Numerical Analysis
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Lecture 12
Numerical Differentiation 3
Operator Method
Numerical Integration 1

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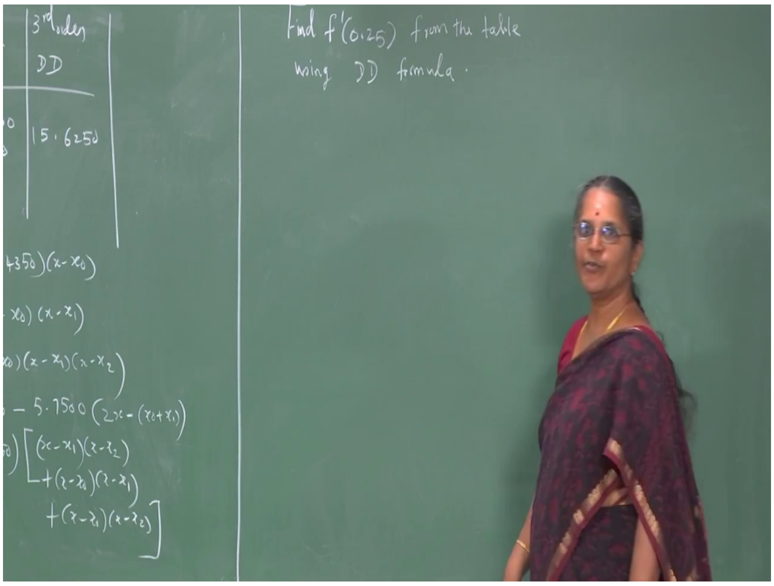

Let us take an example and see how we can obtain an estimate from the derivative. Suppose say we are asked to find f dash (0.25) from the table of values which are given using divided difference formula. So I have used the short notation DD that is divided difference formula.

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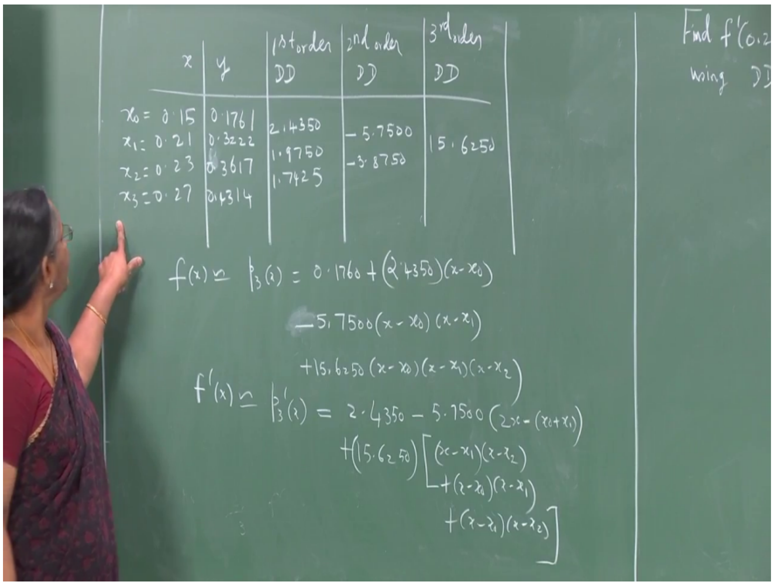

And the table of values are given here corresponding to x 0, x 1, x 2, x 3 the function values are given so I form the divided difference table. So compute the first order difference we know the entry here is this minus this divided by x 1 minus x 0 then the second entry is this minus this by x 2 minus x 0 and so on.

So we compute the first order divided difference. The second order divided difference will be this minus this divided by it involves the points x 2 x 1 x 0 so by x 2 minus x 0 that will give you this difference and so on. So we form the divided difference table. So we require f(x) is which approximated by a polynomial p 3(x) which is of degree at most 3 given information at 4 points. So we know that p 3(x) is given by 0.1761 plus this entry into x minus x 0 the next term will be this entry into (x minus x 0) (x minus x 1) and the last term will be this into (x minus x 0) (x minus x 1) (x minus x 2).

So I compute f dash(x) so f dash(x) will be p 3 dash(x) so we take derivative on the right hand side so we have written down the expression for the derivative on the right hand side.

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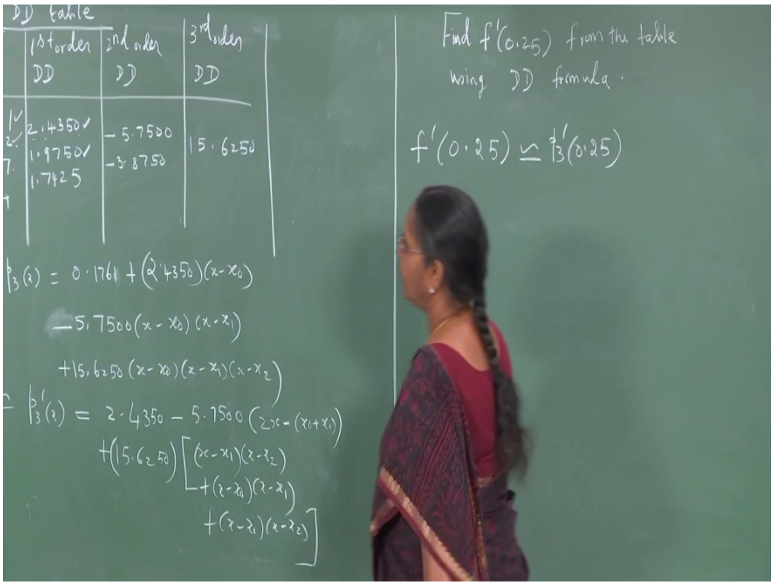

Now we require the derivative at some point f dash(0.25) so that will be estimated by p 3 dash (0.25).

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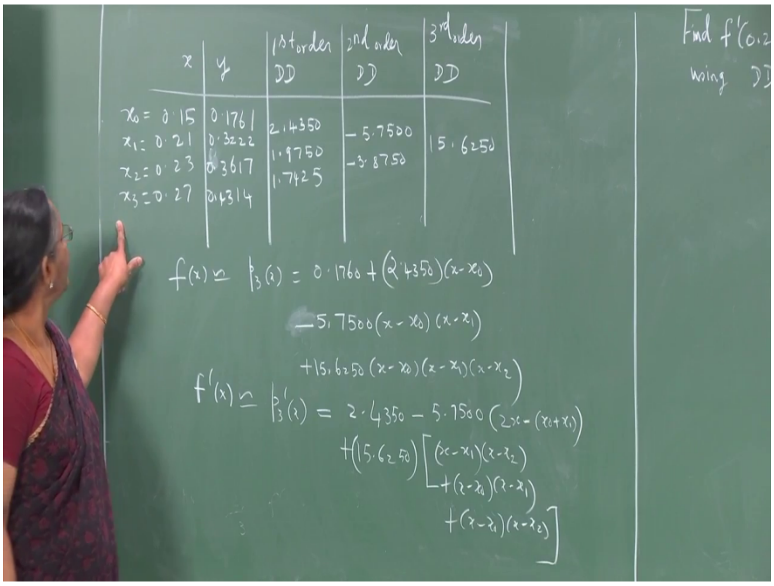

So we observe that we substitute x as 0.25 on the right hand side we will get an estimate for f dash(0.25). And you know what are x 0 x 1 x 2 they are given in the table.

