Numerical Methods and Simulation
Techniques for Scientists And Engineers

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Lecture 10
Numerical integration, Trapezoidal rule

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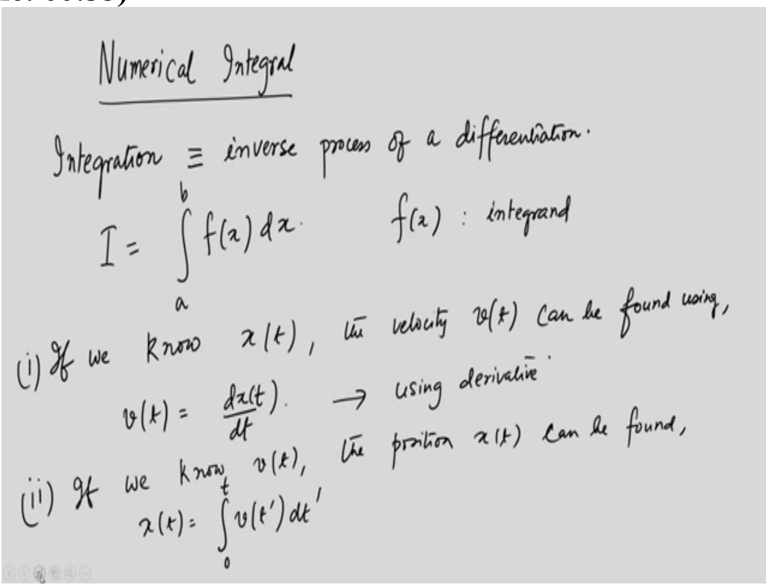

So, we are going to study numerical integration today and it is all well known to anybody who does science or engineering about what an integral is. So, we will see a few techniques to do these perform these numerical integrals in a computer and how computer handles the accuracy of such integrals. So, integral is nothing but the inverse process of derivative or a differentiation or let us write differentiation.

So when we talk about integration, we talk about integration of some function say it is a function of x between 2 intervals say a and b, so we represent it like this so it is between a and b and f of x dx and this f of x is known as the integrand. And it is some function of x may be a polynomial in x or may be a more complicated function with exponentials and logarithms or trigonometric functions of x and that has to be integrated from a lower limit of a to an upper limit of p.

And this is precisely we are we encounter almost in our daily life these kind of integrations. So, basically if you know the position of a particle as a function of time let us call it x t the velocity vt can be found using a simple derivative which is v of t equal to dx dt and so on. So, just in the same spirit as integration being the reverse of differentiation or the inverse of differentiation we can find out the; if we know so this is for the using the derivative.

So, this is using derivative and in a very similar manner if we know v of t then the position x of t can be found using x of t it is from some 0 to p, now I will use a dummy variable t prime because in the integral the upper limit of the integral is t, so we will use a dummy variable it is basically it is a time variable. But using a dummy notation for that as t prime, so this is basically we have to find out.

And in this particular case if you compare between the first line that we have written here, here and what we have written here this a which is a lower limit is taken to be the time t equal to 0 that is the starting time and b is taken as the final time of the ending time which is taken as t and this integral has to be d1over you know over this time variable which is t prime between 0 and t.

