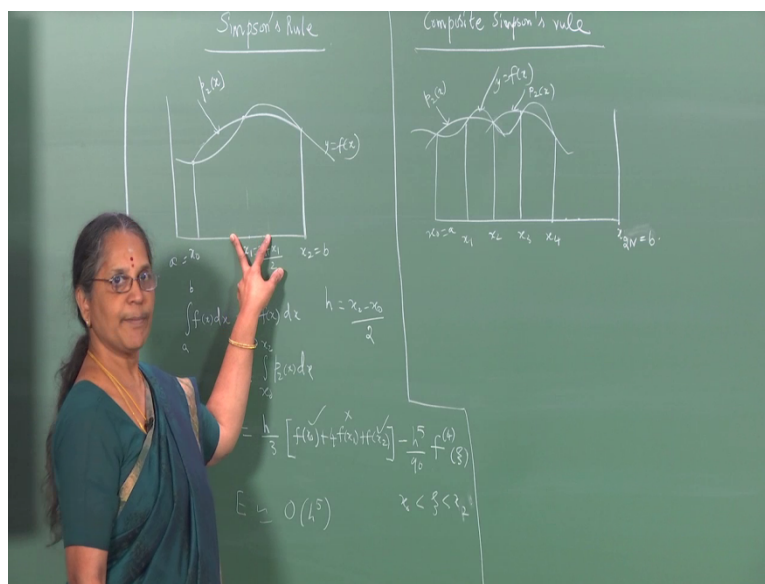


**Numerical Analysis**  
**Prof R Usha**  
**Department of Mathematics**  
**Indian Institute of Technology Madras**  
**Lecture 15**  
**Numerical Integration 4**  
**Composite Simpson's Rule, Error**  
**Method of Undetermined Coefficients**

In the last class we obtained an integration method which is a Newton codes method for equally spaced points.

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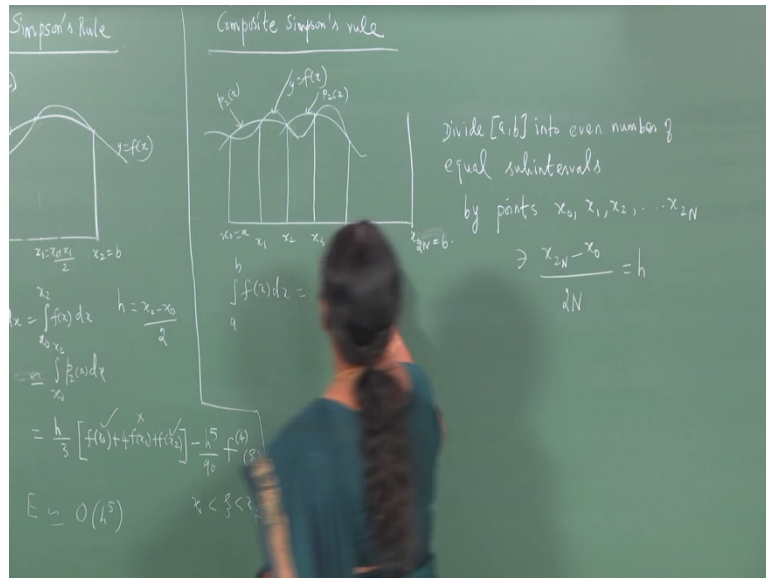


Namely the Simpson's rule in which the curve  $y$  is equal to  $f(x)$  in an interval  $x_0$  to  $x_2$  is approximated by a quadratic interpolating polynomial  $p_2(x)$  and this resulted in Simpson's rule such that  $\int_a^b f(x) dx$  is given by  $\frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)]$  plus the error term where the error term is given by this showing that  $e$  is of the order of  $h^5$  in Simpson's rule. Here  $h$  is  $(x_2 - x_0) / 2$ .

So we divide the interval into two equal parts and get the Simpson's rule. So we would like to see how accuracy can be increased. So in which case the error must be reduced. So that suggest that we must make the step size  $h$  smaller and smaller which is equivalent to dividing the interval  $x_0$  to  $x_2$  into a number of equal sub intervals, but we observe that in Simpson's rule we have to divide the given interval into even number of equal sub intervals because we want to approximate a curve in an interval of the form  $x_0$  to  $x_2$  by means of a quadratic

interpolating polynomial  $P_2(x)$  passing through 3 points and so we have to divide the interval  $x_0$  to the end point or  $a$  to  $b$  into an even number of equal sub intervals and apply Simpson's rule in each of the appropriate intervals and see what we get.

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This results in an integration method which is called Composite Simpson's rule where my integration is between  $a$  and  $b$ . So I divide  $[a, b]$  into even number of equal sub intervals so divide  $[a, b]$  into even number of equal sub intervals by means of points say  $x_0, x_1, x_2$  etc  $x_{2n}$  so that  $x_{2n} - x_0$  divided by, so when we divide it into  $2n$  equal sub intervals so we get the step size  $h$  to be such that  $x_{2n} - x_0$  divided by  $2n$  will be equal to  $h$ .