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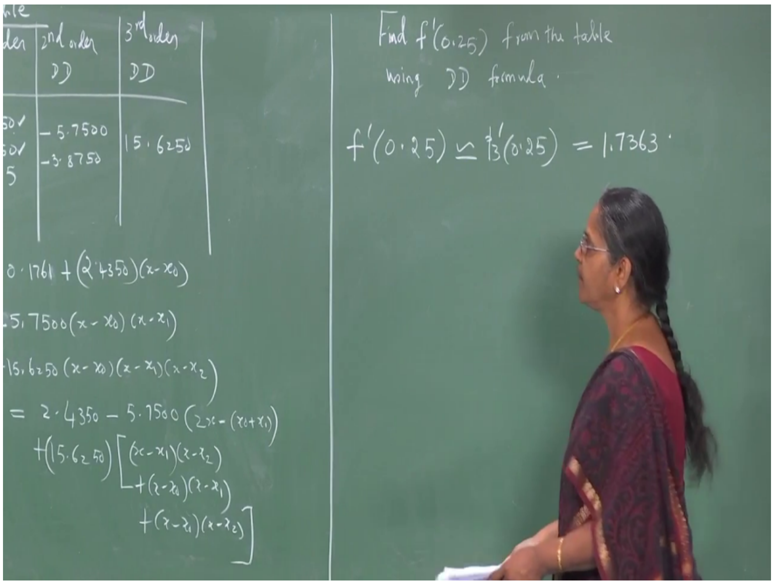

So we should substitute you end up with the value which turns out to be 1.7363. This point x is not any of these nodal points. f dash(0.25) is somewhere here so you require the derivative of the function to the estimated at this point. So you used the divided difference formula and obtained an estimate at any point x in the interval the function derivative can be estimated and the value is the value of the derivative at that point of the interpolating polynomial that interpolates the function. So this illustrates the theorem that we had proved in the previous class.

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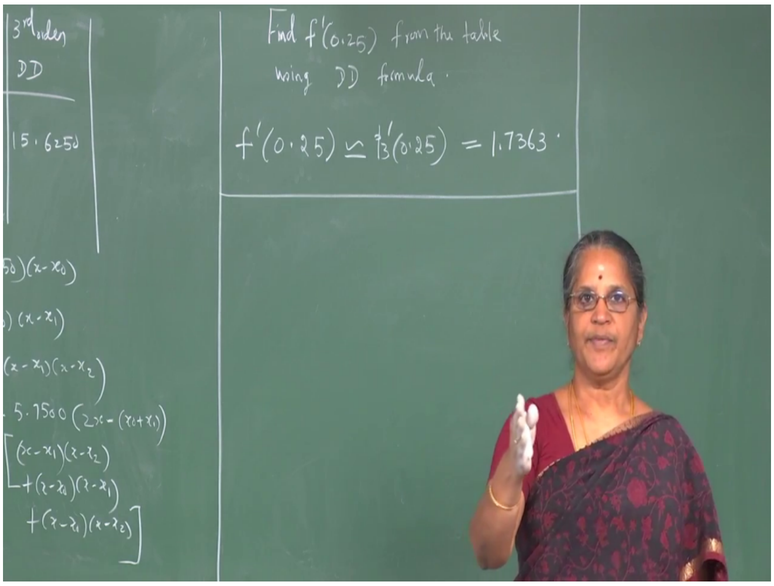

So one can therefore use polynomial interpolation to derive numerical differentiation formula by simply taking the derivative of the interpolating polynomial that reconstructs the function or approximates the function at a set of discrete points and depending upon the order of the derivative from which you require an estimate you can differentiate the interpolating polynomial and then evaluate this estimate at the required point in the interval. So now we move over to another method of getting estimates.

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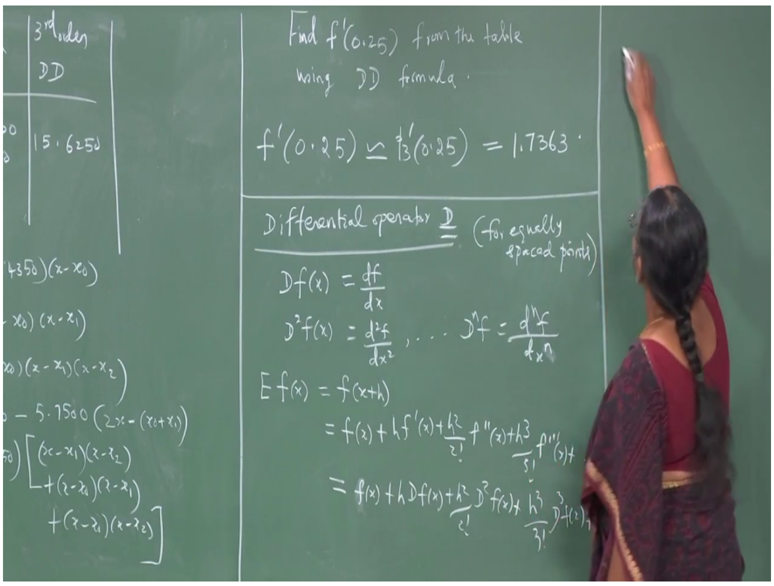

So I introduce what is known as the differential operator. So the differential operator, so let us denote it by D. This operator is such that Df(x) is nothing but d by dx of f, d square f(x) is d square f by dx square, so the n th derivative on f will be the n th derivative of f with respect to x. We know that the shift operator E when it operates on f gives you the value at the mixed point.

So we consider these details for equally spaced points so let the information be given at so E when operates on f (x) is f(x plus h) which by Taylor theorem is f(x) plus h f dash(x) plus h square by factorial 2 f double dash(x) plus h cube by factorial 3 f triple dash(x) and so on. f(x) plus h into f dash is D f(x) plus h square by factorial 2 D square on f(x) plus h cube by factorial 3 into D cube on f(x) plus etc.

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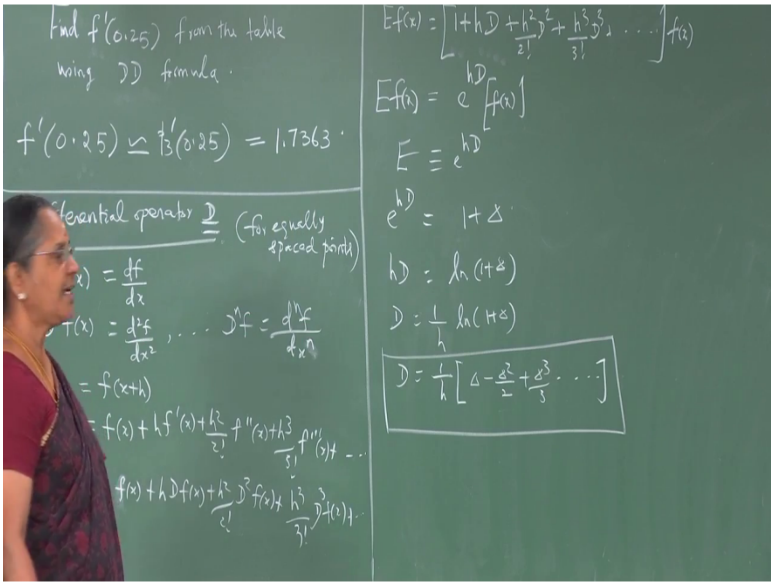

So we have E on f(x) to be equal to [1 plus h D plus h square by factorial 2 D square plus h cube by factorial 3 D cube plus etc] This operator operating on f(x) but we exceed at it is of the form 1 plus hD plus hD the whole square by factorial 2 plus hD the whole cube by factorial 3 and so on operating on f(x) so it is e to the power hD on [f(x)]. So E when it operates on f(x) it plays the same role as we operate an e power hD when it operates on f(x).

