

## Numerical Methods and Computation

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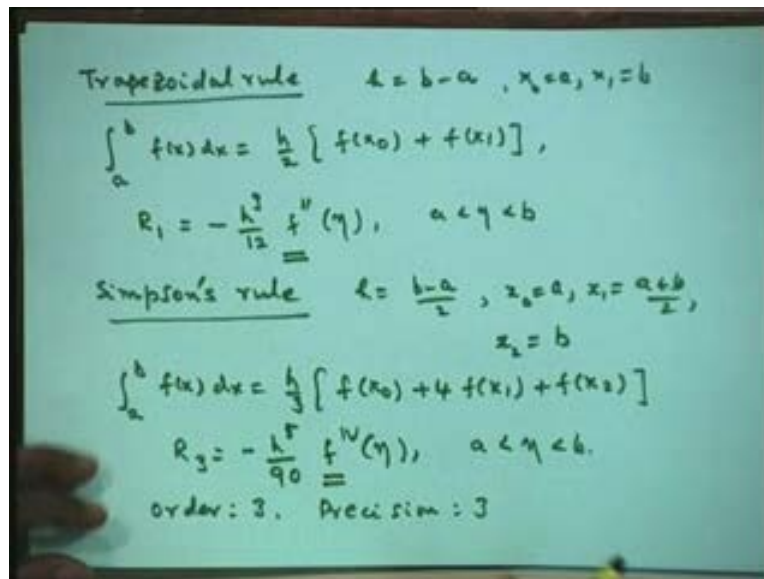
Indian Institute of Technology Delhi

### Lecture No - 38

#### Numerical Differentiation and Integration (Continued)

In our previous lecture we have derived the Newton cotes formulas for a numerical integration; out of this class we have also derived the first two formulas, the trapezoidal rule and the Simpson's rule. Let us just see what are these two formulas that we have derived.

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Trapezoidal rule  $h = b - a$ ,  $x_0 = a$ ,  $x_1 = b$

$$\int_a^b f(x) dx = \frac{h}{2} [f(x_0) + f(x_1)],$$
$$R_1 = -\frac{h^3}{12} f''(\eta), \quad a < \eta < b$$

Simpson's rule  $h = \frac{b-a}{2}$ ,  $x_0 = a$ ,  $x_1 = \frac{a+b}{2}$ ,  $x_2 = b$

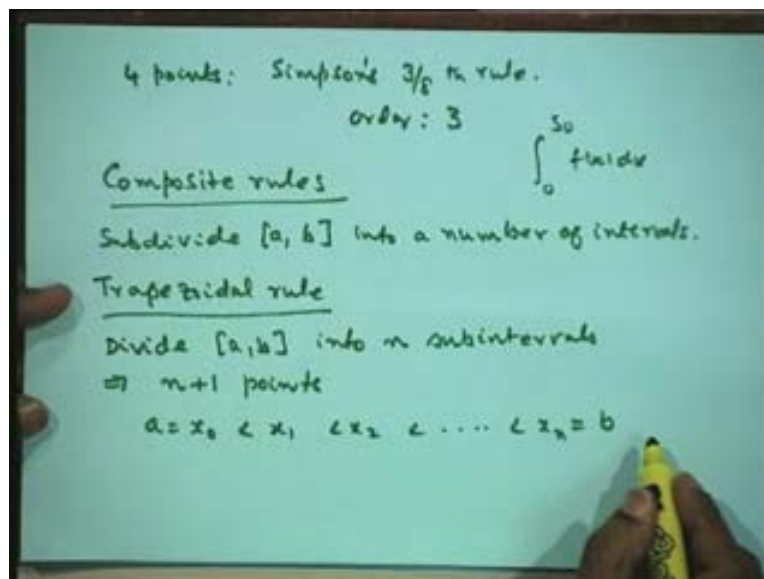
$$\int_a^b f(x) dx = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)]$$
$$R_3 = -\frac{h^5}{90} f^{(4)}(\eta), \quad a < \eta < b.$$

order: 3. Precision: 3

The first formula that we have derived is the Trapezoidal rule in which the step length  $h$  is taken as the total length that is  $b$  minus  $a$  and we have derived the formula as integral  $a$  to  $b$   $f(x) dx$  is equal to  $h$  by 2 of  $[f$  of  $x_0$  plus  $f$  of  $x_1]$ , where  $x_0$  is our  $a$  and  $x_1$  is equal to our  $b$ . We have also derived the error expression for this, the error expression which we have written it as  $R_1$  that is minus  $h$  cubed by 12  $f$  double dash of  $\eta$ , where  $\eta$  is any number between  $a$  and  $b$ . From this we conclude it that the trapezoidal rule integrates exactly polynomials of degree less than or equal to 1 that can be observed from this that the error term contains the second derivative of  $f$ , therefore which will vanish when  $f(x)$  is a polynomial of degree less than or equal to 1.

Now, then we construct the Simpson's rule using 3 points, Simpson's rule in which  $h$  is taken as  $b$  minus  $a$  by 2, so that we have got 3 points  $x_0$  is equal to  $a$ ,  $x_1$  is the middle point  $a$  plus  $b$  by 2 and  $x_2$  is equal to  $b$ . Then we have derived the formula as  $\int_a^b f(x) dx$  is  $h$  by 3  $f$  of  $x_0$  plus 4 times  $f$  of  $x_1$  plus  $f$  of  $x_2$  and the corresponding error we derived it as  $R_3$  is equal to minus  $h^5$  by 90 fourth derivative at some point  $\eta$ ,  $a$  less than  $\eta$  less than equal to  $b$ . Now from this we have concluded that because the error term contains the forth derivative the order of the Simpson's rule, is order is 3 or which we call it also precision 3. Therefore Simpson's rule integrates exactly polynomials of degree less than or equal to 3. This happened because the error constant turned out to be 0 and hence the order of the formula has gone from 2 to 3. Higher order Newton cotes formulas can also be used that means using instead of 3 points we can use 4 points 5 points and so on. The next formula is also called the Simpson's rule but it is called Simpson's 3/8th rule if I use 4 points.