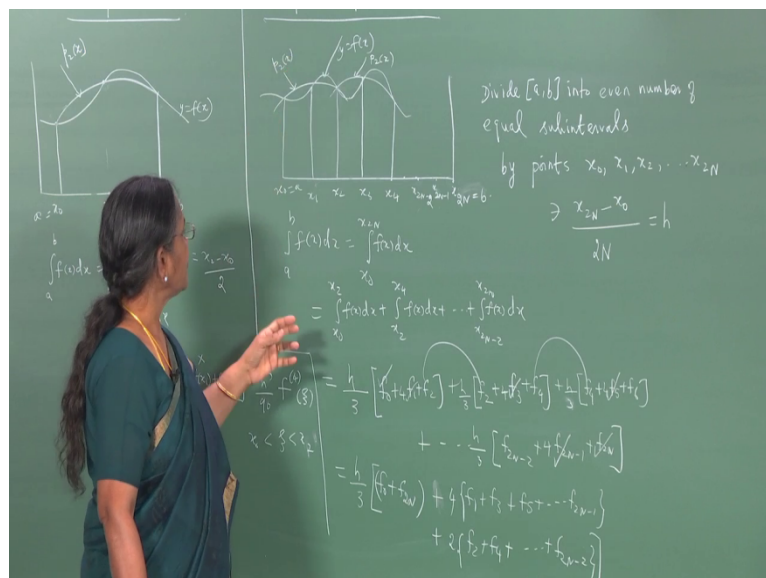
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And now we take the sub interval between  $x_0$  to  $x_2$ , so we have 3 points  $x_0, f(x_0), x_1, f(x_1), x_2, f(x_2)$  so passing through these three points I can get an interpolating polynomial  $P_2(x)$  and the curve  $y$  is equal to  $f(x)$  in this interval is approximated by a quadratic polynomial passing through these three points  $(x_0, f_0), (x_1, f_1), (x_2, f_2)$ .

Similarly in the interval  $x_2$  to  $x_4$  again I approximate the function by a quadratic polynomial that interpolates this function at the points  $x_2, f_2, x_3, f_3, x_4, f_4$  and I continue this and I will have the last interval to consists of the points  $x_{2n-2}, f_{2n-2}, x_{2n-1}, f_{2n-1}, x_{2n}, f_{2n}$  so that in this interval  $x_{2n-2}$  to  $x_{2n}$  the function is again approximated by a quadratic interpolating polynomial that interpolates this function at the points  $x_{2n-2}, f_{2n-2}, x_{2n-1}, f_{2n-1}, x_{2n}, f_{2n}$ .

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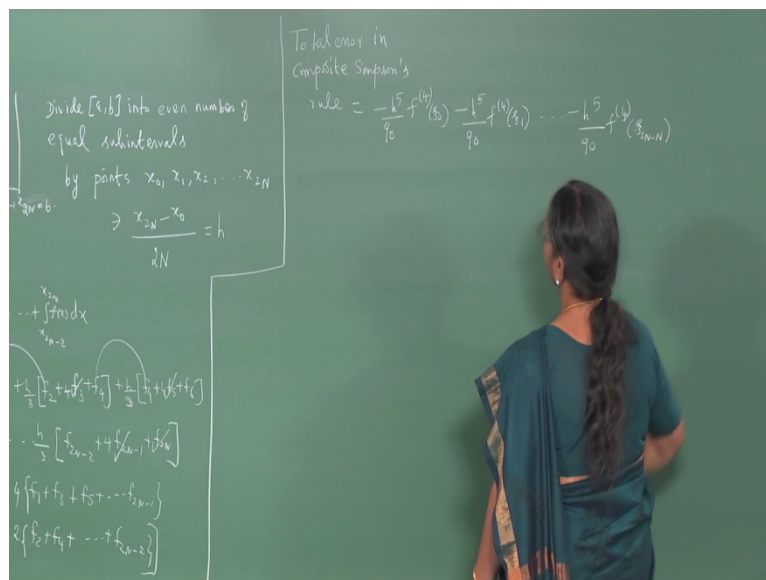
So that suggests that  $\int_a^b f(x) dx$  which is  $\int_{x_0}^{x_{2n}} f(x) dx$  is going to be  $\int_{x_0}^{x_2} f(x) dx + \int_{x_2}^{x_4} f(x) dx + \dots + \int_{x_{2n-2}}^{x_{2n}} f(x) dx$ . So now in each of these intervals I can apply Simpson's rule.

I know how to get the ordinates appropriately and then try this rule on the right hand side which is given by Simpson's rule. So I will have  $h/3$  into in this interval  $f_0 + 4f_1 + f_2$ . In the next interval  $h/3$  into  $f_2$  that is the value of the ordinate at  $x_2$  plus 4 times the intermediate points that is  $x_3$  plus  $f_4$ . What do you think in the next interval it will be  $h/3$  into  $4f_4 + f_5 + f_6$  and continue this and in the last interval it is going to be  $h/3$  into  $f_{2n-2} + 4f_{2n-1} + f_{2n}$ .

So we simplify and see that it is  $h$  by  $3$ . I observe that  $f_0$  and  $f_{2n}$  appear once so just write down this group of terms which corresponds to sum of the end ordinates. Then I observe that I have terms  $4$  times  $f_1$  plus  $f_3$  plus  $f_5$  plus etc plus  $f_{2n-1}$ . I have terms which correspond to sum of the odd suffixed ordinates.

