Engineering Mathematics II Professor Dr. Jitendra Kumar Department of Mathematics Indian Institute of Technology, Kharagpur Lecture 30 Numerical Integration

So, welcome back to lectures on getting Engineering Mathematics 2, and this is lecture number 30 on numerical integration.

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So, in this lecture we will be covering some rules which can be used for integrating a given integral numerically. So, here we have the Trapezoidal rule and the Simpsons one third rule, so these two rules will be discussed in this lecture.

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So, the first question is that, why do we use numerical integration and the idea is that, in many cases, some complicated integrals like e power minus x square 0 to 1 or x power pi sin square root x dx and cannot be integrated exactly so, what we do, we compute them, numerically or we approximate them numerically. So, the idea of the Newton's Cotes integration formula is to replace the integrant or these complicated functions by some simple functions usually polynomial and as we know that these polynomials can easily be integrated.

So, the idea of the Newton's Cotes integration formulas are to replace this f x by some simple polynomials and then to integrate those polynomials and we will get at the end some approximate value of the given integral.

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So, the first Newton's Cotes rule we will discuss as a trapezoidal rule and where we will be talking about single application, meaning that the given integral a to b for instance this f x dx. We will be just considering as a single integral from a to b.

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So, here a to b fx dx and in this trapezoidal rule this f x will be approximated by the polynomial of degree 1 and this is the situation for instance, we have the function f x given and we have these endpoints a to b.

So, between these endpoints, we will be replacing that function or we will be approximating that function by this straight line a polynomial of degree 1. So, we have already discussed before when this point is for instance this a fa, so, this line passing through these two points, we can get as f a plus f b minus f a divided by b minus a into x minus a dx.

So, this can be integrated so, we have fa there and then we have b minus a, the integral and then we have f b minus f a divided by b minus a and here x a minus a whole square by 2 which when we substitute upper limit and then lower limit to lower limit will make that 0. So, upper limit will give half b minus a whole square.

So, here we have f a and then b minus a and then in the second case again we can simplify this. So, this calculation will lead to the simple formula, here we have b minus a that is exactly the difference of these limits, and then f b plus f a divided by 2.

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So, what is exactly this? This is the area of this trapezoid, which is formed by replacing that given function by the straight line. So, instead of getting that actual area under this curve, we are approximating that area basically by the area of this trapezoid and the name of this rule is the trapezoidal rule.

So, this was a single application where we have considered only one interval from a to b, but what we can do? We can improve the accuracy of this integration if we break this interval into several intervals, several sub intervals and then in each sub interval, we can apply the trapezoidal rule. So, in that case this error can be minimized.

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So, exactly that is the idea which we call multiple applications of this trapezoidal rule and in that case, we will split this integral, we will break this integral the range a to b into several points. So, from a we are calling as x naught to x 1 then x 2, x 3, xi minus 1, x i, the last point is b which we are calling xn.

So, we have taken n sub intervals equally spaced points this $x \theta x 1$ xn so, that this h is b minus a over n. So, h is the distance between the two points and it is kept same or equidistant points so this distance is same between any two points. So, the given integral we can split into these n integrals one is from x 0 to x 1, then x 1 to x 2 and so on, we have xn minus 1 to x n.

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And now in each for each interval we can use that trapezoidal rule. So, basically here if we apply that trapezoidal rule we have h by 2 because h is the distance from this x 1 to x 0 and then we have the value of the function f x naught plus f x 1. Similarly, again here we have h and then f x 1 plus f x 2 by 2 here also we have used that trapezoidal rule h into f x n minus 1 plus f xn.

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The Multiple Application of Trapezoidal Rule $I = \int_{0}^{x_1} f(x) dx + \int_{0}^{x_2} f(x) dx + \dots + \int_{0}^{x_n} f(x) dx$ $\approx h \frac{\sqrt{(x_0)^2 + f(x_1)} + h \overbrace{f(x_1)}^2 + \frac{f(x_2)}{2}}{2} + ... + h \frac{\sqrt{(x_{n-1})^2 + f(x_n)}}{2}$ $=\frac{h}{2}\left(\widehat{f(x_0)}+\frac{2}{2}\left(\frac{f(x_1)}{1}+\frac{f(x_2)}{1}+\cdots+\frac{f(x_{n-1})}{1}\right)+\frac{f(x_n)}{1}\right)$ $I = \frac{h}{2} \left[f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n) \right]$

So, having this now we can combine so h by 2 we can take common from each of these terms and then we have here f x naught which is written there, f x 1 here also we have f x 1 so that will be 2 times here again we have f x 2 there will be another term f x 2 and similarly here also we will get f x n minus 1 and there will be a term before also of this f x n minus 1. So, this 2 times f x 1 f x 2 f x n minus 1 and the plus this n the last term f xn.