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That means if I use 4 points in place of 3 that we have used over here then that formula is usually called the Simpson's 3/8th rule that is because the outside this bracket instead of  $h$  by 3 I have 3  $h$  by 8 outside the bracket and it will be containing 4 points. However this formula or the later formulas are not used much because the 4 point formula is also the same order as the Simpson's 1/3rd rule therefore there is no point in doing extra computation that is of evaluating one more value of  $f(x)$ . We have 1 evaluation less for the Simpson's 1/3rd rule, therefore this is also of order 3 only and because of this reason we do not use this formula. Newton cotes beyond a certain order 6, 7 or 8 the weights that is your  $\lambda$ s here they are all positive if you look at this, here  $\lambda_1$ ,  $\lambda_0$   $h$  by 2,  $\lambda_1$   $h$  by 2 here also this is the, all are positive therefore there is no errors due to cancellation, we know mostly errors also errors round off error because of cancellations.

Whereas if you go to higher order Newton cotes formulas, somehow the weights become negative therefore there is a chance of some round off error therefore the most popular methods of numerical integration is a trapezoidal rule, Simpson's rule and some modifications to this to get better accurate methods. Now however if I have an integral in which the length of the integral is large, let us say I want to integrate something like  $\int_0^{50} f(x) dx$  now I can use the trapezoidal rule, I can use Simpson's rule but it is necessary to know how accurate it would be. The accuracy would depend by looking at its error term, if I look at this error term this has got  $h^3$  by 12 here and this has got  $h^5$  by 90 here in these two formulas. when you take the step length in trapezoidal rule as 50 or you take in Simpson's rule 3 points that is step length is 25, now the error in Simpson's rule be 25 to the power of 5 by 90 whereas here it is 50 to the power of 3 and this therefore the error itself is going to be very large in that case when the interval is large therefore application of the trapezoidal or Simpson's rule as it is will give you inaccurate results when the length of the interval is very large.

Therefore we modify this such that this  $h$  is sufficiently small, in other words  $h$  would be sufficiently small if I break the interval, given interval  $a$  to  $b$  into smaller intervals and then use the corresponding formulas for each one of these integrals individually. So such formulas shall be called composite rules, so we shall call them as composite rules. So what we do here is subdivide, subdivide  $[a, b]$  into a number of intervals. Now the, how many number of intervals it depends on you, how small the step length should be, so if you want a step length small corresponding will increase it. Let us first look at the trapezoidal rule, how we are going to get the composite rule for this. Now we have seen that the trapezoidal rule uses only 2 points therefore the way in which we subdivide  $[a, b]$  is immaterial for us, you can divide it into any number of parts. So let us divide  $[a, b]$  into say  $n$  parts, divide  $[a, b]$  into  $n$  subintervals that means this would imply that we are getting  $n$  plus 1 points, so this is  $n$  intervals therefore we will have  $n$  plus 1 points. So let us take this division as, subdivision as  $a$  is equal to  $x_0$  less than  $x_1$  less than  $x_2$  and so on  $x_n$  is equal to  $b$ .

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Subdivide  $[a, b]$  into a number of intervals.

Trapezoidal rule

Divide  $[a, b]$  into  $n$  <sup>equal</sup> subintervals  
 $\Rightarrow n+1$  points  
 $a = x_0 < x_1 < x_2 < \dots < x_n = b$   
$$h = \frac{b-a}{n}$$
  
$$\int_a^b f(x) dx = \int_{x_0}^{x_1} f(x) dx + \int_{x_1}^{x_2} f(x) dx + \dots + \int_{x_{n-1}}^{x_n} f(x) dx$$

Then I will write the given interval into these subintervals that means given this interval  $a$  to  $b$   $f(x) dx$  I will now write this as  $x_0$  to  $x_1$  that is your first point to this  $f(x) dx$  plus integral  $x_1$  to  $x_2$   $f(x) dx$  plus so on  $x_{n-1}$  to  $x_n$   $f(x) dx$ . Furthermore we will, all the subintervals were assumed to be equal when we started to trapezoidal rule its equal so we can still put here  $n$  equal subintervals, they are all of the same length. Therefore if I go a step behind, if they are  $n$  equal subintervals then the length of the interval will be total length  $b$  minus  $a$  that is the total length, there are  $n$  subintervals so that is divided by  $n$  that is equal to  $h$ . These are  $n$  equal subintervals therefore  $b$  minus  $a$  divided by  $n$  is equal to  $h$  therefore the step length that we are talking of is now  $b$  minus  $a$  by  $n$ . So if in the previous problem if we have got  $0$  to  $50$  and I want a step length of point  $5$ , I will now have hundred subintervals  $0$  to  $50$ ,  $100$  subintervals so that step length will be  $50$  by  $100$  that is equal to point  $5$  so we will have a step length half. Therefore this step length  $h$  depends on the number of subintervals that we choose.

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$$\begin{aligned}
 \int_a^b f(x) dx &= \int_{x_0}^{x_1} f(x) dx + \int_{x_1}^{x_2} f(x) dx + \dots + \int_{x_{n-1}}^{x_n} f(x) dx \\
 &= \frac{h}{2} \left[ \{f(x_0) + f(x_1)\} + \{f(x_1) + f(x_2)\} + \dots \right. \\
 &\quad \left. + \dots + \{f(x_{n-1}) + f(x_n)\} \right] \\
 &= \frac{h}{2} \left[ f(x_0) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\} + f(x_n) \right] \\
 R_1 &= -\frac{h^3}{12} \left[ f''(\eta_1) + f''(\eta_2) + \dots + f''(\eta_n) \right] \\
 x_0 &< \eta_1 < x_1, \dots, x_{n-1} < \eta_n < x_n. \\
 |R_1| &\leq \frac{h^3}{12} n M_2 \quad ; M_2 = \max_{a \leq t \leq b} |f''(t)| \\
 &= \frac{(b-a)h^2}{12} M_2 \quad \checkmark
 \end{aligned}$$

Now what we do when once we write this as, this is equal to this I now apply the trapezoidal rule for each of these integrals independently, so I would write this as  $h$  by  $2$ , all of them have  $h$  by  $2$  outside because the step length  $h$   $x_0$   $x_1$  distance is same,  $x_1$   $x_2$  distance is same,  $x_{n-1}$   $x_n$  distance is same that is how we made them as equal subintervals. Therefore  $h$  by  $2$  outside, I will then have corresponding to this I will have  $f$  of  $x_0$  plus  $f$  of  $x_1$  that is the formula for evaluating the first integral  $h$  by  $2$  of this, the formula for the second one is  $h$  by  $2$  of  $f$  of  $x_1$  plus  $f$  of  $x_2$  and so on and the last integral will be  $\{f$  of  $x_{n-1}$  plus  $f$  of  $x_n\}$ . Now I can simplify the whole expression, you can see that there is a  $f(x_1)$  here,  $f(x_1)$  here, they combine and become  $2$  times  $f(x_1)$ , there is  $f(x_2)$  here, there will be  $f(x_2)$  here, they combine, similarly I have a  $f(x_{n-1})$ , there will be  $f(x_{n-1})$  here, so all of them will be multiplied by factor of  $2$  so I will have here  $h$  divided by  $2$  [ $f$  of  $x_0$  plus  $2$  times  $\{f$  of  $x_1$ ,  $f$  of  $x_2$ ,  $f$  of  $x_{n-1}$  plus  $f$  of  $x_n\}$ ].