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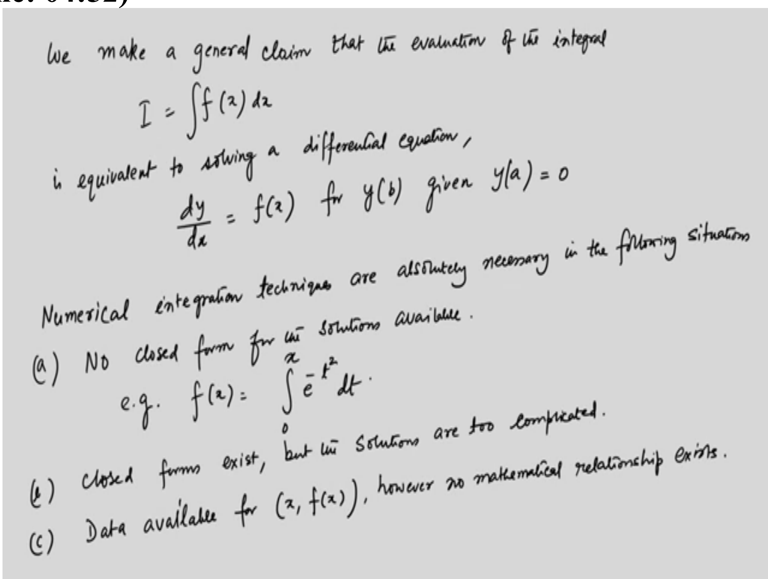

So, we make a general claim that the evaluation of the integral I equal to f of x dx is equivalent to solving a differential equation. So, basically a dy/dx equal to f of x for y at the upper limit be given some value for the lower limit for y at a we can assume it to be 0 without any loss of generality. So, because of this closeness of these 2 formalisms we will take them up 1after another that is first we will talk about numerical integration and then we would go and talk about this solution of differential equations okay.

So, when is numerical integration becomes important or when it is indispensable in a physical problem okay. So, numerical integration techniques are absolutely necessary in the following situations, so what are the situations let us just list them. One that no closed form for the solutions available. What I mean to say is that so for example f of x is equal to exponential -t

Square dt and from say 0 to some x ok. So, this there is no closed form that is available so if you need to do this integral for some value of x you need to do a numerical integration.

It could also be that closed forms are available or closed forms exist but the switch but the solutions are too complicated okay. So, if it is too complicated for you know for us to comprehend what is the nature of this or what is the value of this integral or or the nature of the integrand itself is quite complicated. So, that even if a closed form is available it is very difficult to infer any physical feel out of it.

We would have to go for the numerical integration the third which is probably one of the most important for us is that the data available for x and y we write it x and fx however no mathematical relationship exists okay. This is like you have done an experiment and you got x and y or x and fx and you need to integrate this function f of x over some range and you have no clue what the functional relationship is and you need to do this integration. Of course then the numerical integration is the only possible way.

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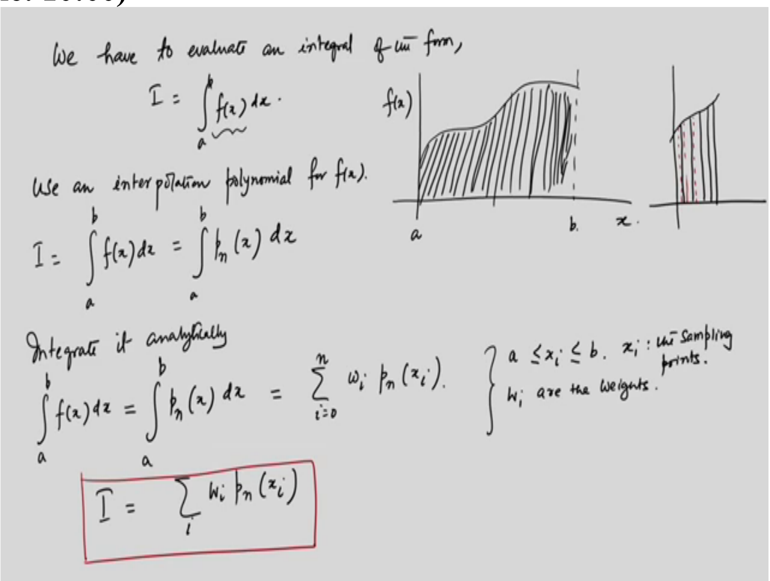

So, let us just see what we mean graphically by numerical integration so we have to evaluate an integral of the form I equal to a to b f of x dx okay. So, what it means is that let us have a f of x which is simply like this and so this is f of x versus x and said this drain or this end is a having a value x equal to a. And say we have a value which is x equal to b and we need to know by this integral what it means for this particular case is that we need to know the area under the curve.