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The Multiple Application of Trapezoidal Rule $I = \int_{x_0}^{x_1} f(x) dx + \int_{x_1}^{x_2} f(x) dx + \dots + \int_{x_{n-1}}^{x_n} f(x) dx$ $\approx h \frac{f(x_0) + f(x_1)}{2} + h \frac{f(x_1) + f(x_2)}{2} + \dots + h \frac{f(x_{n-1}) + f(x_n)}{2}$ $=\frac{h}{2}\big[f(x_0)+2\big(f(x_1)+f(x_2)+\cdots+f(x_{n-1})\big)+f(x_n)\big]$ $I = \frac{h}{2} f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n)$

So, finally, our formula looks like that we have the h by 2, we have f x naught the value of the function at the first node, the value of the function and the last node and the internal nodes we have just the doubling here. So, the double of the sum of the value of the function at those internal points.

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Now, we will discuss the or we will get the formula for the error how much error do we have when we approximate a given integral by this trapezoidal rule for that we need some theorems the one is some results one is this Weighted Mean Value Theorem.

Here we call that, we say that if f and g are continuous in this interval a b and this g never changes sign in this interval, then this Weighted Mean Value Theorem says that a to b f x gx dx will be equal to this fc the f we can bring to outside the integral and there will be a point c somewhere between a and b where we can have this equality there and the integral this gx dx, where this c belongs to somewhere in between the integral and obviously g must be integrable.

So, that is the mean value Weighted Mean Value Theorem around which we require for deriving the formula of the error in trapezoidal rule.

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The second result we need there the discrete mean value theorem which says that if f is a continuous function and let this x j be n plus 1 points in this interval a b and there are Cj n plus 1 constants, all having the same sign, then there exist a Xi in this interval a b such that we have this result.

So, the summation from j to 0 to n Cj f xj will be equal to again the similar situation that this f can be taken outside and then there will be a point xi again lies between that a and b interval and then summation here j 0 to n and Cj. So, here instead of integral now we a have summation.

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And there is a particular case that when all C_l are 1, then we have actually this result that 1 over n plus 1 j 0 to n f x j and this kind of average is equal to this f Xi and Xi is somewhere in this domain from a to b.

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So, now we will be talking about the error bounds for this trapezoidal rule and in the single application, first we will discuss and then we will go for the multiple applications. So, we already know from this interpolation that the error between the function and the its approximation as polynomial of degree 1 is given by x minus x naught x minus x 1 and the double derivative of f t divided by 2 and this t, naturally again lies between this x naught to x 1 if we are talking about the range of our integral from x naught to x 1.

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So, now we integrate the this function from x naught to x 1 and here this t as I said this depends also on x and this lies between 0 and x 1 because there is x there. So, this error will naturally depends on this x also. So, this t is also a function of t also depends on x naturally. So, now if we integrate this so, we will get this error from x naught to x naught plus h f x dx. So, that is the actual integral and minus this is the trapezoidal rule. So, this is the numerical value which we will get.

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So, the difference between the two we are talking about now. So, this will be equal to x naught to x naught plus h and then we can write using this result here that f x minus this P1 x will be equal to this x minus x naught x minus x 1 and this f double prime t dx naturally this t also depends on x, it is not free from x.

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So, having this integral now, we can just notice that is x minus x naught and x minus x 1, so, this x minus x naught and here we have x minus x 1. So, this is always positive and this is always negative because x naught plus h is nothing but x 1. So, we are talking about a single interval. So, this does not change signs, sign and we can use the mean value theorem the Weighted Mean Value Theorem which we have just discussed before.

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Error bounds for the Trapezoidal rule Single application: We know, $f(x) - P_1(x) = (x - x_0)(x - x_1) \frac{f''(t)}{2}$ Integrating (1) from x_0 to $x_1 = x_0 + h$ gives t depends on x and lies between x_0 & x_1 $E = \int_{x_0}^{x_0+h} f(x) dx - \frac{h}{2} [f(x_0) + f(x_1)] = \int_{x_0}^{x_0+h} (x - x_0)(x - x_1) \left(\frac{h}{2} \right) dx$ Note that $(x - x_0)(x - x_1)$ does not change the sign in $[x_0, x_0 + h]$ Applying weighted mean value theorem, we get $\mathscr{L} E = \frac{\mathscr{L}''(\tilde{t})}{2} \int_{0}^{x_0+h} (x-x_0)(x-x_0-h) dx$ Substitute $x = x_0 = v \implies dx = dv$.