Now you can see that this is the first ordinate with a multiplied factor  $1$ , the last ordinate with multiplicative factor  $1$  only but all the middle ordinates are multiplied by  $2$ , so  $2$  times of this one, so this is called the composite trapezoidal rule. And the effect of the error, we must be able to write down the effect of the error on the trapezoidal rule, now let us write down the error what would be for this. I would write down the contribution of each  $1$  of them individually, we had earlier obtained the trapezoidal rule error at minus  $h$  cubed by  $3$   $f$  double dash of  $\eta$ , now I will have  $\eta_1$ ,  $\eta_2$ ,  $\eta_3$  corresponding to each  $1$  of the subintervals, so I would therefore have  $h$  cubed by  $12$   $f$  double dash of  $\eta_1$  plus  $f$  double dash of  $\eta_2$ , there are  $n$  subintervals therefore I will have  $\eta_n$ . Where  $\eta_1$  lies in the first interval and so on  $x_{n-1}$  less than  $\eta_n$  less than  $x_n$ , so each  $1$  of them would lie in that particular interval.

Now it is easier for us **now** to write down what is the bound on this error, so I can just take the magnitude of this as magnitude of  $R_1$ , this will be less than or equal to  $h^3$  by 12,  $h^3$  by 12, let us take the maximum of  $f''$  over the entire interval as some  $M_2$ , so let us define  $M_2$  as the maximum of  $f''$  of  $x$  over the entire interval  $a \leq x \leq b$ . Then  $f''(\xi_1)$  is less than or equal to  $M_2$ , this is also less than or equal to  $M_2$ , this is also less than or equal to  $M_2$  and there are  $n$  factors therefore it will be  $n$  times  $M_2$ . There are  $n$  factors here each one contributing  $1 M_2$  but  $n$  into  $h$  is a known value. If you look at it this is  $n$  into  $h$  is  $b - a$  so we would like to throw away this  $n$ ,  $n$  should not come into picture here, so out of this  $n h^3$   $n$  into  $h$  will be replaced by  $b - a$  therefore this is same as, I will put equal now,  $b - a$  that is  $n$  into  $h$  is equal to  $(b - a) h^2$  by 12  $M_2$ ,  $b - a$   $h^2$  by 12. It is independent of the number of intervals except that  $b - a$  is the total length of the interval.

Therefore in practical computation the order of the formula is still 1 because this is  $M_2$ , this is second derivative therefore order of the formula is the same that is 1, it is going to integrate polynomials of degree 1 only but now if you look at this power of  $h$ , this power of  $h$  is the one that shows really how the trapezoidal rule is behaving. In the earlier case when it is very rough it is we are showing it as  $h^3$  but  $h^3$  as no meaning when  $h$  is very large but here  $h$  is small therefore the trapezoidal rule is really behaving like an order of  $h^2$  expression and it is integrating polynomials of degree less than or equal to 1 exactly. Therefore this is the expression which we are going to use later on when we say that we are using composite rule to get still better results. Now while doing the numerical differentiation we were repeatedly cautioning against the round off errors that it is possible that the round off error can actually swallow the actual solution and finally we may have very bad results but let us see what would happen here in the round off error, let us first see what is effect of the round off error in the trapezoidal rule.

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Effect of round off

$$\begin{aligned}
 I &= \frac{h}{2} \left[ (f_0 + \epsilon_0) + 2 \{ (f_1 + \epsilon_1) + \dots + (f_{n-1} + \epsilon_{n-1}) \} + (f_n + \epsilon_n) \right] \\
 &\quad - \frac{h^3}{12} \left[ f''(\eta_1) + \dots + f''(\eta_n) \right] \\
 &= \frac{h}{2} \left[ f_0 + 2(f_1 + f_2 + \dots + f_{n-1}) + f_n \right] + R.E. + T.E. \\
 |T.E.| &\leq \frac{h^3(b-a)}{12} M_2 \\
 R.E. &= \frac{h}{2} \left[ \epsilon_0 + 2(\epsilon_1 + \epsilon_2 + \dots + \epsilon_{n-1}) + \epsilon_n \right]
 \end{aligned}$$

So let us see what would be the effect of round off error, effect of round off. So our I the value of the integral  $h$  by 2, let us write down  $(f_0 + \epsilon_0)$  that is corresponding to this, round off error corresponding to the first one plus 2 times corresponding to  $f(x_1)$  we have  $(f_1 + \epsilon_1)$  plus so on corresponding to this we have  $(f_{n-1} + \epsilon_{n-1})$  plus  $(f_n + \epsilon_n)$  and add to this the truncation error  $h$  cubed by 12 that we have it here this expression that is your  $f$  double dash  $\eta_1$  plus so on  $f$  double dash of  $\eta_n$ . This is how our integration rule is going to look up when we include your round off error and the truncation error in this particular expression. Now this is equal to our  $h$  by 2 of  $[f_0 + 2(f_1 + f_2 + \dots + f_{n-1}) + f_n]$  plus round off error plus truncation error, so this is our actual formula that we are using and to this we are going to add our round off error and the truncation error. Now we have already derived the truncation error here, so the truncation error bound is here so the magnitude of the truncation error is less than or equal to  $h^3(b-a)$  by 12  $M_2$ , this is the bound for the truncation error. Now let us write down round off error, round off error is  $h$  by 2, outside  $h$  by 2 I have,  $[\epsilon_0 + 2(\epsilon_1 + \epsilon_2 + \dots + \epsilon_{n-1}) + \epsilon_n]$ , this is our round off error from here.