Then I look at the even suffixed ordinates I observe that each of these even suffixed ordinates appears twice. So I had twice  $f_2$  plus  $f_4$  plus etc plus  $f_{2n-2}$ . So I can say that Composite Simpson's rule gives you a method for evaluating integral  $a$  to  $b$   $f(x) dx$  approximately and it is given by  $h$  by  $3$  into sum of the  $n$  ordinates third times the odd suffixed ordinates plus  $2$  times the even suffixed ordinates.

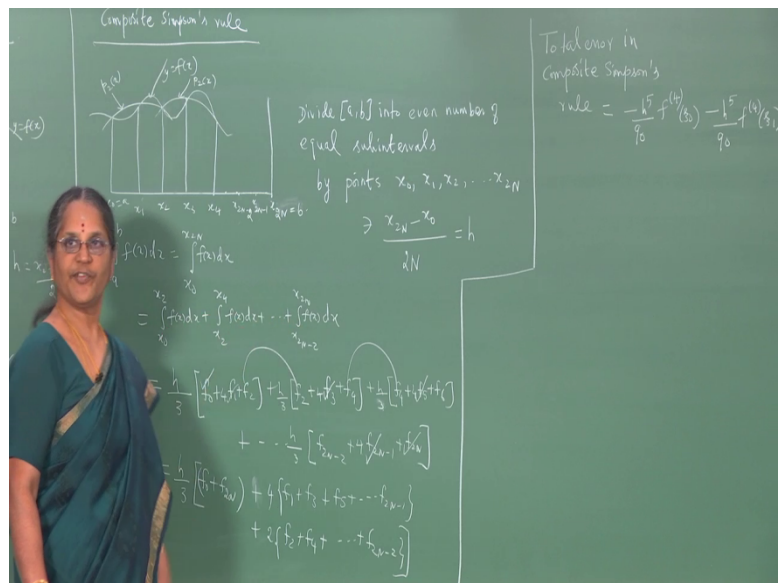
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So it is now important to see what is the error in Composite Simpson's rule that can be easily obtained because we have applied Simpson's rule in each of these intervals and we already have computed the error term in Simpson's rule so I apply the error in each of the intervals.

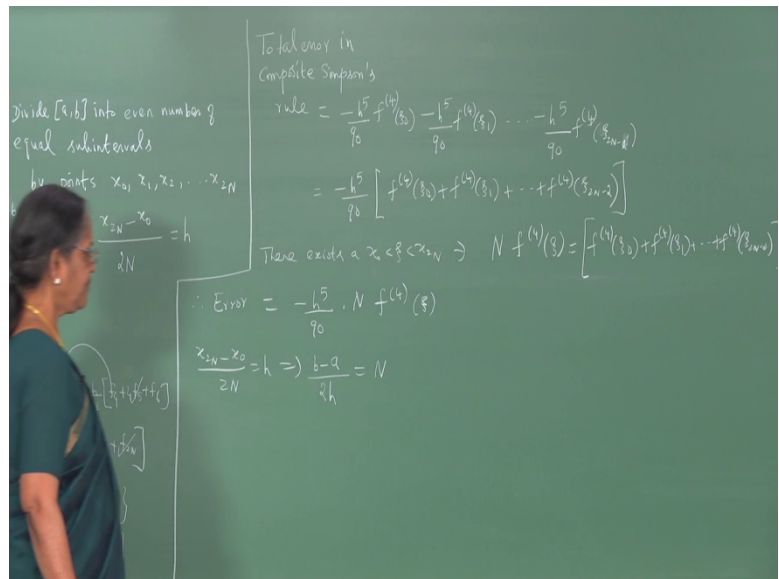
And so I get the total error in Composite Simpson's rule is going to be the error that occurs due to integration in this interval and that will be minus  $h^5$  by  $90$  into the fourth derivative at say some  $(\Psi_0)$ . Then the error that arises due to this integration so minus  $h^5$  by  $90$  into fourth derivative say  $(\Psi_1)$  and so on.. And then from the last integral we will have the fourth derivative appearing at some  $\Psi$  which is  $2n \Psi_{2n-2}$ .

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So I have added the errors that occur due to application of Simpson's rule in each of these integrals.

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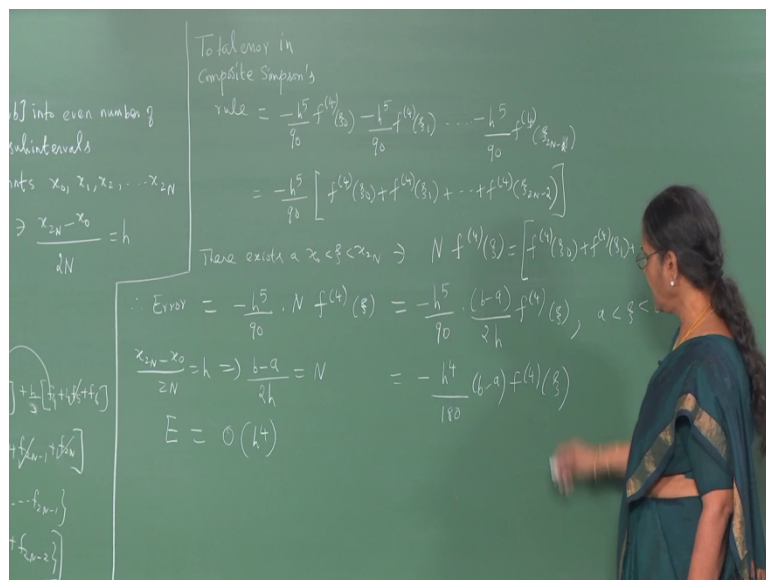


So that gives you minus h power 5 by 90 into the fourth derivative at (Psi 0) plus fourth derivative (Psi 1) and so on the fourth derivative of f (Psi 2n minus 2) ]. So since the requirement for the function f in order that this formula is valid is that the first derivative exists and is continuous in that interval.