So, the mean value theorem says that this f this function f double prime we can bring outside the integral and then we have this integral from x naught to x naught plus h, x minus x naught and this also we have written as x minus x naught minus h, because x 1 is x naught plus h. So,

having this we can now simplify by substituting this x minus x naught as v that means dx is dv.

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So, by doing so, dx is equal to dv we will just simplify this to this expression f double prime this t tilda divide by 2 and this integral 0 to h v v minus h dx and now we can integrate this. So, after this integration what we will get? We will get this error as minus h cube by 12 and there will be this double derivative evaluated at some point here t tilda between this interval x naught to x 1.

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So, this is the error in single application of trapezoidal rule and it is of h cube.

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Now, we will see the error in multiple applications, so, there will be addition now, so, we have error in each step. So, this interval is broken from x naught to x 1 then x 2 and so on then we have here xn. So, in each sub interval we are applying the trapezoidal rule and then we have error as a result in each interval. So, that error will be naturally which we have computed just h cube by 12 and the double derivative t i we are denoting now for ith interval.

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So, what we have i equal to 0 to n minus 1 and minus h cube, this f double prime. So, this h cube by 12 we can bring out of the summation and then summation is from 0 to n minus 1 f double prime and this t i tilda and now, we will use the discrete mean value theorem which is just discussed.

So, that will say that the value of the sum here will be n times because we can have like 1 over n and then multiplied by n there. So, this 1 over n and this 1 will give us this f double prime t hat.

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Where this t hat will be somewhere in the whole interval a and b.

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So, now we got the formula which says that because this n times h here now again n times h is nothing but the b minus a the whole interval, so, that we have given here b minus a divided by 12 and then h square and then we have double derivative at some point t hat which is between a and b.

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So, having this formula we can get at least the upper bound, because this t hat is not exactly known, but the what we can find, we can find the maximum value of this double derivative and then we can estimate the error in this in the given approximate value.

So, if we let this M 2 is this maximum of this double derivative between the points x naught to x n or a to b in that case this error we can bound by this b minus a h square by this 12, and then we have M 2 so this formula can be used for approximating the value of with to give the error bound in our numerical integration.

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So, we will do some numerical example now, or at least this one. So, here we have evaluate the following integral using trapezoidal rule, taking n is equal to 2 and n is equal to 4. So, first we will take 2 intervals, then we will go with 4 intervals and then we will compute the numerical value compare the numerical value so it is compare, compare the numerical values with the exact solution and then finally, we will find the error bound on the error.

Also find the number of sub intervals required if the error is to be less than 5 into 10 raised to power minus 4. So, using the error bound formula we will see that we can also estimate that how many sub intervals do we require if we want our error to be less than 5 into 10 raised to power minus 4.

Case 1, we will consider when we take number of intervals 2 that means the h will be 0.5 because our interval is 0 to 1 and then this will be 0.5. So, we have 2 intervals interval 1 interval 2. So, in that case h is 0.5 and then we can apply this trapezoidal rule. So, f naught 2 times the internal point plus the f 1 and then this h by 2, h is 0.5. So, this can be evaluated and we will get the value here 0.25833.

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When we take the number of subintervals, as 4 so then our h will be 1 by 4 because now 0 to 1 is divided into 4 intervals. So, naturally, this will be 1 by 4 then 2 by 4, then we have 3 by 4 and 1. So, in that case, we can apply this f naught and then f 1 there and the 2 times all internal nodes 2 times or internal nodes and then this can be simplified and we will get this value as 0.25615.

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So, we have the two in taking this h is equal 0.5 we have 0.25833 and then taking that h is equal 0.25 smaller h we are getting 0.25615. The actual value in this case is 0.25541. So, if we compute the error now, just to compare, so in the first case the error is 0.00292, in the second case, we have smaller error which is obvious or which is expected because in the second case we have taken 4 sub intervals, in the first case we have taken only 2 sub intervals. So, here the error is more whereas in this case error is less.

Now, coming to the error bounds. So, we have the formula which is derived just before so b minus a over 12 h square M2 where M2 is the maximum value of the second derivative. So, we have this f x 1 over 3 plus 2 x we can compute the second derivative as 8 over 3 plus 2 x square and now we need the maximum of this 8 over 3 plus 2 x square. So, the maximum will be when we have this minimum there, that means x equal to 0. So, we have 8 over 27 the maximum value of this double derivative.