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$$\begin{aligned}
 & - \frac{h^3}{12} [f''(\eta_1) + \dots + f''(\eta_n)] \\
 & = \frac{h}{2} [f_0 + 2(f_1 + f_2 + \dots + f_{n-1}) + f_n] + RE + TE \\
 & |TE| \leq \frac{h^3(b-a)}{12} M_2 \\
 & |R.E| = \left| \frac{h}{2} [e_0 + 2(e_1 + e_2 + \dots + e_{n-1}) + e_n] \right| \\
 & \leq \frac{h}{2} [1 + 2(1 + 1 + \dots + 1) + 1] E ; \quad E = \max |e_i| \\
 & = \frac{h}{2} [1 + 2(n-1) + 1] E = nhE = \underline{(b-a)E}.
 \end{aligned}$$

Now let us write down its magnitude also, let us put the magnitude. Now if I denote by epsilon the maximum of all these epsilon<sub>i</sub>'s, if I take this maximum of this then this will be less than or equal to h by 2, epsilon comes out so I will have 1, 2 into 1 plus 1 plus so on 1 plus 1 into epsilon. I have taken now common epsilon throughout and I have here 2 into 1 plus 1 plus 1 and so on. Now the total number of points are n plus 1 points therefore the number of these are n minus 1 because this is 1 point, 1 point, so n plus 1 minus 2, so these are n minus 1 quantity so this will be equal to h by 2 [1 plus 2 times (n minus 1) plus 1] into epsilon. This is 2 n minus 2, 2 2 cancels I will have 2 n, 2 also cancels, I will simply have n h into epsilon but n into h is (b minus a) therefore this is (b minus a) into epsilon.

Now you can see that we really do not have to worry at all about the round off error, the integration is a quite stable process because the error at the most is multiplied by (b minus a). If you have taken 10 plus accuracy all the f(x) at the most of the length of the interval is say 50 or each one of them is say 10 so you are just multiplying 10 times at particular epsilon that we have got. Therefore we have, we are quite safe with respect to the round off error, round off error here would really does not affect that much as in the numerical differentiation and hence we normally say that numerical integration is usually a stable process unlike numerical differentiation which can often be an unstable process. The same thing is true whether I consider the Simpson's rule or any of the other Newton cotes formulas.



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Simpson's rule  
Divide  $[a, b]$  into even number  $(2n)$  of equal subintervals.  
$$\frac{b-a}{2n} = h, \quad b = a + 2nh$$
$$a = x_0 < x_1 < x_2 < \dots < x_{2n} = b$$
$$\downarrow$$
$$x_0 + 2nh$$
$$I = \int_a^b f(x) dx$$
$$=$$

Now let us derive the composite Simpson's rule, let us derive the composite Simpson's rule. Now when we derived the Simpson's rule, Simpson's rule required 3 points and we have taken  $h$  is equal to  $b$  minus  $a$  by  $2$  so I need for each sub interval 3 points that means I should have only odd number of points in order that the Simpson's rule can be extended. Odd number of rules means we must have even number of subintervals so therefore to derive the composite Simpson's rule we divide  $[a, b]$  into even number of sub intervals, so divide  $[a, b]$  into even number of, let us take this as  $2n$ , even number of equal subintervals. That means we are taking  $b$  minus  $a$  divided by  $2n$  is equal to  $h$ . We are taking  $2n$  subintervals therefore  $b$  minus  $a$  by  $2n$  will be  $h$  and therefore we have the points  $a$  is equal to  $x_0$  less than  $x_1$  less than  $x_2$  so on  $x_{2n}$  is equal to  $b$ , so that we have total of  $2n + 1$  points. Of course this is our  $x_0$  plus  $2n$  into  $h$  that is you have got  $b$  is equal to  $a$  plus  $2nh$ , so this is  $x_0$  plus  $h$ ,  $x_0$  plus  $2h$  and so on, we have  $x_0$  plus  $2nh$ , all of them are equal subintervals. Therefore we divide  $I$  integral  $a$  to  $b$   $f(x) dx$  as equal to, each one of them should contain 3 points, therefore I would take the first integral as  $x_0$  to  $x_2$   $f(x) dx$ .

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$$\begin{aligned} \frac{b-a}{2n} &= h, \quad b = a + 2nh \\ a &= x_0, < x_1 < x_2 < \dots < x_{2n} = b \\ &\quad \downarrow \\ &\quad x_0 + 2nh \\ I &= \int_a^b f(x) dx \\ &= \int_{x_0}^{x_2} f(x) dx + \int_{x_2}^{x_4} f(x) dx + \dots + \int_{x_{2n-2}}^{x_{2n}} f(x) dx \end{aligned}$$

Then the next integral from starting from  $x_2$  to  $x_4$   $f(x) dx$  and the last interval will be  $x_{2n-1}$ , **2n minus 2** to  $x_{2n}$   $f(x) dx$ . Now when once you have subdivided into this on each one of them now I can use the Simpson's rule, therefore if I apply the Simpson's rule and the each one is subdivided into 3 parts therefore that is, which is nothing but  $h$  therefore step length here in all the integrals is the same.

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$$\begin{aligned} &= \frac{h}{3} [(f_0 + 4f_1 + f_2) + (f_2 + 4f_3 + f_4) + \dots \\ &\quad + (f_{2n-2} + 4f_{2n-1} + f_{2n})] \\ I &= \frac{h}{3} [f_0 + 4(f_1 + f_3 + f_5 + \dots + f_{2n-1}) \\ &\quad + 2(f_2 + f_4 + \dots + f_{2n-2}) + f_{2n}] \\ R_3 &= -\frac{h^5}{90} [f^{(4)}(\eta_1) + f^{(4)}(\eta_2) + \dots + f^{(4)}(\eta_n)] \\ x_0 &< \eta_1 < x_2, \dots, x_{2n-2} < \eta_n < x_{2n} \\ |R_3| &\leq \frac{h^5}{90} \cdot n \cdot M_4 \quad M_4 = \max_{a \leq x \leq b} |f^{(4)}(x)| \\ &= \frac{(b-a)h^4}{180} M_4 \quad nh = \frac{b-a}{2} \end{aligned}$$