There is exists a Psi in this interval  $x_0$  to  $x_{2n}$  such that how many intervals in which you have applied Simpson's rule? You have applied Simpson's rule in each of the  $n$  capital  $N$  sub intervals because you have divided the entire interval into  $2n$  equal sub intervals. You apply the Simpson's rule in  $n$  capital  $N$  sub intervals.

So there exists a Psi in this interval such that capital  $N$  times the fourth derivative (Psi) will be equal to the fourth derivative (Psi 0) plus fourth derivative (Psi 1) plus etc plus the fourth derivative (Psi  $2n$  minus 2). So I can use this and then get therefore the error to be equal to minus  $h$  power 5 by 90 into  $n$  times the fourth derivative (Psi). But I know that  $x_{2n}$  minus  $x_0$  by  $2n$  is  $h$ . So that will give me  $x_{2n}$  is  $b$   $x_0$  is  $a$  divided by  $2h$  to be equal to capital  $N$ .

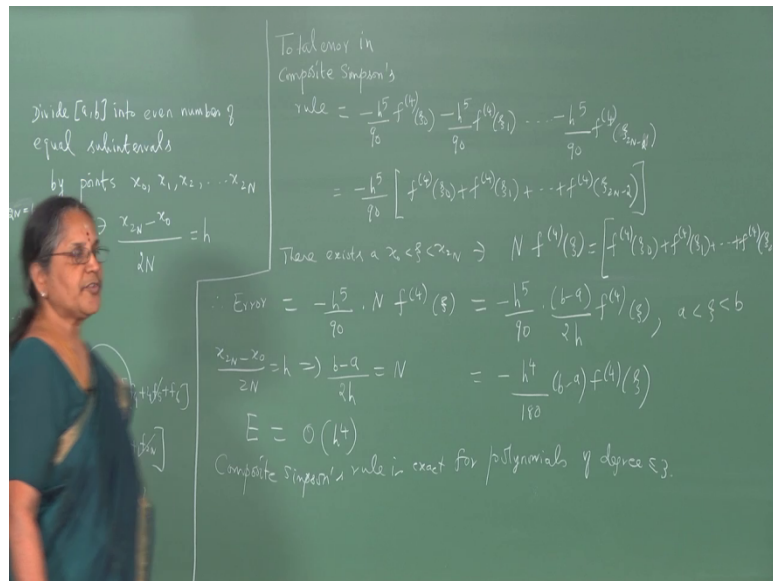
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So we substitute that here so minus  $h$  power 5 by 90 into  $N$  is  $b$  minus  $a$  by  $2h$  into fourth derivative (Psi) where Psi is in the interval  $a$  to  $b$ . So this gives you minus  $h$  power 4 by 180 into  $b$  minus  $a$  into fourth derivative (Psi). So you observe that the error in Composite Simpson's rule is of order of  $h$  to the power of 4.

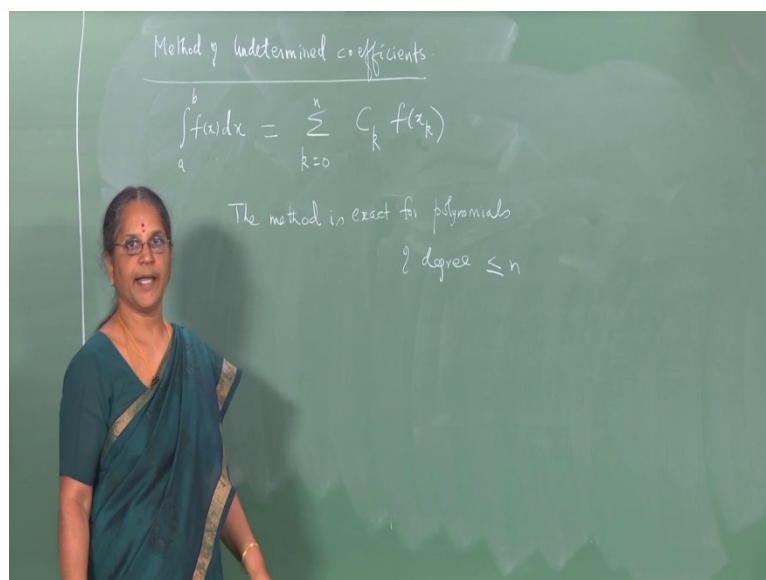
And the error term clearly shows that Composite Simpson's rule is exact for polynomials of degree upto 3. So upto cubic polynomials the method is exact the error will be 0 if  $f(x)$  is a polynomial of degree less than or equal to 3, that is what the error term tells.

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So composite Simpson's rule is exact for polynomials of degree less than or equal to 3. So far we have used the polynomial interpolation in deriving numerical integration methods where the polynomial interpolation is done with equally spaced points. So we shall now explain another method which is called method of undetermined coefficients using which one can derive integration methods where the points mainly the nodes  $x_i$  need not be equally spaced.

