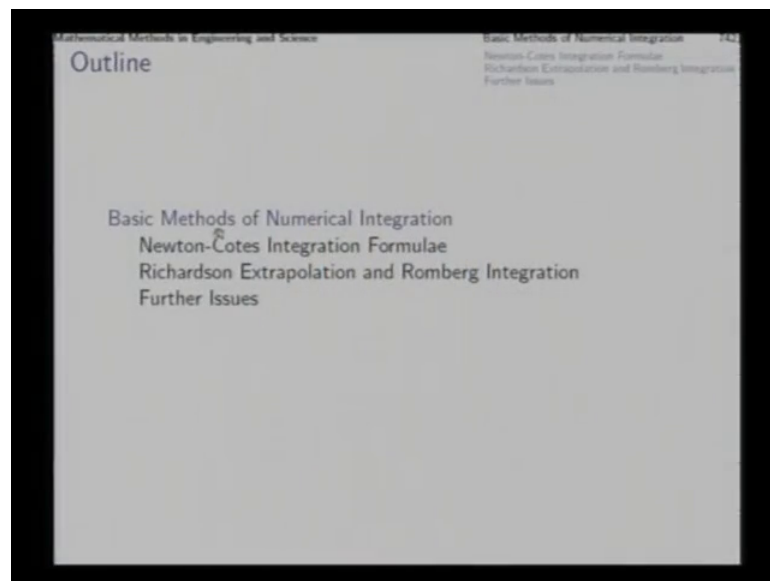


Mathematical Methods in Engineering and Science
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Module – V
Selected Topics in Numerical Analysis
Lecture – 02
Numerical Integration

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Good morning, in this lecture we will study methods of numerical integration. So, first we start with Newton cotes integration formulae.

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Newton-Cotes Integration Formulae

$$J = \int_a^b f(x) dx$$

Divide $[a, b]$ into n sub-intervals with

$$a = x_0 < x_1 < x_2 < \dots < x_{n-1} < x_n \hat{=} b,$$

where $x_i - x_{i-1} = h = \frac{b-a}{n}$.

$$J = \sum_{i=1}^n hf(x_i^*) = h[f(x_1^*) + f(x_2^*) + \dots + f(x_n^*)]$$

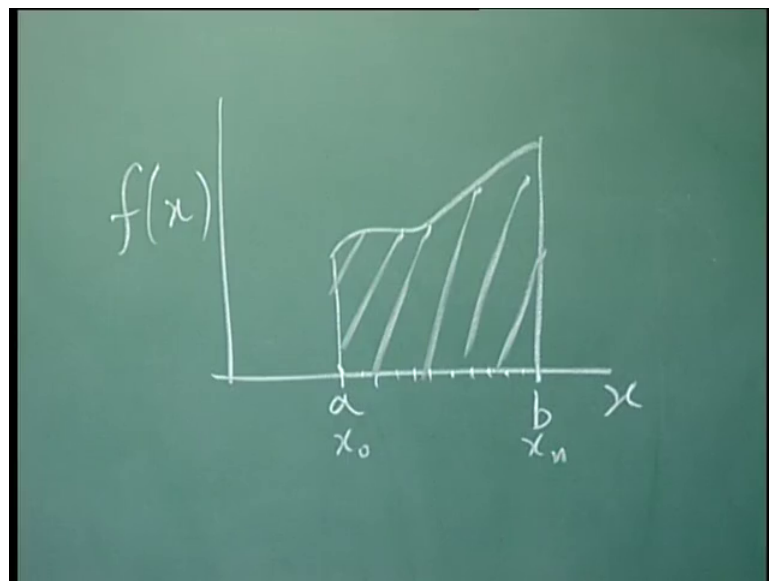
Taking $x_i^* \in [x_{i-1}, x_i]$ as x_{i-1} and x_i , we get summations J_1 and J_2 .

As $n \rightarrow \infty$ (i.e. $h \rightarrow 0$), if J_1 and J_2 approach the same limit, then function $f(x)$ is integrable over interval $[a, b]$.

A rectangular rule or a one-point rule

So, the problem here is to integrate a function of a single variable from a to b.

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Now as you understand if the function is like this then the integral of $f(x)$ from a to b is this area. So, we need to find out this area or find out the integral of function $f(x)$ from a to b that is this.

Now, we will start from the definition and the numerical integration procedure basically works directly on the definition. Now, if you divide this interval a to b into a number of sub intervals say n sub intervals of equal size and then you call this a as x_0 and b as x_n

and in between you have got n equal intervals right of size h then that will mean that x_n minus x_0 is n into h and; that means, this that is for every in sub interval we have the size h which is b minus a by n . Now, an estimate of the integral you can find by taking one point from every interval and summing up the function values over all the intervals that is one point from the first interval one point from the second interval one point from the third interval and so on.

