied by a 1 multiplied by minus delta x, a 2 multiplied by 0, because there is no f dash term over here and a 3 multiplied by plus delta x plus f double dash of i and the terms in f double dash of i are going to be a 1 multiplied by delta x square by 2.

So, a 1 delta x squared by 2 plus a 2 multiplied by 0 plus a 3 multiplied by delta x square by 2 and then, we will have other terms, which is f triple dash of i, and there we will have minus a 1 delta x cube by 6 plus a 3 delta x cube by 6 and so on and so forth plus dot dot dot.

So, now, what we have? we have On the right hand, right hand side we have and f dash of i term; on the left hand side, we have terms in f dash f i f dash of i, f double dash of i so on and so forth. So, what we will do is, we will identify each individual term with different colors f dash of i and we have this as f dash of i.

So, what this means is that the coefficient of f dash of i is nothing but 1 multiplied by f dash of i and that coefficient should be equal to this particular guy over here. So, we will equate that; we will equate the red box term in this particular- on the right hand side with the red number over here. All the other terms appearing should be equal to 0, keep in mind that because we do not know a 1 a 2 and a 3, we require three equations.

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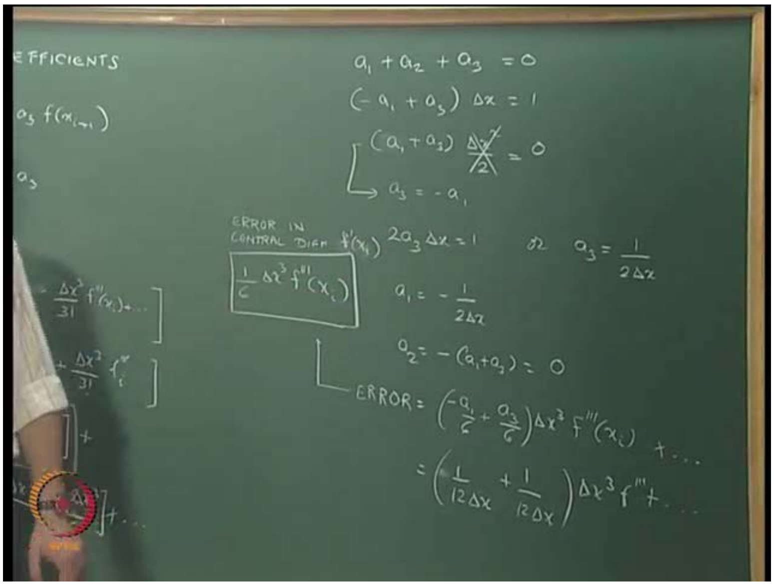

So, the first equation is going to be a 1 plus a 2 plus a 3 equal to 0; the second equation is going to be minus a 1 delta x plus a 3 delta x equal to 1 minus a 1 plus a 3 multiplied by delta x is going to be equal to 1, and the third equation is going to be a 1 delta x squared by 2 plus a 3 delta x squared by 2 equal to 0.

So, a 1 plus a 3 multiplied by delta x squared by 2 equal to 0 that is going to be our third equation. So, based on this we will be we will write a 3 equal to minus a 1; based on this equation substitute it over here; so, we will have 2 a 3 equal to 2 a 3 delta x is going to be equal to 1 or a 3 is going to be equal to 1 by 2 delta x. Based on this equation, we will have a 1 is going to be equal to minus 1 by 2 delta x and a 2. Based on this particular equation, is going to be minus of a 1 plus a 3, which will be 0, because a 1 is minus 1 by 2 delta x and a 3 is equal to 1 by 2 delta x. So, the value of a 1 is this; value of a 2 is 0 value of a 3 is 1 by 2 delta x.

So that is the overall equation that we get using the method of undetermined coefficient. So, we substitute a 1 over here, a 2 over here, a 3 over here and this is the result that we will get; essentially it is going to be the central difference formula.

Now, the question is what about the error term? And the error term to figure out what we have to do is substitute the value of a 1 a 2 and a 3 in this particular term. The terms that we have neglected, keep in mind that this has become zero; this term has become 0 this term has become 1, all the above all these terms are actually non zero, but we are neglecting it.

So, error is going to be equal to minus a 1 by 6 plus a 3 by 6 multiplied by delta x cubed multiplied by f triple dash of x i plus we have other terms as well. Now, if we substitute a 1 and a 3 in this particular equation, and this term turns out to be 0; then we will have to look at the next term; if this term does not turn out to be 0, this becomes the leading error term and we stop our error analysis at this point. So, let us substitute a 1 equal to minus 1 by 2 delta x and a 3 is equal to 1 by 2 delta x.