So, an integral always means an area under the curve, so this is that area under the curve which we have to find out okay. So, this shaded area that is shown here is to be found out and this is what is meant by the numerical integration and the a and b are shown here. And of course we what we can do is that we can break this whole interval between a and b into several sub intervals such that every interval, so I will let me show you a little broader picture so let us say only a little bit of f of x is shown.

Now if we make this things make it grid like this and make the grid small enough so that they each of them look like a say rectangle or trapezium or you know a quadrilateral then of course we can find out the area of a quadrilateral and sum all of them up in order to get the area under the curve. So, this is quite easy to do and you can increase the accuracy of the method by choosing smaller and smaller intervals.

So that if in case of this you choose an interval which is smaller than this so let us show it with a different colour if I choose an interval which is smaller than this and so on. Then I am going to get a more accurate result because finally your f of x is a continuous function and we are discretizing it by making mesh of it. And so this is a discrete you know elements that we consider should be as small as possible.

Of course sometimes numerically it is not possible to choose them to be extremely small because that would probably take a lot of time to integrate or it could lead to other problems but ideally we want it to be small. So, that you get a better accuracy for this and so this is a finer mesh as its called is required for this kind of things for doing this kind of integrals. Even if it looks you know simple it still is a very cumbersome process why because you have to split it up into several trapezoids or quadrilateral and things like that.

And the more Wiggly the function is the chances that you will be able to form a quadrilateral a uniform quadrilateral is questionable especially when the function is very rugged. So, the other way of doing it is that we can approximate this f of x by interpolation polynomial. And we can do it so we will use an interpolation polynomial for f of x okay. So, what we mean to say is that your I equal to a to b f of x dx is equal to a to b a pn of x that is a polynomial nth order polynomial.

Now I am no longer saying that I am going to use small grids which eventually I will show that but this f of x is actually approximated by a polynomial and then you integrate it analytically okay. So, this is the main idea behind this so a to b f of x dx is to be replaced by a polynomial this and a to b and this is written as I equal to 0 to n and w i p n x i, so where several things are to be noted here it is a < x i < b w i are the weights okay.

So, this polynomial actually comes with different weights for different regions and these x i's are called as the sampling points okay. So, let us say that this is the so the integral has to be evaluated using sum over i and w i and p n x i and that is the formula for evaluating an integral numerically using you know numerical methods by assigning the weights and interpolating a polynomial okay.

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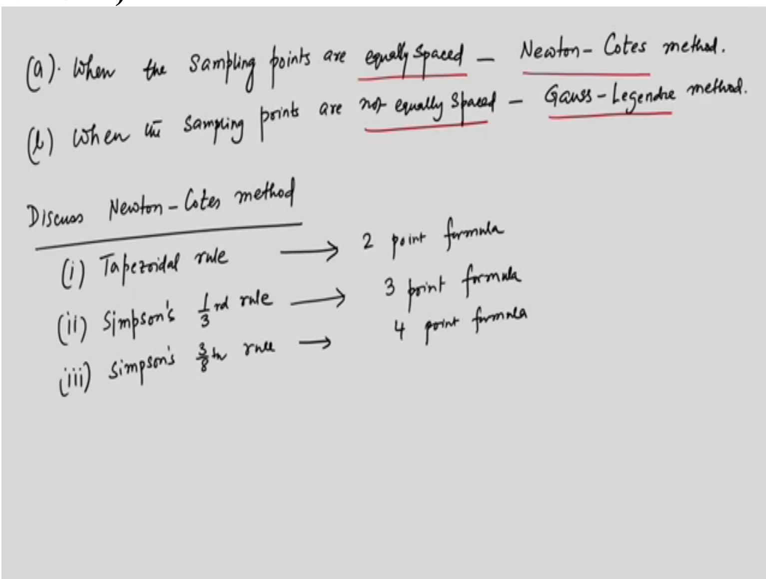

So, let us see this more carefully there are of course various ways of selecting the location and the number of sampling points that is x i but there are 2 things that are important for us one is that when the sampling points are equally spaced. So, what it means is that you have taken data at regular intervals of time and then all these x i points are equally spaced and this method is known as Newton Cotes method.