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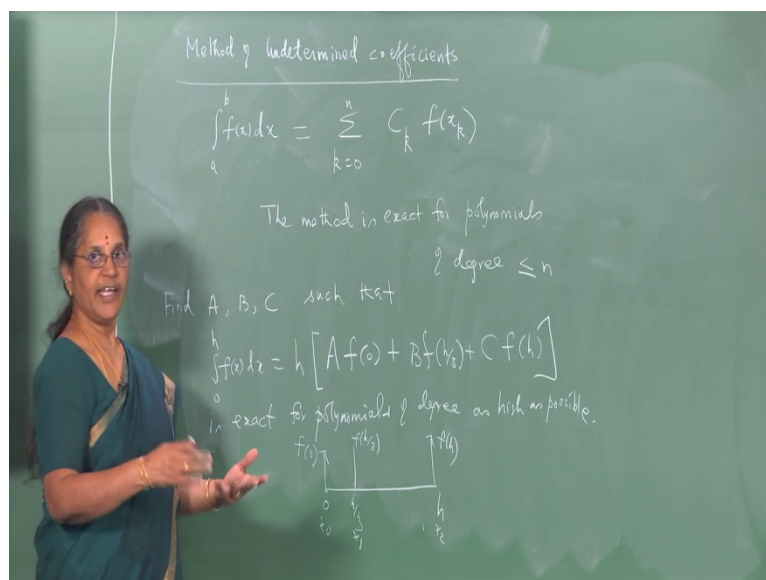
So let us explain what is the method of undetermined coefficients? So using this method one can obtain integration formulas for evaluating integral  $\int_a^b f(x) dx$  by requiring that this integral is of the form say  $\sum_{k=0}^n C_k f(x_k)$ .

And the constants  $C_k$  can be determined in such a way that the method is exact for polynomials of degree so let us upto what how many unknowns are there  $C_k$  are  $n+1$  in number  $k$  runs from 0 to  $n$  so there are  $n+1$  unknowns which have to be determined. The  $x_k$  need not be equally spaced.

But there location of the points will be specified to you in the interval  $a$  to  $b$ . So derive an integration method by seeking the constants  $C_k$  in such a way that this method is exact for polynomials of degree so you require  $n+1$  conditions so for polynomials of degree less than or equal to  $n$ .

So you will have  $n+1$  conditions coming from here when you use those conditions you will be able to determine the constants  $C_k$ . So since you determine the coefficients in the integration method which are unknown by requiring that the method is exact for polynomials of degree less than or equal to  $n$ , the method derives its name that it is a method of undetermined coefficients. So we shall illustrate this by means of the following example.

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So let us obtain constants  $a, b$  and  $c$  such that  $\int_0^h f(x) dx$  is  $h$  into  $A$  times  $[f(0) + B$  into  $f(h/3) + C$  into  $f(h)]$ . So derive integration method of the form  $\int_0^h f(x) dx$

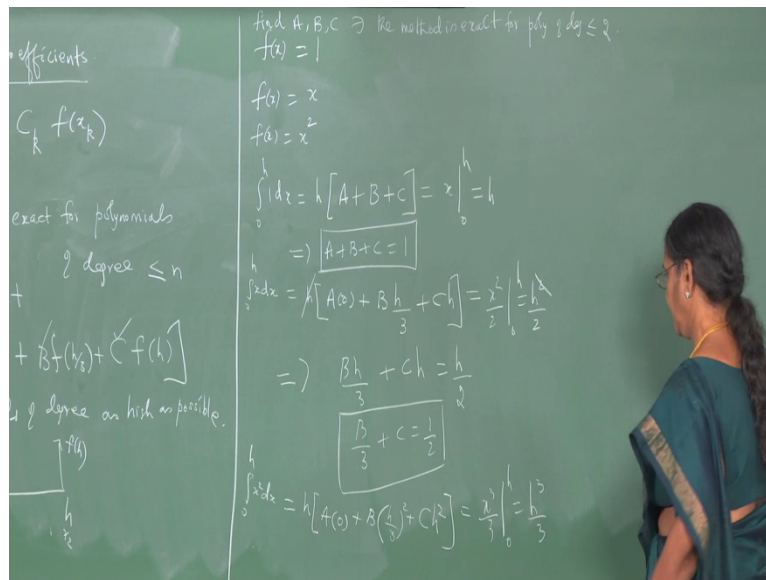


is equal to this where A B C are constants such that this integral method is exact for Polynomials of degree as well as possible.

And you observe that this integral of integration is from 0 to h the ordinates that appear here are f(0) and f(h by 3) and the third ordinate is f(h). So the points say x 0, x 1, x 2 they are not equally spaced they are located in that interval namely 0 to h.

So this illustrates how method of undetermined coefficients can be used to derive integration methods where the nodes need not be equally spaced. Of course the method can be applied to the case where the nodes are equally spaced also. But in case the points are not equally spaced then the method works well.