And if you sum up these and multiply with h , then you get one estimate of the integral that is in the first sub interval you take one value and then suppose you take this value this value of the function multiplied with h gives you this area; this rectangular area, similarly for this next interval, if you take this value and then you get this area. Now, like that if you go on summing up the rectangular areas then you get one estimate of this entire area. Now, if you have the steps if you have the number of sub intervals large and each sub interval of very small size that is h is extremely small, then you get a better and better estimate.

Now, this is an estimate say \bar{j} ; now the question is what is our policy of taking this x_i star whether we take it in the beginning of the interval sub interval or at the end of the sub interval or somewhere in the middle now depending upon which points of the sub interval we take say if we take the starting point of the sub interval. Then we get one such estimate say j_1 and if we take the endpoint of each sub interval, then we get another estimate j_2 . Now, these 2 estimates might slightly differ depending upon how the function changes.

Now, as n tends to infinity that is as the number of sub intervals become very large and; that means, and the size of the sub interval tends to 0 then in such a situation if the 2 summations that is 2 estimates of the integral approach the same limit, then by definition we call the function to be integrable over the interval a to b that is the definition of integrability and the definition of integral that is if the 2 summations approach the same value same limit as n tends to infinity and h tends to 0. Then we say that a function is integral integrable and the common limit to which these estimate approach that limit is the integral.

So, this is how you define the integral as a limit of a sum apart from giving the definition this also gives us a rule for conducting numerical integration and that rule can be called a

rectangular rule or a one point rule why rectangular because it is the sum of rectangular element and why one point because in every sub interval we are considering a single point now. So, for as the question of selecting the point is concerned we may ask this question let us make one point clear that if the function is integrable by this definition then in the analytical way of integration. We typically try to look for affordable expression for this function if there is such an expression and then if that expression can be organized in the form of a function which we know is the derivative of some known function, then we typically conduct the integration in analytical form to analytical means as an anti differentiation formulation.

Now, it may happen that there is an expression for $f(x)$, but then we by the normal school a calculus methods we cannot frame it in the form in which it is recognized to be the derivative of some other known function in that case the analytical methods of integration will not work apart from that there may be situations where you can evaluate the function at whatever point you want, but then you cannot frame an analytical expression there is analytical expression for the function is not available. For example, the function that we are talking about may be the result of an experiment that is you provide x and as with the value of x taken as one of the parameters in the experiment the result of the experiment turns out to be the function value $f(x)$.

So, that way you can evaluate the function at a value of x , but you cannot get an expression of it. So, that way if you can evaluate the function at several points through experimentation or through some complicated calculation in a computer program then we can say that effective have, but you do not have an expression for the $f(x)$. So, in both of these cases, one when you do not have an expression for the $f(x)$ and 2 when you have an expression, but tackling that by the integration methodologies of the school calculus is not enough not possible.

So, in both of these cases, you have to rely on numerical integration, if you need the integral; now we come back to this question that is if whichever point we take as the single point in every sub interval like this we find that the sum approaches the same limit if we take a large number of steps of extremely small size h . But then in actual practice we would like to evaluate the integral with now going into extremely large number of steps that is we would not like n to be extremely large. So, what will be efficient neither the starting point of each sub interval nor the end point of each sub interval.

So, the best result you will find by taking the midpoint of every interval if you want to take a single point in the every in every interval and therefore, to answer this question which point to take as x_i star a common sense answer will be take the midpoint as the best representative and therefore, one special case of the rectangular rule which is most commonly used that is obtained which is the midpoint rule.

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Newton-Cotes Integration Formulae

Mid-point rule
 Selecting x_i^* as $\bar{x}_i = \frac{x_{i-1} + x_i}{2}$,

$$\int_{x_{i-1}}^{x_i} f(x) dx \approx hf(\bar{x}_i) \quad \text{and} \quad \int_a^b f(x) dx \approx h \sum_{i=1}^n f(\bar{x}_i).$$

Error analysis: From Taylor's series of $f(x)$ about \bar{x}_i ,

$$\int_{x_{i-1}}^{x_i} f(x) dx = \int_{x_{i-1}}^{x_i} \left[f(\bar{x}_i) + f'(\bar{x}_i)(x - \bar{x}_i) + f''(\bar{x}_i) \frac{(x - \bar{x}_i)^2}{2} + \dots \right] dx$$

$$= hf(\bar{x}_i) + \frac{h^3}{24} f''(\bar{x}_i) + \frac{h^5}{1920} f^{(4)}(\bar{x}_i) + \dots$$

third order accurate!
 Over the entire domain $[a, b]$,

$$\int_a^b f(x) dx \approx h \sum_{i=1}^n f(\bar{x}_i) + \frac{h^3}{24} \sum_{i=1}^n f''(\bar{x}_i) = h \sum_{i=1}^n f(\bar{x}_i) + \frac{h^2}{24} (b-a) f''(\zeta).$$

for $\zeta \in [a, b]$ (from mean value theorem): second order accurate.