And the second is that when equally so when the sampling points are not equally spaced and this is known as Gauss-Legendre. So, we will be mostly talking about these 2 methods when the sampling points are equally spaced which is given by this Newton Cotes method. And when they are not equally spaced they are given by this Gauss Legendre method. So, let us just talk about the Newton Cotes method to begin with.

So discuss first so this is very efficient algorithms and they are known as 1is the trapezoidal rule. So, which uses this Newton Cotes method trapezoidal rule and we can also use the Simpsons 1/3 rule and as a third Simpsons so basically this is called as a 2 point formula and this is called as a 3 point formula and finally the Simpson’s three-eighth rule which uses a 4 point formula okay.

So, let us discuss one by one and so let us just start or get ahead with this Newton's formula for interpolation or Newton Cotes formula.

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Newton's formula for interpolation.

Given $(n+1)$ points $(x_0, y_0) \cdots \cdots (x_n, y_n)$.

Need to find $y_n(x)$: a polynomial of nth degree.

Let the values of x be equidistant, i.e.

$$x_i = x_0 + ih \qquad i = 0, 1, 2 \ldots n$$

The polynomial can be written as,

$$y_n(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \cdots\cdots a_n(x - x_0)\cdots(x - x_n).$$

$$a_0 = y_0, \quad a_1 = \frac{y_1 - y_0}{x_1 - x_0} = \frac{\Delta y_0}{h}; \quad a_2 = \frac{\Delta^2 y_0}{2!\,h^2} \cdots\cdots a_n = \frac{\Delta^n y_0}{n!\,h^n}$$

$$\Delta^2 y_0 = \frac{(y_1 - y_0)(y_2 - y_1)}{(x_2 - x_0)(x_2 - x_1)}.$$

Substitute these and $x = x_0 + ph$.

$$y_n(x) = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_1 + \cdots\cdots \frac{p(p-1)(p-2)\cdots\cdots(p-n+1)}{n!}\Delta^n y_0.$$

Let us just write it as Newton's formula for interpolation so we have n + 1 points that those are experimental data point starting from x 0 y 0 all the way till x n y n so need to find y n x so which is a polynomial of nth degree. And let the values of x, x be equidistant so that is x i equal to say x 0 + i h where i equal to 0 1 2 and all the way n, so these data points are equally spaced as we have said that this is a formula that we are going to derive for equally spaced data points.

So, the polynomial can be written as why n x equal to a 0 + a 1 x - x 0 + a 2 x – x 0 into x - x1 a n x – x 0 x - x n and so on okay. So, this is the polynomial since this y n of x that should agree at the tabulated point we have a 0 equal to y 0 a 1 is just the slope which is y 1 – y 0, x1 - x 0 equal to delta y 0 by h a 2 equal to Delta square y 0 2 factorial by h Square and so on. And if you go I will tell you what the meaning of was the meaning of Delta Square and a to the power n is Delta to the power n y 0 and divided by n factorial into h to the power n.

Whereas of course Delta is equal to so we have this can be written as so our so Delta's 0 Delta square y 0 its equal to y 1 – y 0 y 2 – y 1 divided by x 2 – x 0 x 2 – x 1 and similarly Delta cube y 0 would be the y 0 should come right here. so, delta cube y 0 would be y 1 y 2 - y 0 y 2 – y 1 and so you know I mean it will have 3 terms in the numerator and will have 3 terms in the denominator and they are sort of you know are they are defined in this particular fashion.