So W is e to the power hD. So e to the power hD what is e we have already shown in terms of the forward difference operator delta as e is 1 plus delta. So we have hD to be equal to log (1 plus delta). So D is 1 by h log 1 plus delta so it is 1 by h into delta minus del square by 2 plus del cube by 3 and so on. So that is the derivative operator in terms of the forward difference operator.

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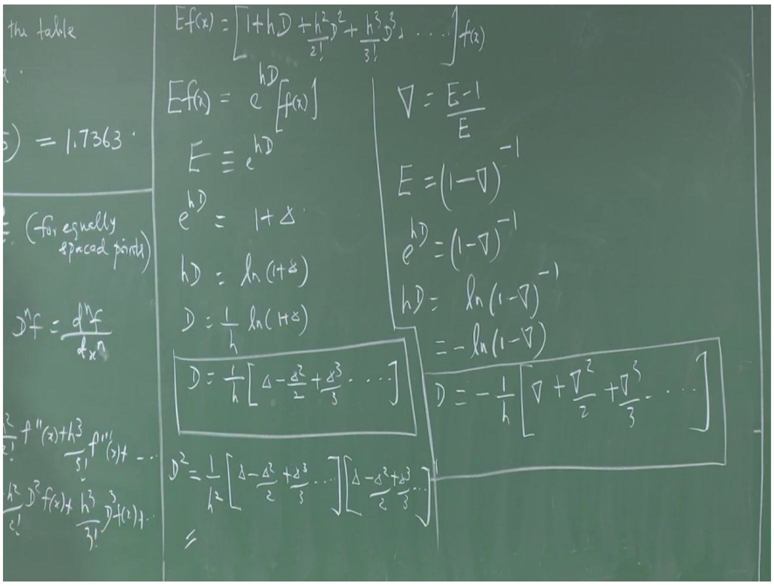

We also have obtained the relationship that connects delta with E that is it is E minus 1 by E or I can give E in terms of backward differnce operator as (1 minus delta) power minus 1. So if I substitute that e power hD is 1 minus delta power minus 1 so hD will be log 1 minus delta power minus 1. So minus log (1 minus delta) so D is also minus 1 by h into log (1 minus delta) is [delta plus del square by 2 plus del cube by 3] and so on. So the operator D can also be given in terms of the backward interpolation operator.

So these relations can be used to obtain derivative of a function. So here we have obtained the expression for the first derivative namely D what will be D square if I want the second derivative it is D on D so this operating on itself so i can write down it is 1 by h square into delta 1 by del square by 2 plus del cube by 3 etc] operating on delta minus del square by 2 plus del cube by 3.

So I can compute the result and write down D square in terms of the forward difference operator and higher order derivatives can be successively obtained in terms of the forward difference operator. The same thing can be done in respect of the backward difference operator and higher order derivatives can be obtained if we know information about the backward difference operators of different orders.

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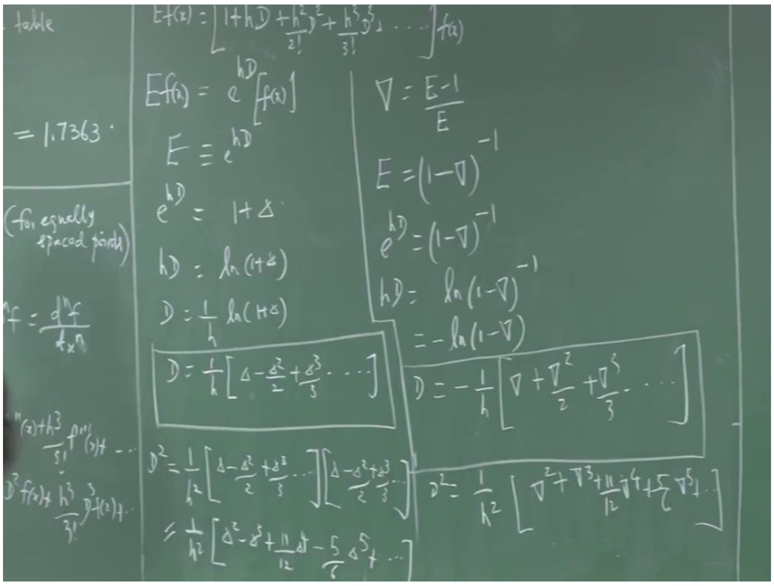

So 1 by h square into [del square minus del cube plus 11 by 12 del power 4 minus 5 by 6 del power 5 plus etc]. And similarly in terms of the backward difference operator it is 1 by h square into [del square plus del cube plus 11 by 12 del power 4 plus 5 by 6 into del to the power of 5 plus etc.]

Again note that use these expressions for the first order derivative second order derivative which is given in terms of the forward difference operator if you require an estimate of the derivative of a function very close to the beginning of the table of values and similarly use the information here for computing the derivatives of a function whose values are descried near the end of the table.

Then you will be able to get an estimate which make use of the information in the beginning of the table as well as the information at the end of the table according as you use the forward difference table or a backward difference table. So let us now take an example and compute an estimate for certain derivatives.

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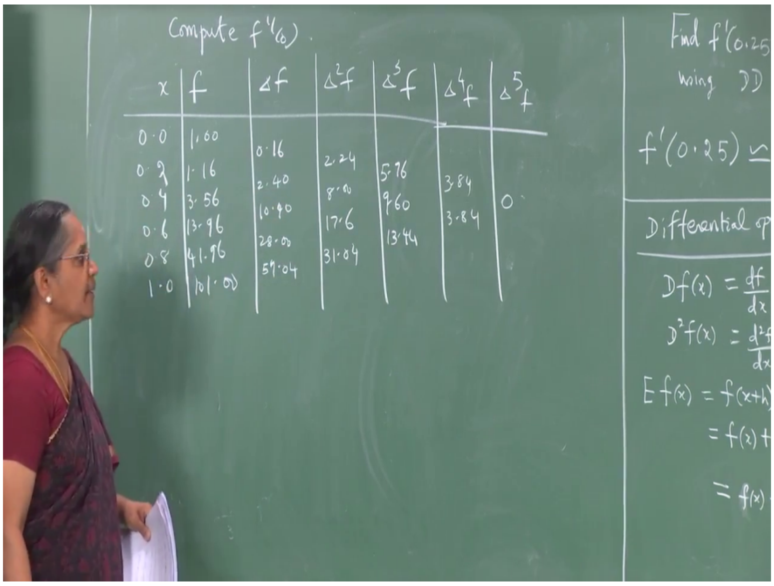

So suppose say you are asked to compute f double dash (0) and the table of values are given at 0.0,0.2,0.4,0.6,0.8 and 1.0. And the function values are 1.0 1.16 3.56 13.96 41.96 101.00. So f double dash (0) is asked it is in the beginning of the table so I shall form the forward difference table and use that information. So first order forward difference will give me 0.16 , 2.4,10.4,28, 59.04 then the second order differences will be 2.24,8, 17.6 and 31.04. The third order differences are 5.76,9.6,13.44. The fourth order differences will be 3.84,3.84 and the fifth order differences will be 0.