So, error is going to be equal to minus a sorry it is going to be equal to minus 1 by 2 delta x multiplied by minus 1 by 6. So, it is going to be 1 by 12 delta x plus 1 by 12 delta x multiplied by delta x cube f triple dash plus dot dot dot. And this becomes equal to 1 by 6 multiplied by delta x squared; this is delta x and 1 of the delta x is over here will get cancelled multiplied by f f triple dash. As a result of this, the error that we write over here is going to be equal to 1 by 6 delta x cube f triple dash of x i.

So, this is the error in central difference of f central difference f dash of x i. So, this is the overall derivation using the method of undetermined coefficients. Now, sometimes what we need is, we need either a higher order method using forward difference formula or higher order method using backward difference formula so on and so forth. So, what I am going to do is, I am going to show you one more result using what is known as three point difference formulae.

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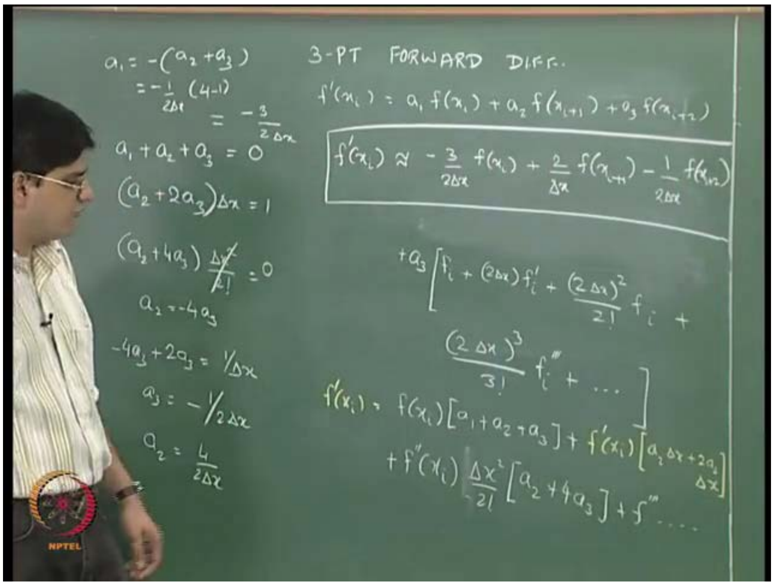

So, we are going to use the method of undetermined coefficients to get three point forward difference formulae for f dash of x i. We will write f dash of x i equal to a 1 f of x i plus a 2 f of x i plus 1 plus a 3 f of x i plus 2. Why is it called the three point forward difference formula, is because in order to get the derivative at this point x i, we are going to use the values at x i plus 1 and x i plus 2.

So, we are using for getting the derivative at this point; we are using this point, this point and this point. So, we are using three points ahead or forward of x i that is why it is called a three point forward difference formula for f dash of x i.

So, we substitute f of x i plus 1 and f of x i plus 2 in this particular equation. So, we will have a 1 f i plus a 2 multiplied by f i plus delta x f dash of i plus delta x squared f double dash of i by 2 factorial plus delta x cube divided by 3 factorial f triple dash of x i plus dot dot dot plus a 3 multiplied by f i plus. Now, we in this particular case x the difference between x i plus 1 and sorry the difference between x i and x i plus 2 is 2 times delta x.

So, it will be 2 times delta x multiplied by f dash of i plus 2 delta x whole squared divided by 2 factorial f double dash of i plus 2 times delta x the whole cube by 3 factorial f triple dash of i plus dot dot dot. Now, we collect the terms in f i, f dash i, f double dash i so on and so forth together. So, we will write f dash of x i is going to be equal to f of x i multiplied by a 1 plus a 2 plus a 3 plus f dash of x i; f dash of x i multiplied by a 2 times delta x plus 2 a 3 times delta x plus f double dash of x i; f double dash of x i multiplied by a 2 delta x squared by 2 factorial, I will take delta x squared by 2 factorial outside the bracket.

So, we will have a 2 multiplied by delta x square f double dash by 2 factorial; so that multiplied by a 2 plus a 3 multiplied by 4 delta x squared by 2 factorial multiplied by f double dash. So, 4 a multiplied by delta x square by 2 factorial plus 4 a 3 is what we get for f double dash plus terms in f triple dash. So, our three equations are going to be a 1 plus a 2 plus a 3 equal to 0; a 2 delta x plus a 2 2 a 3 delta x equal to 1; and a 2 plus 4 a 3 equal to 0.

So, I will write down the three equation over here; a 1 plus a 2 plus a 3 equal to 0; a 2 plus 2 a 3 times delta x equal to 1; and a 2 plus 4 a 3 times delta x squared plus 2 factorial equal to 0; this particular term gets cancelled, a 2 equal to minus 4 a 3 substitute this over here, we will get minus 4 a 3 plus 2 a 3 equal to 1 by delta x. So, a 3 is going to be equal to minus 1 by 2 delta x; a 2 is going to be equal to 4 by 2 delta x; and a 1 is negative of a 2 plus a 3, which is going to be equal to negative of 1 by 2 delta x, a 4 minus 1, which is equal to minus 3 by 2 delta x.