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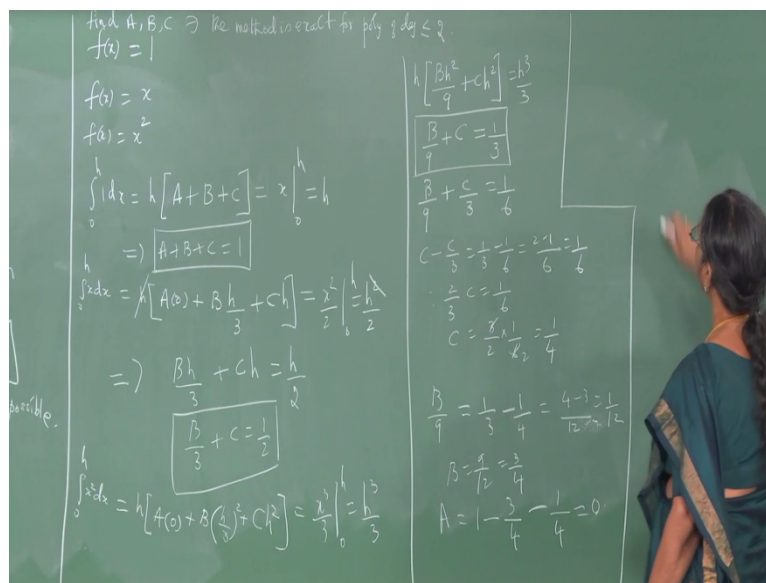
So let us obtain the constants, what does it say? we want this method to be exact for polynomials of degree as high as possible and we observe that the method involves 3 arbitrary constants so we require three conditions so we make the method exact for polynomials of degree 0,1, and 2 that would say that when f(x) is a constant f(x) is x and f(x) is equal to x square.

The method must be exact. So find A B c such that the method is exact for polynomials of degree less than or equal to 2. So let us substitute integral 0 to h f is 1 that will give you h into [A f(0) plus B f(h by 3) plus C and that gives you integral 0 to h dx is h between 0 to h dx is x between 0 and h. So that is h so that gives you the first equation A plus B plus C equal to 1.

Then let us take  $f(x)$  to be  $x$  so  $\int_0^h x \, dx$  is equal to  $h$  into  $[A \text{ times } f(0) + B \text{ times } f(h/3) + C \text{ times } f(h)]$  and so it is going to be  $h$  and what is this it is  $\int_0^h x^2 \, dx$ , so  $x^2$  by  $2$  between  $0$  and  $h$  so it is  $h^2$  by  $2$ .

So which gives you a condition I can cancel the factor  $h$  so this gives you  $B$  into  $h$  by  $3$  plus  $C$  into  $h$  is equal to  $h$  by  $2$ . So  $B$  by  $3$  plus  $C$  must be equal to half that is the second condition and thirdly we require that  $\int_0^h x^2 \, dx$  must be equal to  $h$  into  $A f(0) + B f(h/3) + C f(h)$  so  $(h/3)^2$  plus  $C$  into  $h$  this must be equal to  $\int_0^h x^2 \, dx$  so  $x^3$  by  $3$  between  $0$  and  $h$  so it is  $h^3$  by  $3$ .

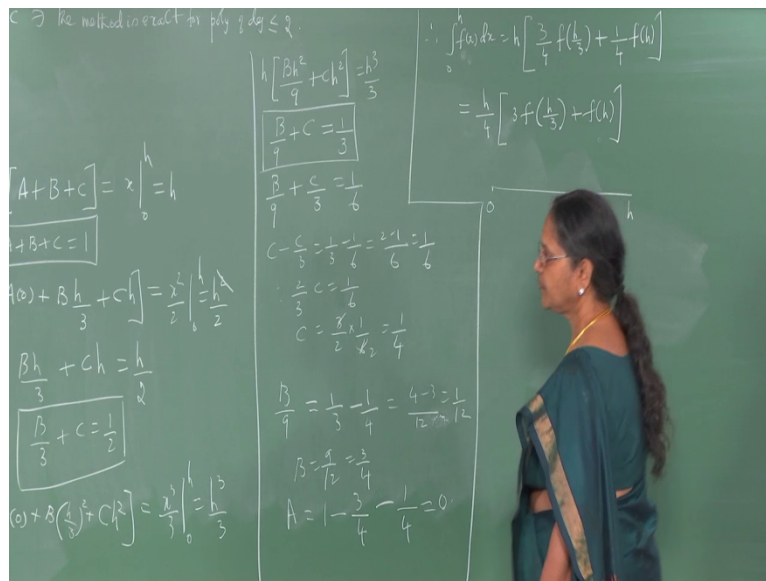
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So that gives you  $h$  into  $Bh$  square by  $9$  plus  $C$   $h$  square] is  $h^3$  by  $3$ . So cancelling  $h^3$  on both sides we get  $B$  by  $9$  plus  $C$  is  $1$  by  $3$ . So we have 3 equations to determine the 3 unknowns  $A$ ,  $B$  and  $C$ . So we have  $B$  by  $3$  plus  $C$  is half so multiplying by  $1$  by  $3$  I get  $B$  by  $9$  plus  $C$  by  $3$  is  $1$  by  $6$ .

So subtracting this from here I get  $C$  minus  $C$  by  $3$  is  $1$  by  $3$  minus  $1$  by  $6$ , so which is  $1$  by  $6$  so  $2$  by  $3C$  is  $1$  by  $6$  so  $C$  is  $1$  by  $4$  and therefore  $B$  by  $9$  must be  $1$  by  $3$  minus  $C$  so that gives you  $1$  by  $12$  and so  $B$  is  $9$  by  $12$  or  $3$  by  $4$ . But I know  $A$  plus  $B$  plus  $C$  must be  $1$  so  $A$  must be  $1$  minus  $B$  minus  $C$  and so  $A$  must be  $0$ .