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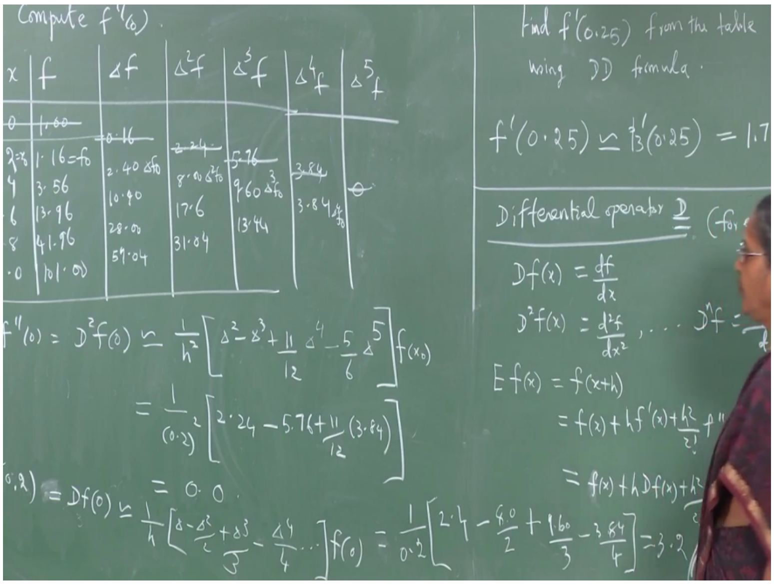

So I require now f double dash(0). So it is D square f evaluated at 0 and estimate can be got using the forward difference operator which is 1 by h square into [del square minus del cube plus 11 by 12 del power 4 minus 5 by 6 del power 5] right plus etc the higher order differences will all be 0 so I can close this so this on where we require the second derivative of f at 0. So this on f(x 0) so that will be 1 by h square what is h?

The difference between any 2 successful nodes namely 0.2. So 1 by 0.2 the whole square into del square f(x 0) so it starts with del square f(x 0) which is [2.24 minus del cube f(x 0) so 5.76 plus 11 by 12 del power 4 f(x 0) into 3.84 then minus 5 by 6 into del power 5 f(x 0) which is 0.

So this is what I need to evaluate and if you compute this the result turns out to be say 0. So the second derivative evaluated at 0 is 0 is an estimate which is obtained from this table of values. In addition if you are asked to say compute f dash(0.2) suppose say you are asked to get f dash(0.2) So you can still make use of this forward difference table where you can forget about the information that is given to you along this leading diagonal. Say think back you are given the table of values starting from 0.2 so f dash(0.2) will be approximated that is equal to Df(0) and it is approximated by 1 by h into delta minus del square by 2 plus del 2 by 3 minus del power 4 by 4 and so on or f(0).

So this will be your x 0 no and also this is f 0 so this is the first order difference, the second order difference the third order difference and this will be the first order difference. So the information is available at all these points. And so substituting this we will get this will be 1 by h again 0.2 multiplied by delta on f(x 0) so it is 2.4 then minus del square so 8 by 2 then this del cube by 3 on f (x 0) so it is 9.60 by 3 minus del power 4 so minus 3.84 by 4. So evaluate this and that turns out to be 3.2.

So we are able to make use of information given about the function at a set of discrete points in estimating the derivative of the function at any of these nodes using the operators. We need forward difference operators and the backward difference operator. So this is just to illustrate that one can get an estimate of the derivatives of a function for which interpolation polynomials which interpolate the function are available to us. One can get the corresponding table of differences depending upon where the information about the derivative is required and then the estimate can be obtained.

So we almost have come to the end of our discussion on numerical differentiation so I will close this section on numerical differentiation with a small remark. So it all looks nice namely one can obtain numerical differentiation methods using method of undetermined coefficients for the derivatives of a function whose values are specified only at a certain set of discrete points.

And these formulas can involve any number of points namely you can get a 3 point formula or a 2 point formula or if you want to specify the accuracy then depending upon what accuracy and what class of functions f that you have been given then you can accordingly write down the numerical differentiation formula using method of undetermined coefficients.

In addition polynomial interpolation gives us an estimate of the derivative at the nodes and also at any point x in the interval where the function f(x) is known which was discussed in the theorem that we considered in the previous class. Or one can also get an estimate of the derivatives in terms of the operators. So it all looks nice we will be able to get an estimate of any order derivative of the function provided f satisfies requirements so that we will be able to compute the derivatives which exist in a continuous.

So now we now give a remark by saying that this numerical differentiation formulas are right and stable in a sense that if the given set of values about the function have rounding errors about the function values then our method is likely to become unstable namely even for small round off errors in the function values we make it large errors or large deviations so that the method is an unstable method. So we would like to illustrate by the following example.

So we should take care to see the example essentially informs you that you should make sure that the information about the function that is given in the form of a table right are correct and then you can use the numerical differentiation methods that we have discussed to get an estimate of the derivative of the function. So it is important to ensure that the information about the function which are specified in the form of a table are correct, otherwise your numerical differentiation methods can become unstable.

So we illustrate this by the following example. So let us take the following simple example.

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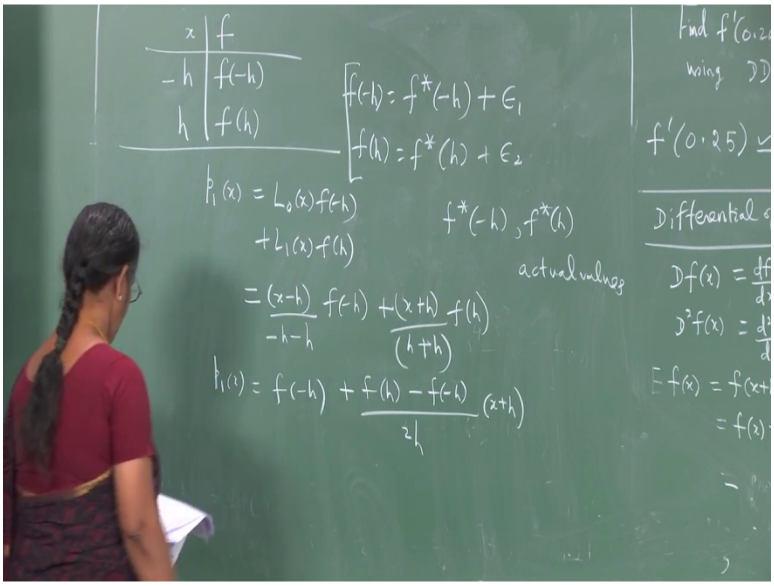

Suppose say we are given the function values at 2 points namely minus h and plus h. I can interpolate this function by a linear polynomial p 1(x). Remember that f(minus h) and f(h) they involve rounding errors namely the actual value let us denote it by a star(minus h).

So that f(minus h) is this plus some epsilon 1 which is the rounding error and similarly f(h) is a star(h) plus some error which is epsilon 2 f star (minus h) and f star(h) are the actual values. The information given to us has rounding errors that is how we start because we would like to show that when there are rounding errors and the set values given to us is not correct then numerical differentiation may lead to unstable process.

So I have information at two equal points so I can approximate this function by a linear polynomial passing through these two points. So I write down the Lagrange polynomial that is L 0(x) into f(minus h) plus L 1(x) into f(h).

What is L 0(x)? It is (x minus h) by minus h minus h into f(minus h) plus L 1(x) will be x minus (minus h) by minus (minus h) into f(h). So this is the first degree linear polynomial that approximates this function. p 1(x) is equal to f(minus h) plus f(h) minus f(minus h) divided by 2h into x plus h.