And then every order you go you will have more and more terms coming in the numerator and denominator in a multiplicative fashion and this is what the definition of this is, so if you substitute these and x equal to x 0 + p h then what I get for y n x which is the approximate polynomial for the data set that has been given to me it is equal to a y 0 + p delta y 0 + a p into p - 1 by 2 factorial Delta square y 0 + so on.

P into p - 1 p - 2 and so on so this is like a p - n + 1 and divided by n factorial and there is a delta n y 0 okay. So, that is the in nth order polynomial that we are looking for which could appropriately substitute or replace the f of x that have been found out from the experiment ok.

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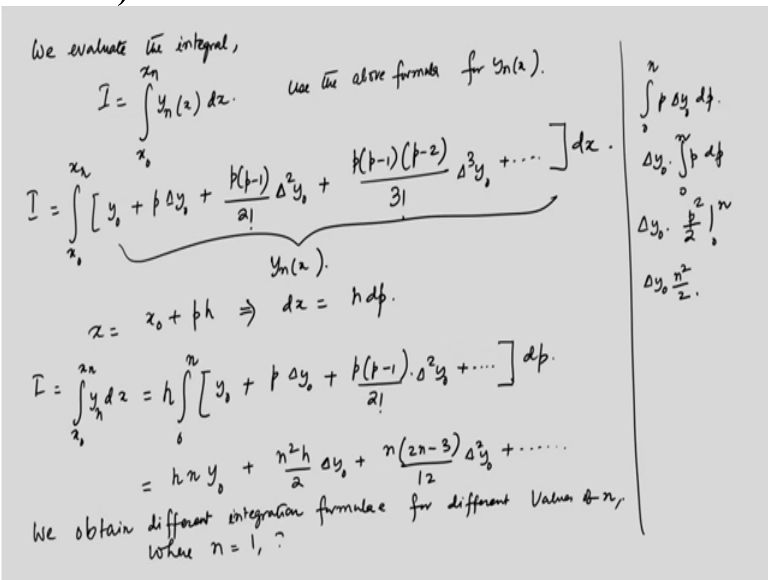

So, now we evaluate the integral why n x and dx so use the above formula for y n x and so basically this is particularly useful when we do not know what is f of x or what represents was a mathematical form of f of x. So, I simply now go ahead and substitute this from earlier so it is x 0 to x n and then we have a y 0 + a p delta y 0 + a p into p - 1 by 2 factorial a delta square y 0 + p into p - 1 a p - 2 by 3 factorial delta cube y 0 and so on.

And then there is a dx that is there so it is this is your nothing but the Y n of x. Now if you remember your x is equal to x 0 + p h, so that tells you that dx is equal to h dp and we can replace this there, so your i becomes equal to x 0 to x n y dx or Y n dx this is equal to h 0 to n so this is actually h let us write it properly h nd then you have a y 0 + a p Delta y 0 + a p into p - 1 by 2 factorial a delta square y 0 and so on and then alright.

So let us see that this is of course h into n y 0 because this is just a 1 and then you have a dy here or rather a dp here. So, this is that h dp, so the first term becomes h n y 0 ok. The second term can be found out if you just note that 0 to n p delta y 0 dp so this is like delta y 0 p Square dp from 0 to n so this is delta y 0 sorry this is p dp not p Square, this p dp so this is p Square over 2 0 to n and this is like Delta y 0 n square by 2.

So, this will become equal to n square h by 2 delta y 0 and the next term if you do it carefully it becomes this by 12 and then the delta y 0 and so on, ok. So, that is the third term and so on. So, the important thing is that we obtained different integration formula for different values of n let us see how so where n can be 1 2 3 and so on okay.