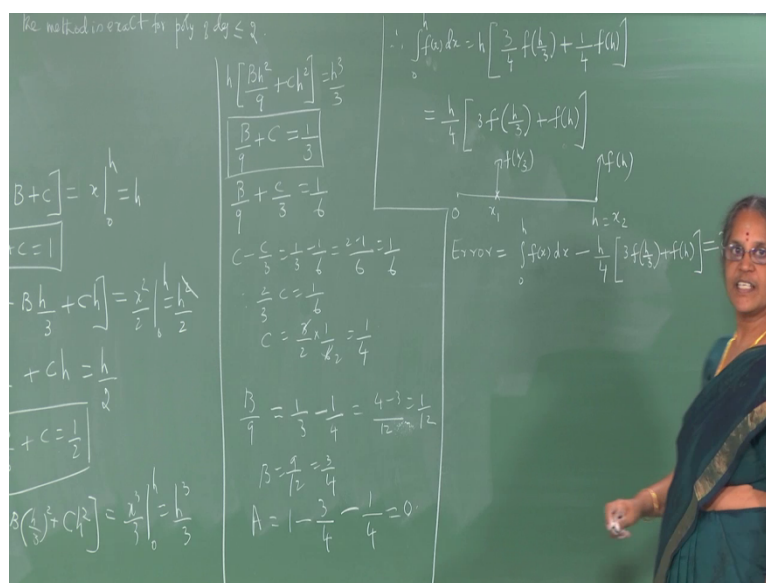
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So we have evaluated the constants A B C so we can write down the integration method so  $\int_0^h f(x) dx$  is  $h$  into  $A$  is  $0$   $B$  turned out to be  $\left[ \frac{3}{4} f\left(\frac{h}{3}\right) + \frac{1}{4} f(h) \right]$  so it is  $h$  by  $4$  into  $\left[ \text{thrice } f\left(\frac{h}{3}\right) \text{ plus } f(h) \right]$ .

So this integral is approximately the value on the right hand side. So what does this involve if you want to integrate between  $0$  and  $h$  then this says it is  $h$  by  $4$  what is that  $h$  the  $h$  appears as the upper limit right? It is not the step size it is what appears as the upper limit so  $0$  to  $h$ .

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So that gives you  $h$  by  $4$  into [thrice  $f(h$  by  $3$ ) plus  $f(h)$ ]. In fact since the interval of integration is  $0$  to  $h$  the length of the integral is  $h$  so the ordinates are taken at the total length of the interval by  $3$  that is one of the points which is our  $x_1$  and the other one is at this end point. So evaluate these two ordinates and then apply this rule you will get the value of the integral approximately.

So we compute the error and we see that it is  $\int_0^h f(x) dx$  minus  $h$  by  $4$  into [thrice  $f(h$  by  $3$ ) plus  $f(h)$ ]. That is one way of computing the error namely we will say that we make use of the fundamental theorem of integral calculus and say there is a capital  $F(x)$  such that  $F'(x)$  is equal to small  $f(x)$  and then  $f'(x)$  evaluate the integral and then use Taylor's theorem and compute what is the first neglector term or what is the leading order error term.

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$$\int_0^h f(x) dx \approx h \left[ \frac{3}{4} f\left(\frac{h}{3}\right) + \frac{1}{4} f(h) \right]$$

$$= \frac{h}{4} \left[ 3f\left(\frac{h}{3}\right) + f(h) \right]$$

$$f(x) = x^3$$

$$\int_0^h x^3 dx = \frac{h^4}{4} \left[ \frac{3}{4} \left(\frac{h}{3}\right)^3 + \left(\frac{h}{4}\right)^3 \right]$$

$$= \frac{h^4}{4} \left[ \frac{3}{4} \left(\frac{h^3}{27}\right) + \frac{h^3}{64} \right]$$

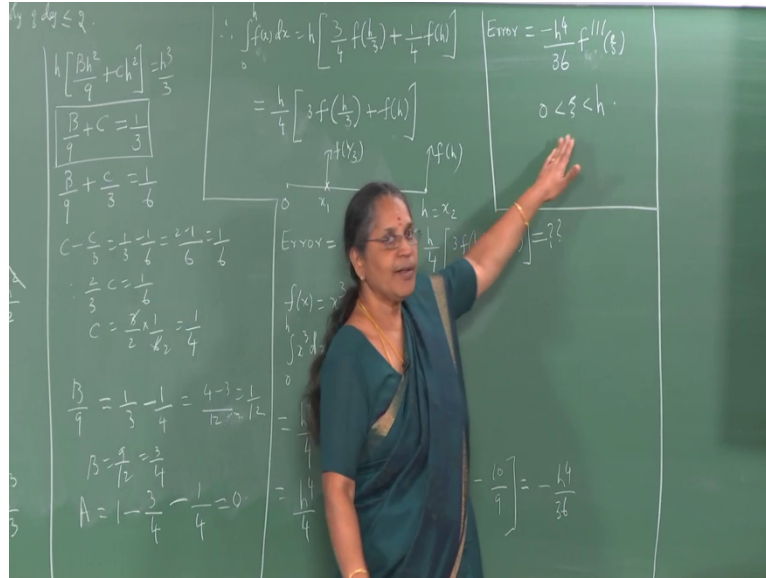
$$= \frac{h^4}{4} \left[ \frac{3h^3}{108} + \frac{h^3}{64} \right] = \frac{h^4}{4} \left[ \frac{10}{9} \right] = \frac{h^4}{36}$$