Therefore I would have  $h$  divided by 3, this is  $(f_0 \text{ plus } 4 f_1 \text{ plus } f_2)$  that is the contribution of the first integral plus the contribution of second integral starting  $x_2$  to  $x_4$  that is  $(f_2 \text{ plus } 4 \text{ times } f_3 \text{ plus } f_4)$  plus so on, from the last integral we will have  $(f_{2n-2} \text{ 4 times } f_{2n-1} \text{ plus } f_{2n})$ . Now we can simplify this and write this as  $h$  by 3 or let us write down  $I$  is equal to  $h$  by 3  $f_0$ , now we can see that the odd suffixes of  $f$  all are multiplied by 4,  $f_1, f_3, f_5, f_7$  up to  $f_{2n-1}$ , all the odd suffixes ordinates they are all multiplied by 4, so we will have this as  $(f_1 \text{ plus } f_3 \text{ plus } f_5 \text{ so on } f_{2n-1})$ . Except the first and the last all the even suffixes are multiplied by 2,  $f_2, f_4$  there are 2 of them,  $f_4$  there are 2 of them, so all the even number suffixes are multiplied by 2,  $f_2, f_4$  plus so on  $f_{2n-2}$  and the last one again is simply  $f_{2n}$ . Therefore this is the first ordinate, this is the last ordinate, they have only multiplied to factor of 1, all the odd number suffixes ordinates have multiplied by 4 and the even number suffixes ordinates have got factor of 2 so this is called the composite Simpson's rule.

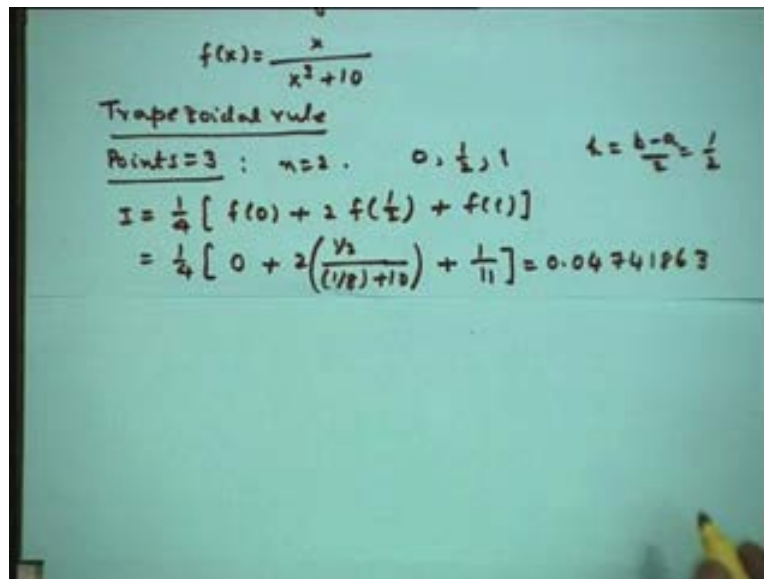
Let us also obtain the expression for the error in the composite rule so that we can make some comments about the behavior of the error. Now let us write down the error  $R_3$ , we had written it as minus  $h^5$  by 90, minus  $h^5$  divided by 90 of 4<sup>th</sup> derivative at some  $\eta$ , fourth derivative at  $\eta_1$ , fourth derivative at  $\eta_2$ , forth derivative at  $\eta_n$ . Now they are divided into  $2n$  equal subintervals to have the  $2n + 1$  points but each interval is containing 3 points. Total number of integrals that we have are only  $n$  integrals therefore each one will contribute one of these terms as  $\eta_1, \eta_2, \eta_3, \eta_n$ , where  $\eta_1$  is lying in the first interval  $x_0$  to  $x_2$  and so on, the last one  $\eta_n$  lies in this interval  $x_{2n}$ , so each of these integrals containing 3 points. Therefore I can now bound this also and write magnitude of  $R_3$  is less than or equal to, again let us denote by  $M_4$  the maximum of the fourth derivative in the interval given interval  $a$  is less than  $x$  less than or equal to  $b$ . Then I can write this  $h$  to the power of 5 by 90 into  $n$  times  $M_4$ , there are  $n$  of this terms so each 1 will be contributing 1 so  $n$  times  $M_4$ . Again you can see  $n$  into  $h$  is  $b$  minus  $a$  by 2 so we will have here  $n$  into  $h$  is equal to  $b$  minus  $a$  by 2 that is the expression here, so I would through away  $n$  into  $h$  from here so that I will have here  $h$  to the power of 4 by 180, this is 2 coming from here  $M_4$  into  $b$  minus  $a$ , into  $b$  minus  $a$ , I will write it once more here.

(Refer Slide Time: 29:01)

The image shows a whiteboard with handwritten mathematical notes. At the top, the error formula for Simpson's rule is written: 
$$= \frac{(b-a)h^4}{180} M_4$$
 where the  $h^4$  is circled. Below this, an example is given: "Example Evaluate  $\int_0^1 \frac{x}{x^2+10} dx$ ". The text continues: "Using Trapezoidal and Simpson's rules with number of points taken as 3, 5 and 9." At the bottom, the function is defined as 
$$f(x) = \frac{x}{x^2+10}$$
. A hand holding a yellow pen is visible at the bottom right of the whiteboard.

That is equal to  $(b - a)h^4$  by 180  $M_4$ . This is the actual indicator of the error in the composite Simpson's rule and it is therefore of the order of  $h$  to the power of 4 and integrates of course polynomials of degree less than or equal to 3 because we have got  $M_4$  which is nothing but the fourth derivative therefore Simpson's rule in the composite form also integrates polynomials of degree less than or equal to 3. However this is the real indicator of the error because now  $h$  is going to be sufficiently small, very often much less than 1 therefore the actual error, truncation error in the Simpson's rule is going to be very very small because this  $h$  to the power of 4. If you take  $h$  is equal to point 1 this itself is going to 10 to the power of minus 4 therefore the error is, even though  $(b - a)$  is large even then the error is going to be extremely small. Now let us first take an example on this, so let us take an example. Let us say evaluate 0 to 1  $x$  upon  $x$  cubed plus 10 using trapezoidal and Simpson's rules with, let us fix the number of points, either we fix the number of points or you fixed a number of sub intervals, with the number of points taken as 3, 5 and 9. Now here  $f(x)$  is  $x$  upon  $x$  cubed plus 10.