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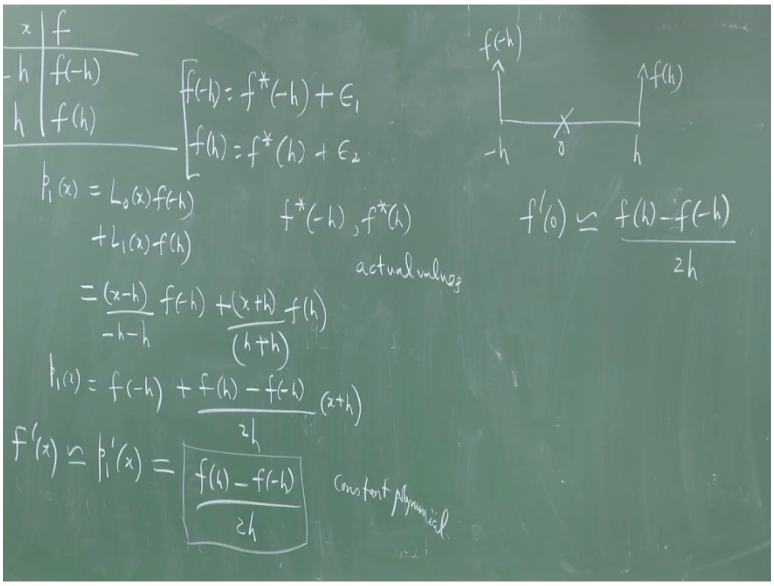

So I compute f dash(x) which is the derivative of f and we know that it is approximated by the derivative of p 1(x) so p 1 dash(x) will be f(h) minus f(minus h) by 2h into the derivative is 1 here. So p 1 dash(x) is the term on the right hand side. So it involves the function values which are specified the difference between them by 2h.

So this is a constant so there are two points minus h and h sso the function values are this point minus the function value at this point are used so the difference between that by 2h you recall that this such a formula was derived yesterday using the method of undetermined coefficients namely it approximates the derivative at the center point.

So whatever you have got is an approximation of the derivative of f at the centre points and that is f(h) minus f(minus h) divided by 2h.

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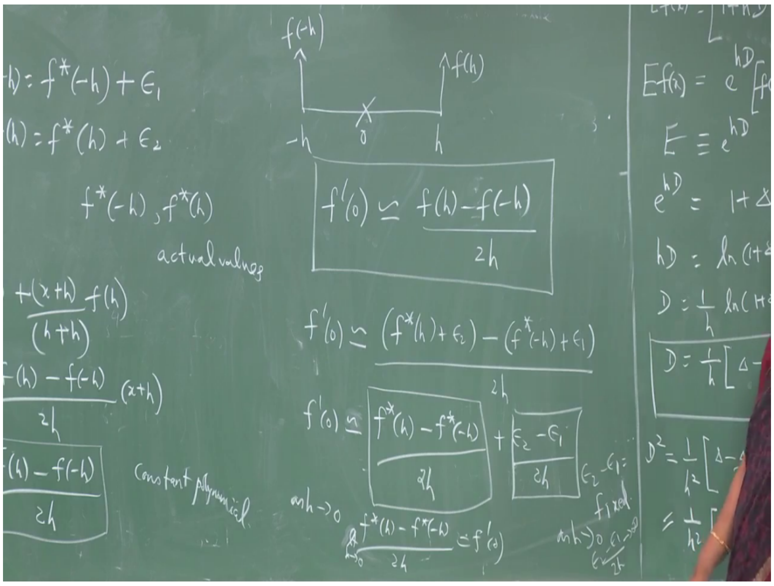

So what is it that you have got by performing differentiation you essentially have a numerical differentiation formula that estimates the derivative of f at the point 0 which is this. So let us see what is it? So f dash (0) is essentially estimated as what is f(h) f star(h) plus epsilon 2 minus f(minus h) is f star (minus h) plus epsilon 1 divided by 2h. So this is f star(h) minus f star (minus h(divided by 2h then plus epsilon 2 minus epsilon 1 divided by 2h.

Recall f star(h) and f star (minus h) are the actual values which must have been given to us in the table of values but there were some round off errors and so f dash(0) which is estimated as this is such that as h goes to 0 the first term f star (h) minus f star (minus h) by 2h in the limit as h goes to 0 will review f dash(0).

However if you look at the second term Epsilon 2 minus Epsilon 1 is some fixed constant and so as h tends to 0 this second term tends to Epsilon 2 minus Epsilon 1 by 2h tends to infinity. So the estimate of f dash(0) is such that as h tends to 0 the first term gives f dash (0) but the second term goes to infinity as h tends to 0. So for small values of h when you take the information at a set of points and take your h to be very very small then the first term does give you f dash (0) it is fine but the second term which occurs due to round off error goes to infinity.

So you think that ok I will make my h large. So if you make h large in such a way that this Epsilon 2 minus Epsilon 1 by 2h may become smaller and smaller but the first term will be a poor approximation for f dash(0). So you neither can have h to be very very small in which case the term coming out of the round off errors become very very large. So that the error becomes large in estimating f dash(0). Or when you make h very very large the term becomes smaller but this is not a good estimate of f dash(0) it is a poor estimate of f dash(0). So this tells you that there is an optimal h that must be taken in order that this numerical differentiation formula will give you an estimate which is accurate enough to be considered for computations.

So this example essentially illustrates the facts that numerical differentiation formulas can become unstable namely for a small changes in the actual values of the form Epsilon 1 Epsilon 2 they are very small say you get a large deviation in your final estimate of the derivative when the step size h becomes very small.

And therefore the method can become unstable. And therefore you must ensure that the infromation that is given to you in the form of table of values when you use them to get an estimate for derivatives of the function whose information is provided to you is accurate is correct, it does not involve any rounding or round off errors are not incorporated in the set of values which are given to you.

So with this we close this section on Numerical differentiation, and we shall move on to the section on Numerical Integration where again we make use of this polynomial interpolation of approximating a function f which has to be integrated between suitable limits. So let us see how we can obtain Numerical integration methods to evaluate certain definite integrals.

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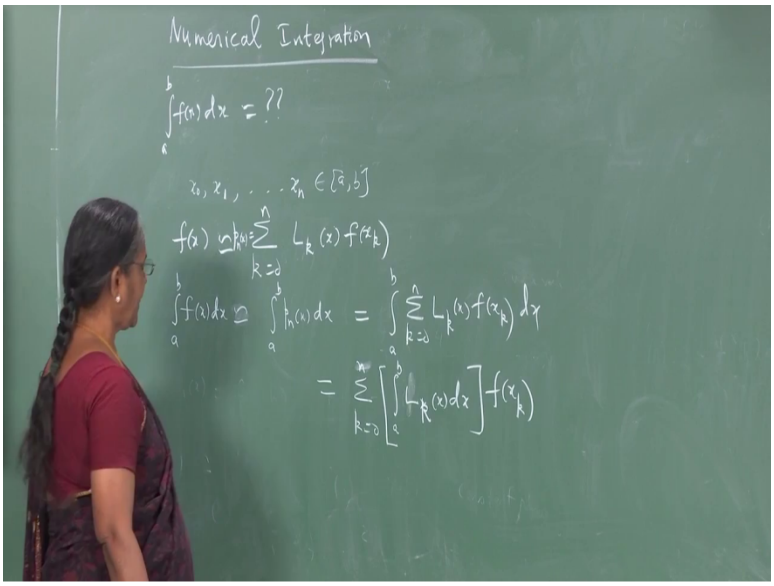

So I am interested in evaluating am integral of the form say integral a to b f(x) dx. So in case f(x) is given at a set of discrete points in the interval [a,b]. Or when f(x) is such that the methods which are known to you like substitution integration by parts cannot be applied to this integral a to b f(x) dx. Then you require some methods by means of which you should be able to have an estimate of this integral. In such cases we resort to the numerical integration methods and use them to get an estimate of this integral.