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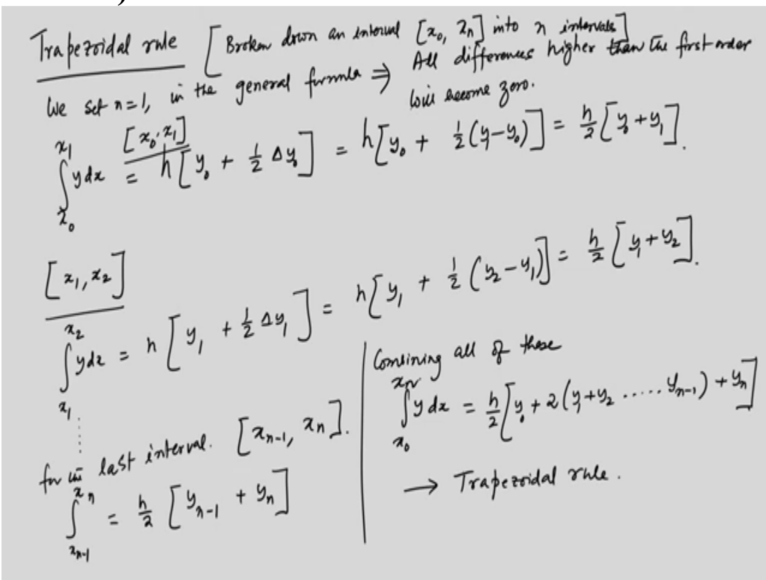

So, let us that takes us to this trapezoidal rule, so what it means is that we set n equal to 1 in the general formula. So, which means that all differences that is deltas will you become 0 y dx in which case if we put n equal to 1 so we have 0 to x n which will now become x 1 because n is equal to 1 this is simply equal to h y 0 + half delta y 0. And so this is nothing but h so this is actually not n this is h.

This h and there is y 0 + 1/2 y 1 - y 0 but this is like a h over 2 and a y 0 + of y 1 and so on okay. So, this is for the interval so we still have you know I mean we can divide an interval into between a and b into as many intervals as we want for the next interval between x 1 to x 2, so this is between x 1 x 0 or let us call it x 0 and x 1, so x 1 and x2 so this is that x 1 and x 2 will be x 1 and x 2 y dx which is equal to h.

And y 1 + 1/2 Delta y 1 which will be h and y 1 + 1/2 y 2 - y 1 its equal to h by 2 y 1 + y 2 okay. So, that is the for the second interval and for the you know carrying on with this for the last interval. So, we have broken down so let us not write this here so just write x 1 interval between x 0 to x n into n intervals. So, for the last interval which is x n - 1 x n this is like x n - 1 x n which is equal to h by 2 and a why n - 1 + y n.

So, if you take the contribution from all these integrals you will see that only the first 1that is y 0 and the last one y n they are counted only once while all others are counted twice, so of combining all of these one gets a y dx between you know x 0 to x n which is equal to h by 2 y

0 + twice of Y 1 + y 2 y n - 1 + y n and that is the formula for the trapezoidal rule or it is also called as a multiple trapezoidal rule, so this is called as a trapezoidal formula for the trapezoidal rule alright.

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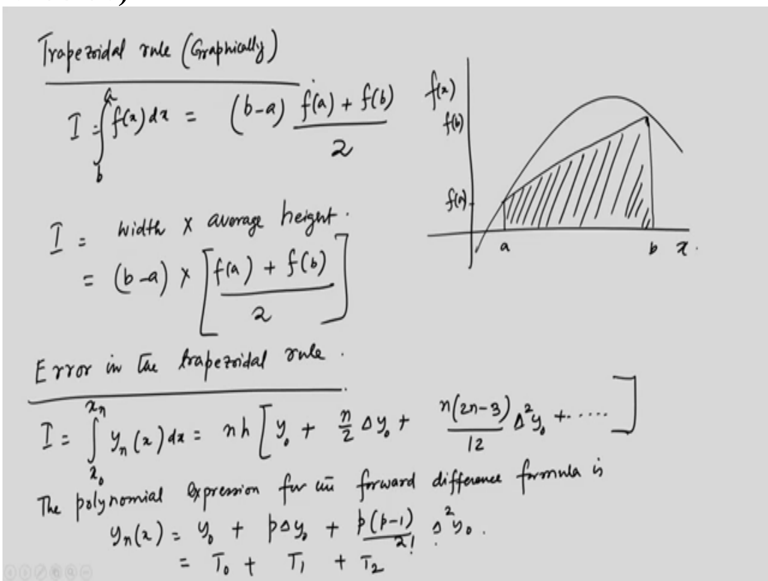