Hence now we can bound the error, so error by this formula and M2 we can substitute so we have b minus a is 1 in that case so 1 over 12 h square 8 over 27. So, this is the error bound depending on h and then we have considered two situations. One was where we have taken h is equal to 0.25, the error bound suggest or says that the error will be less than 0.00617 the actual error was 0.00292. So, naturally that actual error is less than the bound given in this case.

When we take h is equal 0.25 it suggest now the upper bound for the error will be 0.00154 or naturally smaller number than the case when h was 0.5 and this also meets the criteria that the actual error is smaller than this number.

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Now, the last part of the question was that given this error or we want error less than this number, so, how many sub intervals we should have to get this error or error less than this one that means, we want that this error bound here M is the, M2 is the maximum now of f double prime. So, that this should be less than the maximum merit which are getting from our bound this should be less than the given error 5 into 10 raised to minus 4 and we want to get in how many sub intervals do we need.

So, this h is replaced by b minus a by n and having now this inequality b minus a is 1. So, we can compute that, this bound on this n. So, having this inequality we realize that n is greater than or equal to 7.03 means more than 7, n is suggested with this inequality. So, if we take n is equal to 8 for instance, then definitely that error will be met this error bound which is given here 5 into 10 raise to minus 4 will be attain.

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Now, the next rule we are talking about the Simpsons one third rule. So, earlier in this trapezoidal rule we have replaced this f x by a polynomial of degree 1 and now we will replace here a polynomial of degree 2. So, that is the only difference the rest everything the error bound and so on a similar calculations can be made.

So, in this case since we are substituting here the second order polynomial, so, even in the single application of the Simpsons one third rule, we need three points we need x naught, we need x 1 and we need x 2. So, at least three points are required to fit a polynomial of degree 2 which passes through these points.

So, in that case now we will use this polynomial of degree 2 it is a Lagrange polynomial of degree 2 which passes through these points a x 1 and b. So, from x naught to x 2 we are integrating this is a single application of this one third rule and now, we can simplify this or we can integrate this because this is integrated over x and x is setting here in the numerator as a quadratic form, quadratic term.

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Simpson's 1/3rd Rule
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$$
I = \int_{a}^{b} f(x)dx \approx \int_{a}^{b} P_{2}(x)dx
$$
\nLet $x_{0} = a$, x_{1} , $x_{2} = b$
\n
$$
I \approx \int_{x_{0}}^{x_{2}} \frac{\left(\sqrt{(x-x_{1})(x-x_{2})}\right)}{\left(\sqrt{(x_{0}-x_{1})(x_{0}-x_{2})}\right)}f(x_{0}) + \frac{(x-x_{0})(x-x_{2})}{(x_{1}-x_{0})(x_{1}-x_{2})}\left(\sqrt{(x_{1})} + \frac{(x-x_{0})(x-x_{1})}{(x_{2}-x_{0})(x_{2}-x_{1})}\right)dx
$$
\n
$$
= \frac{1}{2h^{2}}f(x_{0}) \int_{x_{0}}^{x_{2}} (x-x_{1})(x-x_{1}+x_{1}-x_{2})dx - \frac{1}{h^{2}}f(x_{1}) \int_{x_{0}}^{x_{2}} \frac{(x-x_{0})(x-x_{0}+x_{0}-x_{2})dx}{x_{0}} + \frac{1}{2h^{2}}f(x_{2}) \int_{x_{0}}^{x_{2}} (x-x_{0})(x-x_{0}+x_{0}-x_{1})dx
$$

So, we can either do direct integration or the way which is done here that x minus x 1. So, this is taken out here, which is all these constant terms, only this numerator is adjusted here x minus x 1 and this x minus x 1 plus this x 1 here also we have done minus x 0 plus x 0 so, that we can get exactly this term as one term there. So, x minus x 0 here x minus x 1 and then integration can be performed.

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So, if we integrate now, what we will get? This kind of terms but if we simplify this we will get h by 3 f x naught and we have 4 times f x 1 then f x 2 so, how this rules, rule can be understood we have h by 3 it is call also one third rule. So, h by 3, the value the first point value at the end point and the internal point here are 4 times f x naught so, there should be

minimum these three points or two intervals x naught, x 1 and x 2 to apply this Newton's one third rule or any multiple of this as we will see in the multiple application that will have.

So, either we have 2 intervals or we have 4 intervals, we have 6 intervals, we can apply Newton's one third, Simpsons one third rule.