Here again polynomial interpolation comes to our rescue. Suppose say we are given integral a to b f(x) dx which has to be evaluated then we can choose points x 0, x 1,x 2 etc x n in this interval [a, b] evaluate this integral by approximating this function f (x) by an interpolating polynomial such that f(x) is sigma k is equal to 0 to n L k (x) into f(x k) namely f(x) is approximated by a polynomial of degree p n whose degree is atmost n. And so we have taken a Lagrange interpolation polynomial.

So integral a to b f(x) dx will be integral a to b p n(x) dx and that is integral a to b sigma k is equal to 0 to n L k(x) into f(x k). So this will be sigma k is equal to 0 to n into [integral a to b L k(x) dx multiplied by f(x k)]. So k is equal to 0 to n integral a to b k (x) into f(x k). So when what are these L k(x) they are all polynomials we have already seen.

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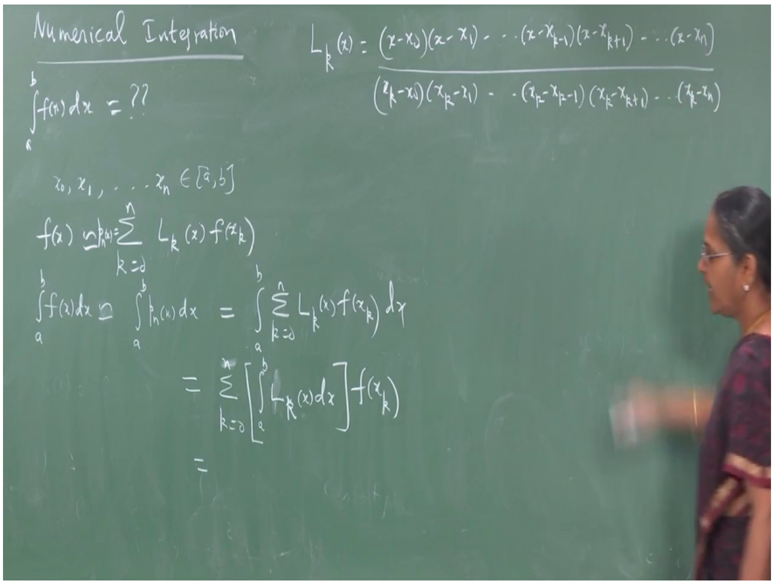

What is this L k(x)? L k(x) will be equal to (x minus x 0) (x minus x 1) etc (x minus x k minus 1)(x minus x k plus 1) into (x minus x n) divided by (x k minus x 0) into (x k minus x

1) etc (x k minus x k minus 1) (x k minus x k plus 1) and so on (x k minus x n). So L k(x) are all polynomials and therefore we know how to integrate these polynomials between a and b.

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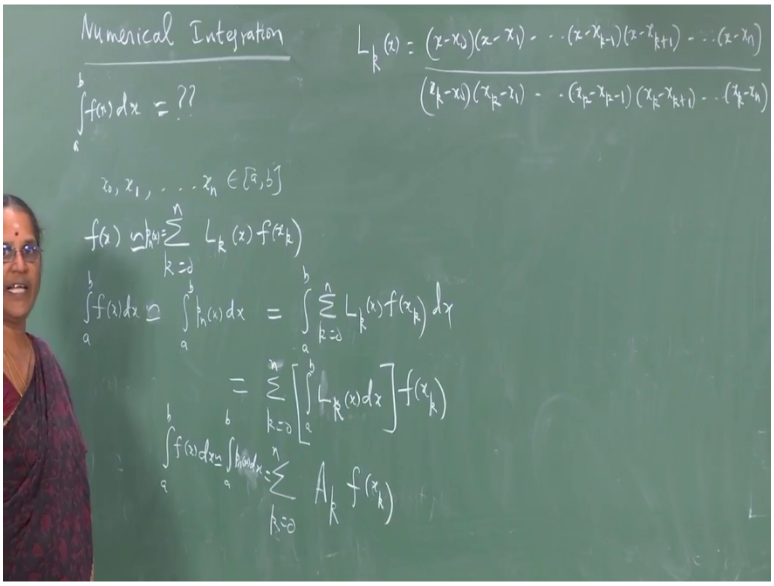

So we write down the result so that will be sigma k is equal to 0 to n we call that value when L k is integrated between a and b as a k so A k into f(x k). So we have integral a to b f(x)dx to be approximated by integral a to b p n(x) dx which is equal to sigma k equal to 0 to n a k f(x k). So find out A k and then take this sum from k equal to 0 to n of A k f(x k) that will give you an estimate of integral a to b f(x) dx.

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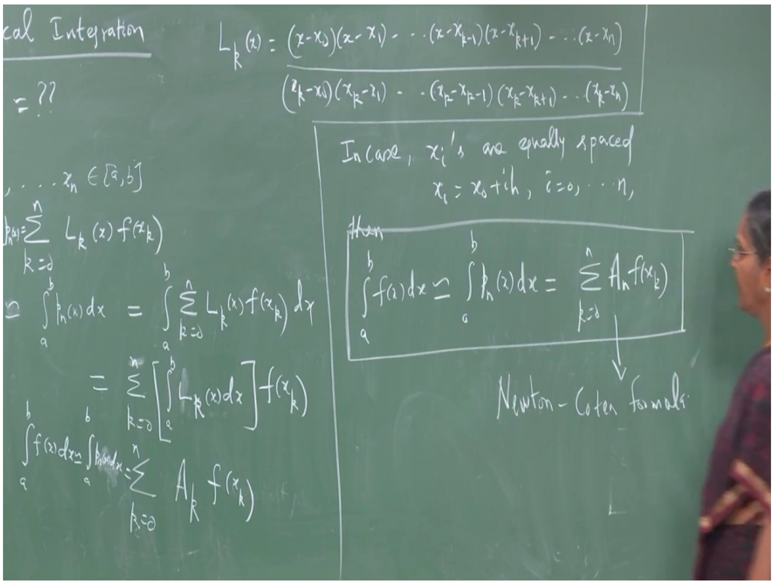

In case the points x 0 x 1 etc are equally spaced then the resulting method is called Newton Cotes formula. So in case x i 's are equally spaced namely x i is x 0 plus i h for i is equal to 0,1,2,3 upto n then integral a to b f(x) dx which is approximated by integral a to b p n(x) dx which is equal to sigma k equal to 0 to n A n f(x k), this is called Newton quotes formula.