So, let us see an example of this trapezoidal rule so suppose we divide the entire range only into one segment that is we entire integration is now into one segment there is a single trapezoidal rule. So, we have a I equal to f of x b to a dx which is according to the trapezoidal rule it is h, h is b - a and the average value of fa and fb divided by 2, so what it means is the following that you have you have a curve like this which is f of x versus x and this is that x equal to a so this is f of a and say this is b and this is say f of b ok.

So we are replacing this curve by a simple trapezoid and by using this trapezoidal rule we are calculating the area of this trapezoid which is shaded here. So, we are approximating by sort so basically this curve has been approximated by a straight line and then we are calculating the area of the trapezoid. So, the integral estimate is given as so I is equal to width into average height this is like b - a into fa + fb by 2 okay.

So, that is the average height fa + fb by 2 and multiply it by the width of this and this gives you the area under the trapezoid. But this is of course very crude how crude it is one can understand but before that let us calculate the error in the trapezoidal rule. So, error of course comes from dropping the higher-order terms in the trapezoid trapezoidal rule. And because we have dropped some terms so there's a truncation error that is bound to come in okay.

So, to remind ourselves of this formula that we have seen x 0 to x n or a to b whichever way one wants to write it n by 2 Delta y 0 + n into 2 n - 3 by 12 Delta square y 0 and so on okay.

So, the trapezoidal rule is for n equal to 1 so the second term onwards I mean basically the you know the term that are the second term onwards are dropped.

So, now the polynomial expression for the forward difference formula is y n x equal to y 0 + p Delta y 0 + a p into p - 1 by 2 factorial Delta square y 0 so this can be actually written as T 0 + T 1 + T 2 and so on.

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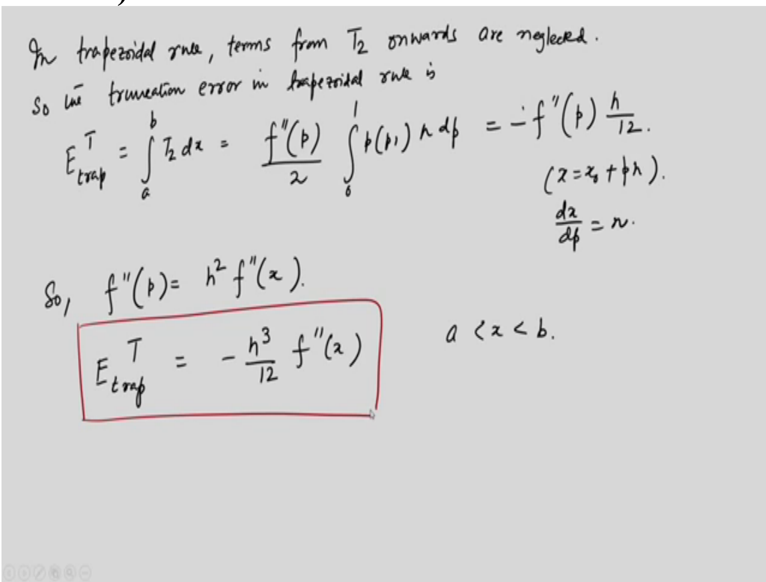

So, in trapezoidal rule terms from T 2 onwards are neglected so the truncation error in trapezoidal rule is e crap crap for the trapezoidal and T for the truncation this is a to b or t to and dx which is f double prime p by 2 0 to 1 p into p - 1 h dp which is equal to - f double prime P and h over 12 because of this I mean this is where we have used x equal to x 0 + ph okay, so your dx dp equal to h.