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So, coming to the multiple applications, so, again the idea is same that we have the range from a to b which we will split into several sub intervals, that means x naught to x 1, then x 2 and so on xi minus 1, to xi and the last point we have xn which is equal to b and we have equidistant points of b minus a is equal to n h.

So, given this I which is splitted now into several parts, considering that in each sub interval we should have three points that mean x naught to x 2, so there is a x naught x 1×2 point here also we have x 2 to x 4, so we have x 2, x 3, x 4, here also we have x n minus 1 then xn minus 2 x n minus 1 and then xn. So, in each for each in integral here we have the three points so, we can apply the Newton's, the Simpsons one third rule in each.

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That means, in the first case we have h by three we have f x naught 4 times f x 1 the middle point and then we have f x 2. Similarly, for the second integral we have f x 2, we have 4 times f x 3, we have f x 4 and again h by 3 similarly for all other intervals.

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And now what we will realize that there are these 4, here also 4 so the 4 times f x 1 f x 3 f x 5 etcetera that means the summation will run on these odd numbers 1, 3, 5 and so on the first term is f x naught, the last will be f x n and then we have this f x 2 and similarly here also we have f x 2 so, that will be doubled. So, 2 times we have f x 2, we have f x 4 again and so on. So, the second summation will run for the even numbers 2, 4, 6 and so on of this f x j.

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Multiple Application of Simpson's Rule $b = x_n$ $x_0 = a$ $x_1 \dots$ x_{i-1} , x_i $I = \int_{x_0}^{x_2} f(x) dx + \int_{x_2}^{x_4} f(x) dx + \dots + \int_{x_{n-2}}^{x_n} f(x) dx$ $\approx \frac{h}{3}\left\{f(x_0)+4f(x_1)+f(x_2)\right\}+\frac{h}{3}\left\{f(x_2)+4f(x_3)+f(x_4)\right\}+\cdots+\frac{h}{3}\left\{f(x_{n-2})+4f(x_{n-1})+f(x_n)\right\}$ $= \frac{h}{3}\left\{f(x_0) + 4\sum_{i=1}^{n-1} f(x_i) + 2\sum_{i=1}^{n-2} f(x_i) + f(x_n)\right\}$ **Error:** Single application: $E = -\frac{h^5}{90} f^{(4)}(\xi)$; $\xi \in (a, b)$ Multiple application: $E = \left(-\frac{b-a}{180}h^4 f^{(4)}(\xi); \ \xi \in (a, b)\right)$

Well, if we compute the error we are not showing all the steps but what comes out to be in this case, the error term in the single application will contain the h 5, the fourth order derivative at the size, size between the given interval and in the multiple application, we have this b minus a over 180 h power 4 and this f the fourth order derivative at this Xi.

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So, as we see from the error itself, now, we have h power 4 terms whereas, in this trapezoidal rule we have h square term. So, naturally this error will be small for small h and which is expected because here we have now approximated with a higher degree polynomial.

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Again we will take the same example and will apply the Simpsons rule taking n, 2 intervals and the 4 intervals and we will compare with the exact solution. So, n is equal to 2 if we take so, the 2 intervals and in that case we will apply this formula f 0 4 times f half and this f1 this is the single application of this Simpson rule. So, after this calculation, we do see that we are getting 0.2556.

Whereas, when we take n is equal to 4 points, what we will get we will get 0.25542 as the answer and just remember the exact solution this case was 0.25541. So, we do see we are getting much better result now, then the trapezoidal rule as even the single application itself we are matching with three digits and whereas, here it is much even better when we take n is equal to 4 points.

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So, these are the references use for preparing the lecture.

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And just to conclude that we have discussed the numerical integration mainly the trapezoidal rule which says that we can integrate this f x from a to this b where we denote this a as x naught and then we have equidistant point x 1, x 2, x 3 and so on and the formula is given here that h by 2 and we take the f x naught and this f x n and all internal points will be just doubled.

Error we have discussed that the error is given by this difference here x n minus x naught divided by 12 and we have h square the second derivative a term.

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Whereas, in the Simpsons rule, we have slightly different formula, where again this first and the last points are exactly same as in the trapezoidal rule. Whereas, the internal points all this having odd indices 1, 3, 5 they will be having 4 times the function value and here 2 times the function value for those having indices 2, 4, 6, etcetera.

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Well, and the error here was of higher order so then this one there was h 2 there and here we have h 4 for the Simpsons rule. So, that is all for this lecture. And I thank you for your attention.