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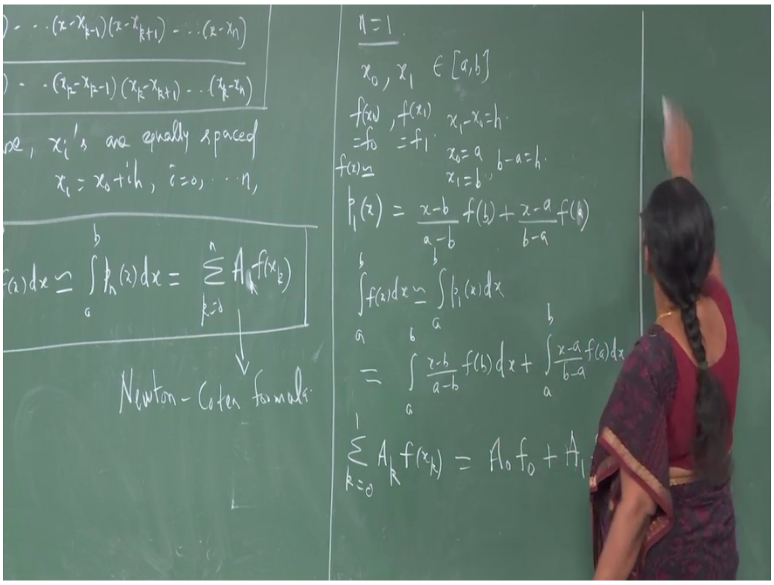

So let us work out the details for a simple case. Say when n is equal to 1, where n is 1 that is given we have given the two points x 0 and x 1, and the corresponding function values which I denote by f 0 and f 1. So I am taking these two points x 0 and x 1 where belonging to the interval a b such that x 1 minus x 0 is h. And I would like to derive a Newton Cotes formula when n is equal to 1 by taking two points x 0 and x 1.

I can take that x 0 and x 1 to be such that x 0 is a and x 1 is b so that b minus a will be equal to h. I can use the n points and then write down this formula, so what will be my p so here n is 1 so I can approximate the function f by a linear polynomial which will be x minus b by a minus b into f(b) plus x minus a by b minus a into f (a). This is a linear polynomial that approximates f.

So f(x) is approximated by this. So I require integral a to b f(x)dx. So that is integral a to b p 1(x)dx and that will be equal to integral a to b x minus b by a minus b into f(b) into dx plus integral a to b x minus a will be b minus a into f(a) into dx. So in our notations what will be the formula. The formula is sigma k is equal to 0 to n is 1 A k into f(x k). So we will get A 0 into f (x 0) plus A 1 into f(x 1) that is f 1. So what is A 0?

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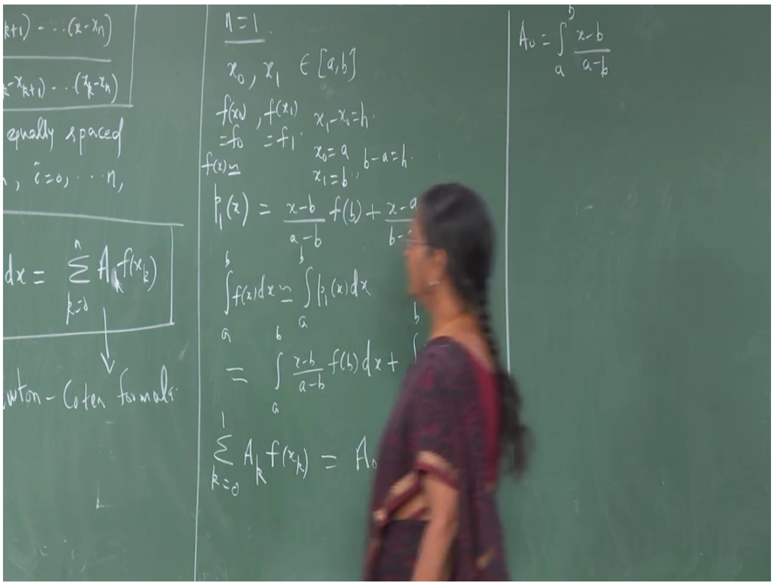

A 0 is going to be nothing but integral a to b x minus b by a minus b.

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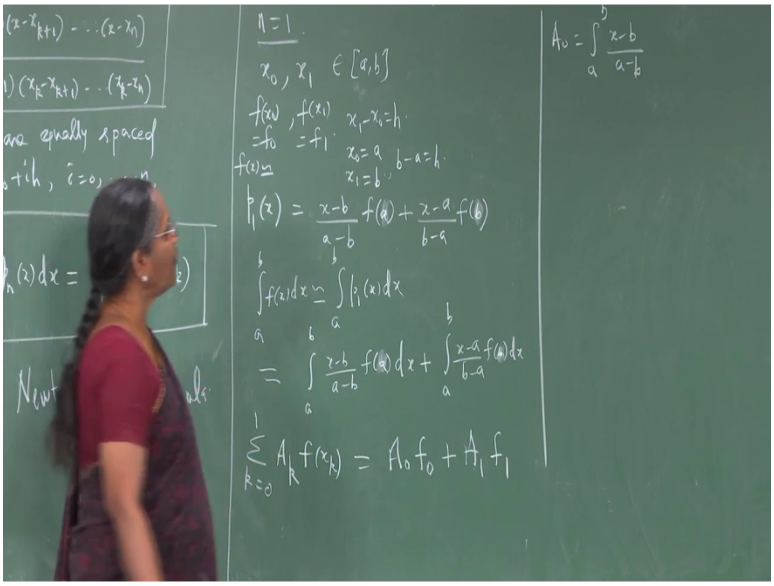

x minus b by a minus b into f(a) plus x minus b by b minus a into f(b) Lagrange interpolation polynomial is written. So the points are a and b so x minus b by a minus b into f(a) plus x minus a by b minus a into f(b). So here this will be a and here it is b. so we have to now evaluate A 0 and A 1.

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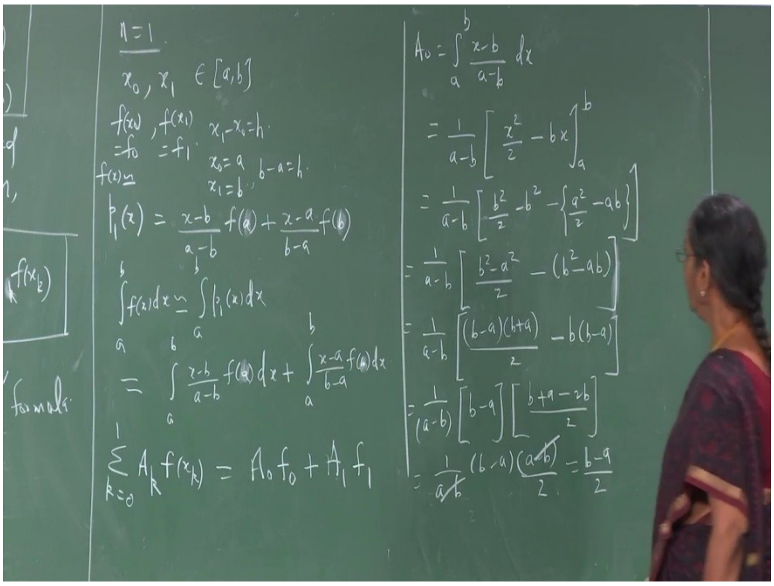

So A 0 will be x minus b by a minus b integration with respect to x. So that is 1 by a minus b into integral a to b x dx minus b into x between a and b So that will give you 1 by a minus b[b square by 2 minus b square minus { a square by 2 minus a b}]. So that will give you 1 by a minus b into [b square minus a square by 2 minus (b square minus ab)].

So this gives you 1 by a minus b into i can write this as [(b minus a) into (b plus a) by 2 minus b into (b minus a)]. So 1 by (a minus b) into[b minus a] can be taken out so I am left with [b plus a minus 2b by 2] So that will give me 1 by a minus b into b minus a into this gives me a minus b by 2, so the value of A 0 is b minus a by 2.