(Refer Slide Time: 31:07)



The image shows a handwritten derivation of the trapezoidal rule. At the top, the function is given as  $f(x) = \frac{x}{x^2 + 10}$ . Below this, it says "Trapezoidal rule". Then, it specifies "Points = 3 : n = 2", with points listed as  $0, \frac{1}{2}, 1$ . The step size is calculated as  $h = \frac{b-a}{2} = \frac{1}{2}$ . The integral is then calculated using the formula  $I = \frac{1}{4} [f(0) + 2f(\frac{1}{2}) + f(1)]$ . The final result is  $I = \frac{1}{4} [0 + 2(\frac{1/2}{(1/2)^2 + 10}) + \frac{1}{11}] = 0.04741863$ .

Now let us first take the results for the trapezoidal rule. Let us take the number of points as 3 that means n is equal to 2. If I take 3 points of the interval 0 to 1 what we are really talking of is the 3 points as 0, half and 1, h is equal to b minus a by 2 that is equal to 1 by 2. So the step length that we are taking is h is b minus a by 2 that is and three, three points are 0, half and 1. Therefore the value of the integral would be I is equal to h by 2 that is 1 by 4 f of at  $x_0$ , f of 0, 2 times f at half plus f at 1, [f at  $x_0$  plus 2 times f at  $x_1$  plus f at  $x_2$ ] that will be the value of the integral. So let us now substitute, so we would get here 1 upon 4 f(x) is this therefore at x is 0 this is 0, 2 times half 1 by 8 plus 10, I am just writing it x is equal to half as it is, plus x is equal to 1, this is 1 upon 11, this gives 1 upon 11. Now we will give you the value of this, it is 0 point 0 4 7 4 1 8 6 3. Now I am giving it intentionally say 8 decimal places because I want to use this later on for some other purposes, so let us write it in 8 decimal places. This is the result obtained by using 3 points and the composite trapezoidal rule.

(Refer Slide Time: 33:21)

$\text{Points} = 5 : n = 4, h = \frac{b-a}{4} = \frac{1}{4}$   
 $= 0, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, 1$   
 $I = \frac{1}{8} [f(0) + 2(f(\frac{1}{4}) + f(\frac{2}{4}) + f(\frac{3}{4})) + f(1)]$   
 $= 0.04794057$

$\text{Points} = 9 : n = 8, h = \frac{b-a}{8} = \frac{1}{8}$   
 $= 0, \frac{1}{8}, \frac{2}{8}, \frac{3}{8}, \frac{4}{8}, \frac{5}{8}, \frac{6}{8}, \frac{7}{8}, 1$

Now let us take 5 and 9 also, so let us take points as 5 therefore this is simple mechanical application now, that is  $n$  is equal to 4,  $h$  is equal to  $b$  minus  $a$  by 4 that is equal to 1 by 4,  $b$  minus  $a$  by  $n$  that is 1 by 4, therefore the points are 0, 1 by 4; retain it as 2 by 4, 3 by 4 and 1. Now when we are actually doing in a class or a test or anything we can retain the values of the previous one, we should write down all the values because they are all repeated because this is a point which is already occurred earlier for 0, half and 1, so the computation that you have performed that is finding  $f(x)$  should be retained so that we do not repeat those computations again. So we really, to apply this 5 point formula I need to compute only these two values of  $f(x)$  1 by 4 and 3 by 4 and the remaining three values are available in the previous step itself.

Now therefore  $I$  will be equal to  $h$  divided by 2 that is 1 by 8 [ $f$  at 0, 2 times, now this is ( $f$  at 1 by 4 plus  $f$  at 2 by 4 plus  $f$  at 3 by 4) plus  $f$  at 1]. So the ordinates, the middle ordinates all multiplied by factor of 2 and the first and the last stays as it is. Now this is simple computation so I will give you the value for this one, this turns out to be 0 point 0 4 7 9 4 0 5 7. Now consider the case with 9 points, let us take points as equal to 9 that is  $n$  is equal to 8,  $h$  is equal to  $b$  minus  $a$  by  $n$  that is equal to 8 that is 1 upon 8. Therefore we will know have the points as 0, 1 by 8, 2 by 8, 3 by 8, 4 by 8, 5 by 8, 6 by 8, 7 by 8 and 8 by 8 that is equal to 1. Now as I mentioned earlier, now all these 5 points are going to appear here again therefore this is, this is the one point that is equal to 1 by 2 you have got 1 also you have, you have 1 by 4 is available and this 3 by 4 is available, so these 5 values are available from the previous step so I need to do only these 4 ordinates to be computed at this particular stage.

(Refer Slide Time: 36:29)

$$\begin{aligned}
 &0, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, 1 \\
 &= \frac{1}{8} \left[ f(0) + 2 \left( f\left(\frac{1}{4}\right) + f\left(\frac{2}{4}\right) + f\left(\frac{3}{4}\right) \right) + f(1) \right] \\
 &= 0.04794057 \\
 &\text{Points } 9: \quad n=8, \quad h = \frac{b-a}{8} = \frac{1}{8} \\
 &0, \frac{1}{8}, \frac{2}{8}, \frac{3}{8}, \frac{4}{8}, \frac{5}{8}, \frac{6}{8}, \frac{7}{8}, 1 \\
 &= \frac{1}{16} \left[ f(0) + 2 \left( f\left(\frac{1}{8}\right) + \dots + f\left(\frac{7}{8}\right) \right) + f(1) \right] \\
 &= 0.04807248
 \end{aligned}$$

Therefore I will have the value of the integral is equal to h upon 2 h is 1 by 8 therefore 1 upon 16, I will have [f of 0 2 times (f of 1 by 8 so on upto f of 7 by 8) plus f of 1] and this value is 0 point 0 4 8 0 7 2 4 8.