So, f double prime p is nothing but h square f double prime x so the E trapezoidal and the truncation error is nothing but h cube by 12 f double prime x for a < x < b okay. So, this is the error in the trapezoidal rule.

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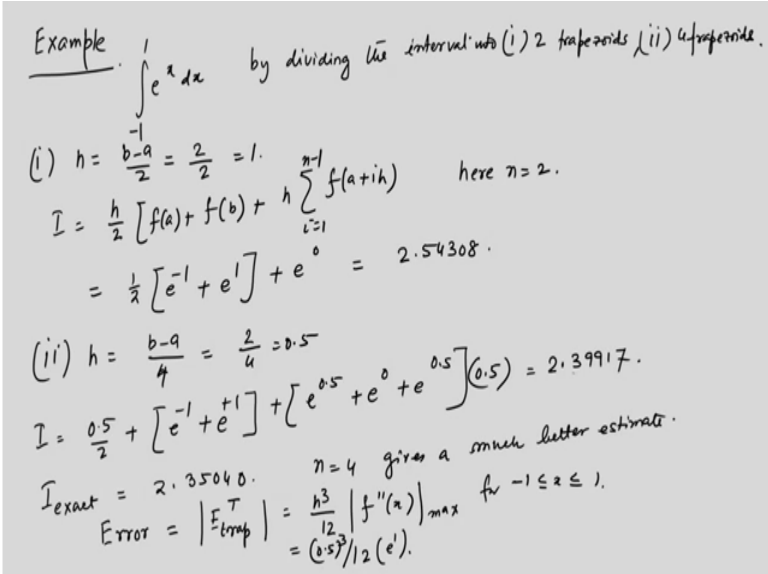

Let us see some 1quick example of this and so we have to evaluate the integral 0 to 1 exponential x dx by dividing the interval into one say 2 trapezoids and second say for example 4 trapezoids. And the way it can be d1so let us just do 1so h is equal to b - a by 2 which is 2 - so this is not from 0 to 1 say from - 1 to + 1 so it is 2 divided by 2 is equal to 1, so I is equal to h over 2 f a + f b + h f a + i h i equal to 1 to n - 1 and of course here n equal to 2 ok, so this is equal to 1/2 exponential - 1 + exponential 1 + exponential 0 so if you simplify this it comes as 2.54308.

Now for the second case when you consider 4 trapezoids in which case your h is equal to b - a by 4 n is 4 here, so this is like 2 by 4 equal to 0.5 so I is equal to 0.5 by 2 + exponential - 1 + exponential + 1 + exponential 0.5 + exponential 0 + exponential 0.5 and multiplied by 0.5 and it came out as 2.39917 okay. So, the exact if you calculate I exact this is equal to 2.35040 okay. So, this is the exact by 2 intervals we calculate it to be 2.54308 and 4 interval itself gets us reasonably close.

So, n equal to 4 gives much better estimate okay, so before we wind up let us see the error according to the calculation that we have done. So, this is equal to E trapezoidal and T integral which is equal to h cube by 12 f and we calculate the maximum for the x - 1 <= x <= 1 and this one actually comes out to be like 0.5 cubed divided by 12 into e to the power 1 and things like that. So, this is if you calculate it this will give you the error.

So you will see that the error from the exact value using this interval 4 interval value that comes out to be pretty close. So, we can calculate the errors from the I exact and - I trap using 4 intervals so this is 2.35- 2.39 etcetera and then you can divide it by the exact value and multiply it by 100 that will give you the relative percent error. And when you calculate the truncation error from the formula that we have derived you will get values that are very close okay.

So, we will carry on with this a little bit more on the trapezoidal rule and then we will go to the Simpsons rules that is one-third rule and 3/8 rule for calculating these numerical integration. You will see that particularly the Simpsons 1/3 rule is very efficient and is mostly used in most of the numeric computation for using or rather evaluating integrals.