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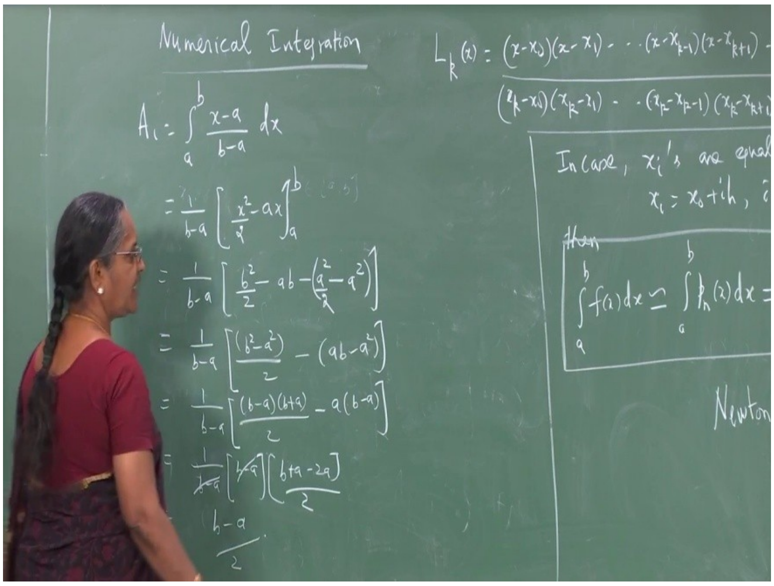

Let us now evaluate the second constant A 1 which is integral a to b x minus a by b minus a. So that will be 1 by b minus a x square by 2 minus A x between a and b. So that will give you [b square by 2 minus ab minus (a square by 2 minus a square)]. So this will give you 1 by b minus a into [(b square minus a square) by 2 minus ab minus a square)]. So which is 1 by b minus a we can write this as [(b minus a) into (b plus a) by 2 minus a into (b minus a)].

So we have removed the factor b minus a so you have a b plus a minus 2a by 2 and that gives you b minus a divided by 2 so that is here A 1. so you have computed A 0 and A 1.

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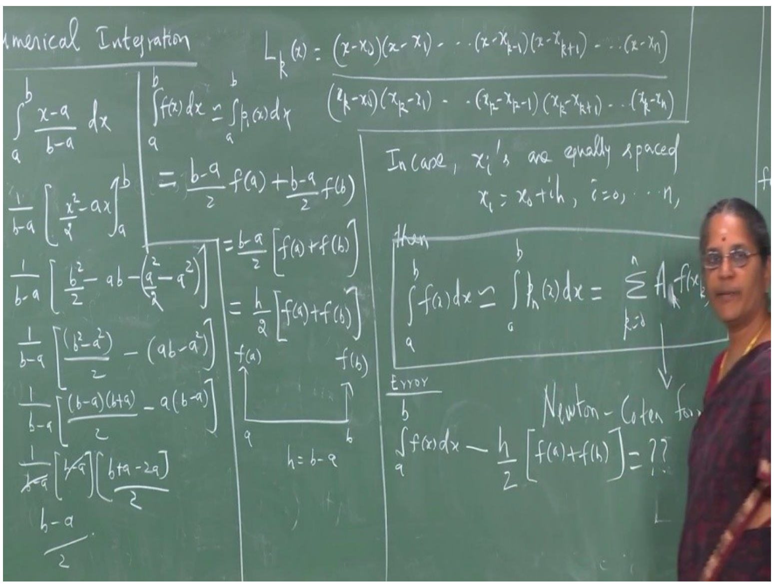

So that gives you the result for approximation of the integral f(x)dx which is integral a to b p n(x) dx which is A 0 into f 0, f 0 is f (x 0) and x 0 is a. So A 0 into f (a), A 0 is b minus a by 2. So b minus a by 2 into f(a) plus A 1 into f 1 x 1 is d so f 1 is b , so that gives you A 1 which is b minus a by 2 into f(b). So it is b minus a by 2 into[f(a) plus f(b)], but b minus a is the length of the interval 100. We have said that is equal to say h so h by 2 into f(a) plus f(b)

so this is an estimate of the integral when you approximate the function by a linear polynomial p 1(x) and what do you observe you have the end points a and b of the interval across and you require the integral of a to b f(x) dx and the function values f(a) and f(b) and the length of the interval is b minus a at the method Newton cotes method that we have derived by taking n is equal to 1 gives you a result which says that this integral is h by 2 into sum of the end ordinates of that interval a and b.

So you simply take the ordinates at the end points say it be length of the interval by 2 so half the length of the interval into the sum of the n ordinates will immediately give you the result namely an estimate of integral a to b f(x)dx. And you surely know that there is some amount of error that is incurred in this estimate so you have to determine what is the error that is incurred namely integral a to b f(x) dx minus h by 2 into f(a) plus f(b), what is this error which has to be determined.

So we will continue with the error analysis of Newton Cotes formula derived when n is equal to 1 and then move on with n is equal to 2 and see how Newton cotes methods can be derived. And note that the method we have derived with n is equal to 1 it is called trapezoidal rule.

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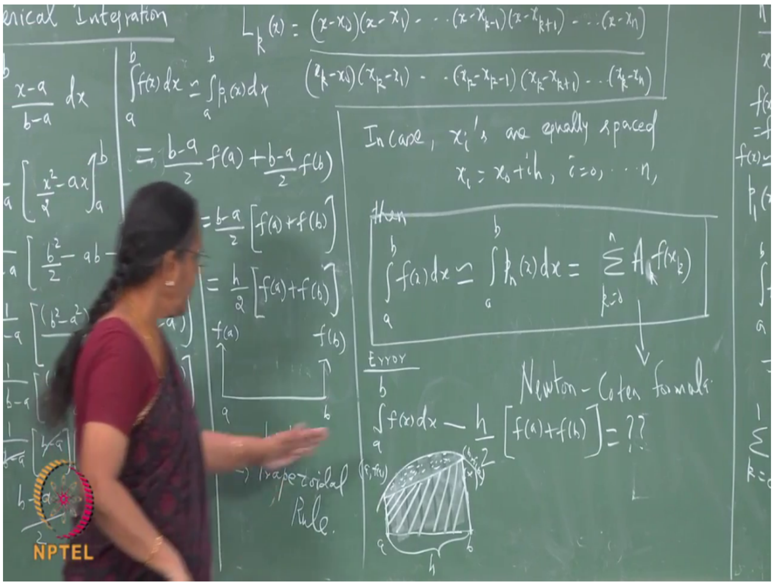

You have approximated this function by means of a linear polynomial namely a straight line passing through the points a, f(a) and b, f(b) and you have approximated what is integral a to b f(x) dx it is the area bounded by the curve y is equal to f(x) and the ordinates at x is equal to a and x is equal to b namely you require this shaded area what did you do?

You approximated f(x) by means of a straight line passing through the point and therefore you computed only the area under this line namely you computed the area of the trapezium bounded by the parallel sides namely at x is equal to a and x is equal to b multiplied by the height which is equal to h.

So h by 2 what is the area of the trapezium it is h by 2 multiplied by sum of the parallel sides. So h by 2 into f (a) plus f(b) and that is what you got as a formula. So you got the area as the area that is given here and therefore the error that has been committed by you is that you have not incorporated the area that is now darked.

So that much amount of error has been committed by you inapproximating this function f(x) by a linear polynomial. So what is it what we need to determine. So we shall perform this error analysis in the next class.