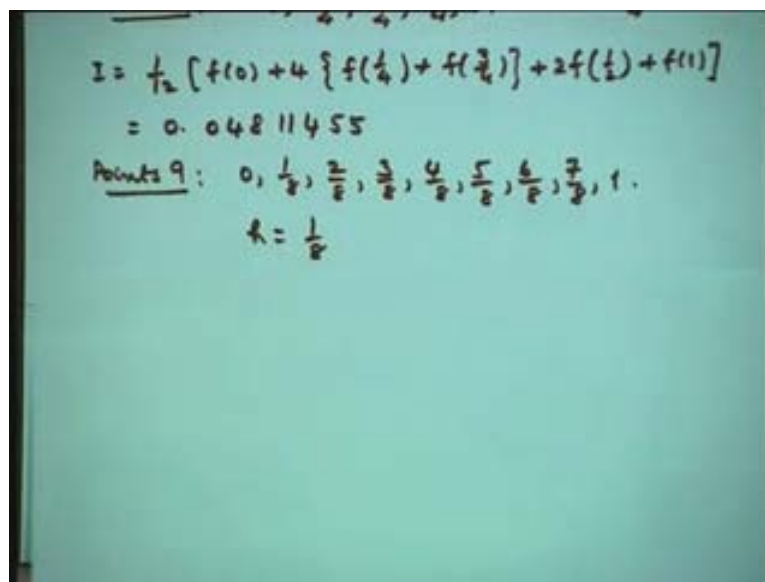
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$$\begin{aligned}
 &\text{Simpson's rule} \\
 &\text{Points } 3: \quad 0, \frac{1}{2}, 1, \quad h = \frac{1}{2} \\
 &I = \frac{1}{6} \left[ f(0) + 4 f\left(\frac{1}{2}\right) + f(1) \right] = 0.04807333 \\
 &\text{Points } 5: \quad 0, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, 1, \quad h = \frac{1}{4} \\
 &I = \frac{1}{24} \left[ f(0) + 4 \left\{ f\left(\frac{1}{4}\right) + f\left(\frac{3}{4}\right) \right\} + 2 f\left(\frac{2}{4}\right) + f(1) \right] \\
 &= 0.04811455
 \end{aligned}$$



Now let us give the application in Simpson's rule, let us take the Simpson's rule. The question was formulated such that you can use the Simpson's rule, we have been asked to take 3 points, 5 points and 9 points; they are all odd number of points so Simpson's rule can be applied on those points. Therefore the Simpson's rule we have, let us take the first one points as 3, therefore the points are 0, half and 1 and h is equal to half that is the distance between this. Therefore I is equal to h by 3 so we will have 1 by 6  $[f_0$  plus 4 times f at half plus f at 1]. Now again I will leave this computation to you, this comes out to be 0.4807333. Now I go to 5 points, so I have the 5 points as 1 by 4, 2 by 4, 3 by 4 and 1 so that h is equal to 1 upon 4. We use these 5 points and write the given integral into 2 integrals each containing 3 points. Therefore h is the step length that we are using there, therefore the value of the integral is h by 3 that is 1 by 12 of f of 0 4 times f of 1 by 4 plus f of 3 by 4 4 times this odd suffixed one's plus 2 times f of the even suffix ordinate that is this plus f of 1. This is 1 and 3 these are the ones multiplied by 4, this is 2 and is multiplied by factor of 2, so this value is, I will give you the value as 0.4811455.

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Handwritten work on a green chalkboard:

$$I = \frac{1}{12} [f(0) + 4 \{f(\frac{1}{4}) + f(\frac{3}{4})\} + 2f(\frac{1}{2}) + f(1)]$$

$$= 0.4811455$$

Points 9:  $0, \frac{1}{8}, \frac{2}{8}, \frac{3}{8}, \frac{4}{8}, \frac{5}{8}, \frac{6}{8}, \frac{7}{8}, 1.$

$$h = \frac{1}{8}$$

Now let us take 9, points so we will again have the points as 1 by 8, 2 by 8, 3 by 8, 4 by 8, 5 by 8, 6 by 8, 7 by 8 and 1 so that h is equal to 1 by 8.



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$$I = \frac{1}{24} \left[ f(0) + 4 \left\{ f\left(\frac{1}{8}\right) + f\left(\frac{3}{8}\right) + f\left(\frac{5}{8}\right) + f\left(\frac{7}{8}\right) \right\} + 2 \left\{ f\left(\frac{2}{8}\right) + f\left(\frac{4}{8}\right) + f\left(\frac{6}{8}\right) \right\} + f(1) \right]$$

$$= 0.04811645$$

Extrapolation      Romberg Integration

Trapezium rule

$$I = I_T = c_1 h^2 + c_2 h^4 + c_3 h^6 + \dots$$

Simpson's rule

$$I = I_3 = c_1 h^4 + c_2 h^6 + c_3 h^8 + \dots$$

Therefore our value of the integral is  $h$  divided by 3 therefore 1 by 24  $f$  at 0 4 times all the odds suffixed ones that is your 1 by 8, 3 by 8, 5 by 8, 7 by 8, so this will be  $\{f$  of 1 by 8 plus  $f$  of 3 by 8 plus  $f$  of 5 by 8 plus  $f$  of 7 by 8 $\}$ . Then 2 times the even ones so even one is 2 by 8, 4 by 8, 6 by 8 so we will have  $\{f$  of 2 by 8,  $f$  of 4 by 8 plus  $f$  of 6 by 8 $\}$  plus  $f$  of 1. I can make this computation and I get this as 0 4 8 1 1 6 4 5. Now we mentioned just now that is in practice we do not use any higher order formulas beyond this Simpson's rule or Simpson's 3/8th rule. The one important reason is that we can apply the extrapolation that we talked of in the numerical differentiation can be carried over directly to numerical integration. The extrapolation idea, extrapolation depends on, write down the error expression for the given method, manipulate the computed results such that the new value comes out to be order higher than what we have obtained in the previous case.

Now therefore if I want to obtain the extrapolation procedures for this it are called, it is not called Richardson extrapolation, here it is a different name it is called Romberg integration, so let us define what is our extrapolation for this, it is called Romberg integration. Now what we really need here is the expression for the error for the trapezoidal rule and the Simpson's rule and that would come from looking at this truncation error for the composite Simpson's rule and that has got factor  $h$  square, so the leading term of the error for the trapezoidal rule is  $h$  square and I can show that the next term  $h$  cubed will vanish,  $h^5$  will vanish and so on. I will take that result only so that I will have for the trapezoidal rule the expression for the truncation error as this,  $I$  is equal to  $I$ , I will call it as  $T$  for trapezoidal rule that will be  $c_1 h$  square that the part we have proved, this part we have proved so now I will take the remaining things as  $h^4$ ,  $c_3 h^6$  and so on. All the coefficients of the odd powers of  $h$  vanish, whereas for the Simpson's rule  $I$  is equal to  $I$  Simpson and for the Simpson's rule we have shown that error is starting with  $h$  to the power of 4, so it starts with  $h$  to power of 4, so I will have here is  $c_1 h$  to the power of 4 plus  $c_2 h$  to the

power of 6 again here odd powers all of them cancel here. Now if this is the result then we know what is the extrapolation procedure, when once this is  $h^4$ ,  $h^6$  we have already derived the formula for this, so I can just carry over the extrapolation formula to this.