So, we substitute these values in this particular expression and the result that we will get for a three point forward difference formula is f dash of x i is going to be approximately equal to minus 3 by 2 delta x f of x i minus 3 by 2 delta x f of x i plus 2 divided by delta x f of x i plus 1 minus 1 by 2 delta x f of x i plus 2.

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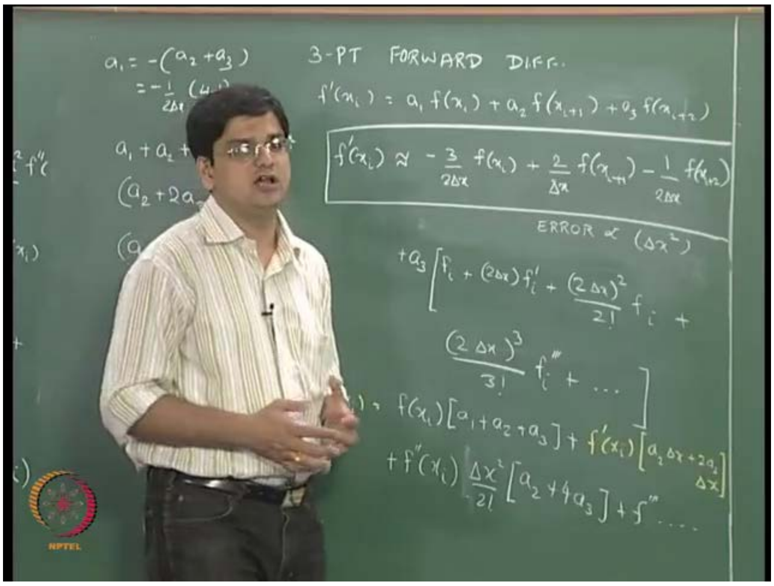

And this is our three point forward difference formula and if we substitute the value of a a 1 a 2 and a 3 in the f triple dash term, we will realize that the error of the leading term is of the order of delta x squared. So, a three point forward difference formula has an error which without derivation I am just stating, error is proportional to delta x square.

So, we now have a forward difference formula, which is more accurate than our traditional two point forward difference formula for f dash x i.

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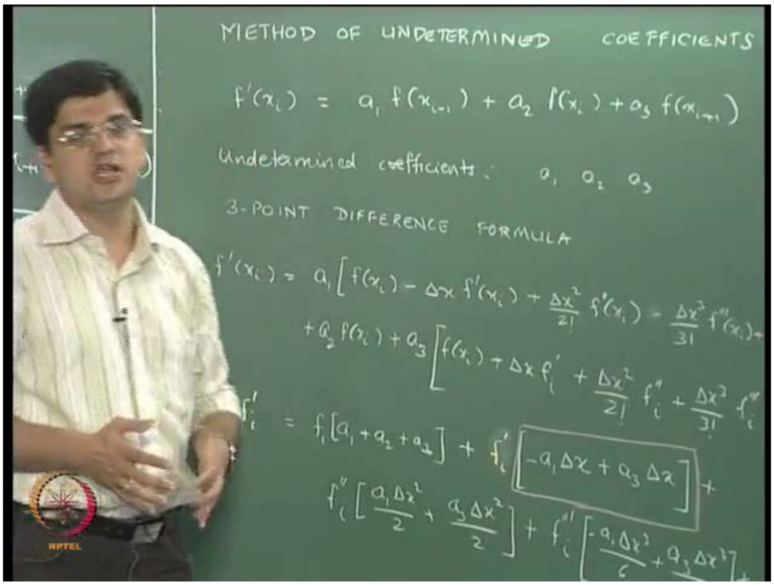

This we have obtained using the method of undetermined coefficients. To summarize what we have done in this particular lecture until now is, we started off with an introduction to numerical differentiation and integration. We motivated the numerical differentiation and integration part saying, where exactly numerical differentiation and integration will be useful and then, we started covering some of the methods for doing getting the numerical differentiation using the forward difference method, backward difference method, central difference method for getting f dash of x; then we talked about the method of undetermined coefficients, where we write our f dash of x as a linear function of f computed at various different points.

And then, we used a method in order to compute this particular or these particular coefficients and finally, we talked about higher order formulae, for example, three point forward difference formula in order to get f dash of x i.

So, that is essentially what we have covered in this particular lecture. In the lecture, I will briefly recap all these formulae and then, I will go on to taking a couple of numerical examples to show what we have derived in these particular equations.

Thank you.