The other way of evaluating is to see is this method exact for polynomials of degree 3 namely when  $f(x)$  is equal to  $x$  cube is the method exact? Let us try. So by taking  $f(x)$  is equal to  $x$  cube in that case  $\int_0^h f(x) dx$  is  $x$  cube  $dx$  and the method gives you  $h$  by  $4$  into thrice  $f(h$  by  $3$ ) so  $(h$  by  $3$ ) the whole cube plus  $f(h)$  which is  $h$  cube.

So this gives you  $x$  power  $4$  by  $4$  between  $0$  and  $h$ . So it is  $h$  power  $4$  minus I have a  $h$  power  $4$  by  $4$  into  $[3$  by  $27$   $1$  by  $3$  cube plus  $1]$ . So that gives you  $h$  power  $4$  by  $4$  minus  $h$  power  $4$  by  $4$  into  $(30$  by  $27)$ , which gives you  $h$  power  $4$  by  $4$  into let us simplify but we can keep  $h$  power  $4$  by  $4$  as it is , so  $[1$  minus  $10$  by  $9]$  which gives you minus  $h$  power  $4$  by  $36$ .

So the difference when evaluated by taking  $f(x)$  to be equal to  $x$  cube is not 0 and it is equal to minus  $h$  power 4 by 36 and we have taken the polynomial of degree 3 here.

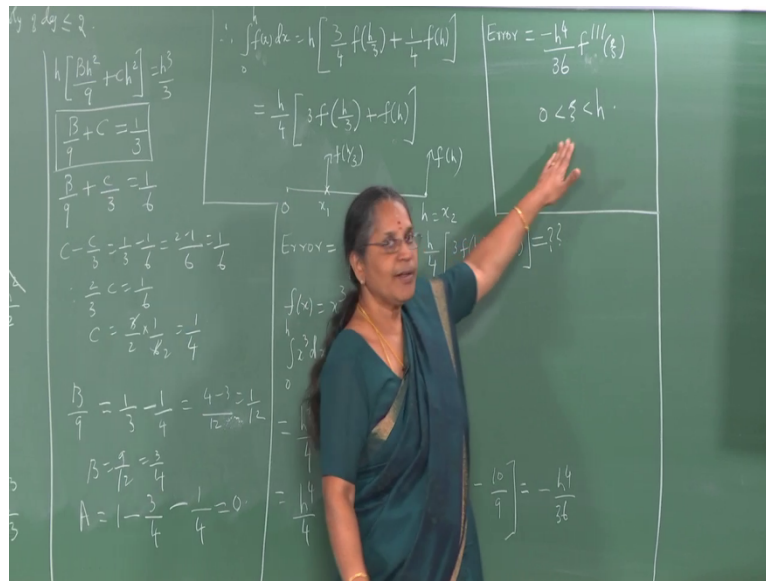
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So we can now write down therefore the error in this method which we have concluded. So the error in this method will be the method is exact up to polynomial of degree 2 the error contributes to a non zero value when  $f(x)$  is taken to be  $x$  cube and it is exact for polynomials of degree less than or equal to 2 so we can write down the error immediately as minus  $h$  power 4 by 36 into the third derivative evaluated at  $\Psi$  where  $\Psi$  lies between 0 and  $h$ .

So this tells us that the function  $f$  or the class of functions  $f$  for which this integration method can be applied and it also tells us that the method is exact for polynomials of degree less than or equal to 2 so that the error will be 0. So using method of undetermined coefficients we have been able to derive an integration method where the nodes need not be equally spaced.

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So now you can try to see what happens if you want a method of the form say integral a to b f(x)dx such that it is capital A times f(A) plus B f(A plus B by 2) plus C into (f(b)). So determine A B and C such that the method is exact for polynomials of degree as high as possible. So here you observe that the points are A B and A plus B by 2, which means this, is the midpoint of the interval so the points are equally spaced.

I would like to derive this integration method using method of undetermined coefficients and find A B and C such that the method is exact for polynomials of degree as high as possible and you would immediately see that you are essentially deriving Simpson's rule for equally spaced points but now using the method of undetermined coefficients.

Earlier you derive Simpson's rule using polynomial interpolation with equally spaced points but now that we have learnt the method of undetermined coefficients I want you to derive Simpson's rule for equally spaced points namely a method of this form which would give you Simpson's rule so that the constants A B and C what do you expect A B C to be A will come out to be h by 3 and B we will come out to be 4 h by 3 and C will be again h by 3.

So derive a method and also compute the error using say once you get the method you know that the method is exact for what polynomials you require three constants so polynomials of degree 0 1 and 2 you will use these three conditions to derive A B and C then check what happens when f(x) is equal to x cube.

You already know result about the error in Simpson's rule check what happens and then work out the details because you want the method to be exact for polynomials of degree as high as possible. So that completes our discussion on method of undetermined coefficients we move on to another method which is called Gaussian Quadrature that we will take up in the next lecture.