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Extrapolation formulas  $h, \frac{h}{2}, \frac{h}{4}, \dots$

$$I_T^{(m)}(h) = \frac{4^m I_T^{(m-1)}\left(\frac{h}{2}\right) - I_T^{(m-1)}(h)}{4^m - 1}$$

$m = 1, 2, \dots$

$$I_S^{(m)}(h) = \frac{4^{m+1} I_S^{(m-1)}\left(\frac{h}{2}\right) - I_S^{(m-1)}(h)}{4^{m+1} - 1}$$

$m = 1, 2, \dots$

Therefore let us write down what is the extrapolation for trapezoidal rule, extrapolation formulas that is for T trapezoidal rule is, it is  $h^2$  therefore we are talking of, we are reducing  $h$ , we are taking  $h$  by 2,  $h$  by 2 square and so on, we are assuming that we are decreasing by factor of 2 each time that we are computing. Then we are shown that this will be nothing but 4 to the power  $m$  because when  $h$  is reduced by factor of 2 that is you are going to have 2 square that is 4 so multiplied by 4, 4 the previous value  $I_T^{(m-1)} h$  by 2 minus  $m$  minus 1  $h$  divided by 4 to the power of  $m$  minus 1,  $m$  is going from 1, 2, 3 and so on. Therefore the first column of extrapolation will have 4 times this next value minus the previous value divided by 4 minus 1 3, the next value  $m$  is 2, 16 minus 1 this is 15 and if I have one more then will have 4 cubed 64 minus 1 and 63. Now whereas your Simpson's rule starts with  $h$  to the power of 4, so let us push this by 1 so 4 to the power  $m$  plus 1 let us make it and this is  $I$  Simpson  $(m$  minus 1)  $h$  by 2 minus  $I$  Simpson  $(m$  minus 1) of  $h$  by 4 to the power of  $m$  plus 1 minus 1,  $m$  again going from 1, 2 and so on. Now this is the formula that we can apply, it is for this reason that we have done the previous example to the number of 8 places so that we can use the Romberg integration on the example that we have done there, so let us take this as an example.

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$$I_T^{(m)}(h) = \frac{4 I_T^{(m-1)}\left(\frac{h}{2}\right) - I_T^{(m-1)}(h)}{4^m - 1}$$

$m = 1, 2, \dots$

$$I_S^{(m)}(h) = \frac{4^{m+1} I_S^{(m-1)}\left(\frac{h}{2}\right) - I_S^{(m-1)}(h)}{4^{m+1} - 1}$$

$m = 1, 2, \dots$

Example: Apply Romberg integration to the previous example.

Apply Romberg integration to the previous example. Now we just go back to the values that we have obtained for the trapezoidal rule.

(Refer Slide Time: 48:14)

$h$	Trapezoidal rule		
	$O(h^2)$	$O(h^4)$	$O(h^6)$
$\frac{1}{2}$	0.04741863		
		0.04811455	
$\frac{1}{4}$	0.04794057		0.04811657
		0.04811645	
$\frac{1}{8}$	0.04807248		

$\uparrow$   
 $\frac{4\left(\frac{1}{2}\right) - (1)}{2}$

$\uparrow$   
 $\frac{16\left(\frac{1}{4}\right) - 4\left(\frac{1}{2}\right)}{15}$

So what we are starting here is the step length that is we have here, let us first take the trapezoidal rule, trapezoidal rule. The order of the formula is  $h^2$ , the first extrapolation gives me order of  $h$  to the power of 4 and the second extrapolation gives me order of  $h$  to the power of 6. We have done the example with starting with  $h$  is equal to half, the 3 point formula so your first value of this is equal to half then we had 1 by 4 and we had 1 by 8, these are the 3 values which we have used and these are the values I **what** retain it there, this is the value that we have obtained for this one that is 0.4741863. Then the next value was, was this 0.4794057 and the third value was this, 7.248. Therefore this column values will be obtained from the formula this for  $m$  is equal to 1, so that is 4 times this value minus previous value by 3 and the next one element will be 4 times this value minus this divided by 3, so this will be 4 times this value minus the previous value divided by 3, this is your  $h$  by 2 corresponding to this and this is corresponding to  $h$ . Therefore if I multiply this by 4, subtract, divided by 3 and this value I will give you as 0.4811455. Similarly 4 times this minus this divided by 3 gives me 0.4811645.

Now the second column would come from this formula by putting  $m$  is equal to 2 the next step that is equal to 16 minus 1 by 15 so I will have here 16 times, you can call it as  $I^{(1)}$   $h$  by 2 minus  $I^{(1)}$   $h$  by 15. So I just multiply this by 16 subtract and divide by 15, I would get here 0.4811657. This result is actually correct upto this last decimal place, except this last decimal place it is correct to 7 decimal places. As we observed in the numerical differentiation here also the Romberg integration along with this formulas can really work wonders in getting the resolution very very fast, in fact in an example you can take a very complicate examples, if it takes about few thousands of points to get a certain accuracy say  $10^{-6}$  by using Romberg integration you can get it in few hundreds of points. You can evaluate that integral which 50, 100, 200 and 400, 4 steps and then when if you do the 4 steps with Simpson's rule for example it will be order of  $h^4$  we started with,  $h^6$ ,  $h^8$ ,  $h^{10}$ , so you have got as if you obtained a formula with order of tenth order formula that you have got that is it integrates polynomials of degree less than or equal to 10 and the value that would have obtained, the value, the last value here in the first column will be, I mean the error from this and this will be so large that the convergences has been obtained very very fast. Therefore the Romberg integration or Richardson extrapolation in the other cases works wonders in most of this integration and differentiation formulas. We would stop at here.