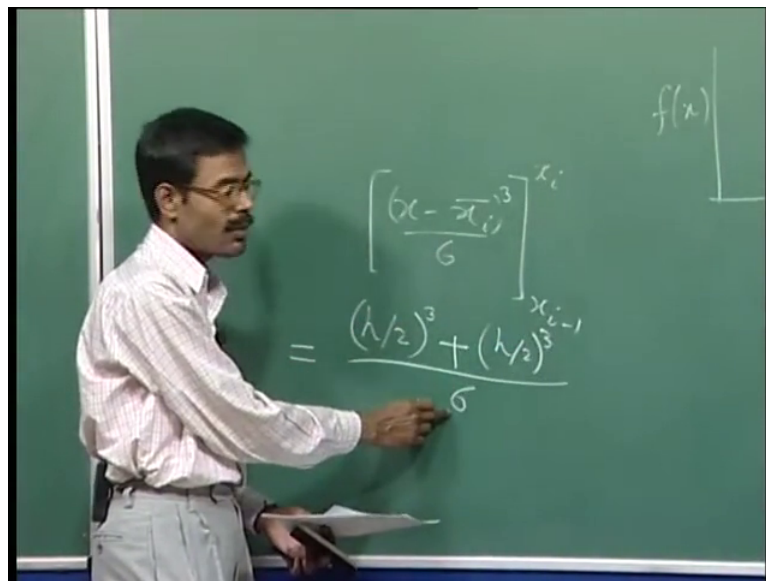
So, selecting x_i star as the midpoint of the sub interval you get over one such sub interval you get a integral as h into that value that is neither in the beginning nor in the end, but in the midpoint the understanding is that whatever is the trend of the function whatever is lost in this half is compensated in this half to a good extent. So, with that intention with that background we typically take the midpoint for a single point rule. So, this is the estimate of this integral over a particular sub interval and over the entire domain from a to b these things will be added from x_0 to x_1 , x_1 to x_2 , x_2 to x_3 and So on. So, that sum over the entire domain is given by the summation of this for i equal to 1 to n , right.

Now, after we have found this midpoint rule or single point formula for the numerical integration we need to figure out how good it is now the way we conduct this error estimate is through the Taylor series. So, suppose we from the Taylor series of $f(x)$ about this point about this midpoint then Taylor series of $f(x)$ around this midpoint is f at the midpoint plus f prime at the midpoint into x minus midpoint plus second derivative into

delta x square by 2 and so on, right. So, this is the Taylor series of f x around xi bar the midpoint.

Now, the correct integral of this Taylor series would be this; this is constant; constant into h; h is xi minus xi minus 1 that is the size of the interval plus noun node; what will be the integral of this the integral of this will be this is constant number and the integral of this will be x minus xi bar whole square by 2, but then that is a whole square. Now when you evaluate the square at this and this in both cases.

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We will get the same value; that means, x minus xi bar whole square by 2, now this is xi and this is xi minus 1 right.

So, when we put xi in this place then we find this is h by 2 because the size of the interval is h. So, midpoint is h by 2 away from the endpoint. So, this is h by 2 right. h by 2 square by 2 and when we put this value we get this as minus h by 2, but it is square. So, it will be the same thing and so, when you subtract we get that cancelled. So that means, h square by 2 h square term will be absent from the error because you can simply see that this is an odd function. So, its integral from minus h by 2 to h by 2 is 0. So, this part will go missing in the integral.

The leading term in the integral after this will be different right and this one will be this is square. So, it will be cubed by 3, right. So, the integral of this term we will get as cube

by 3 and already there is a 2 sitting here. So, we will get it as 6 right and outside we will have this f'' , right. So, then when you evaluate this at x_i , we will find this is h^2 when you evaluate it at x_{i-1} we will find it minus h^2 . So, we will get h^2 minus minus h^2 which will give us 6, right.

So, here the terms will survive. So, h^3 plus h^3 that is h^3 divided by 6; that means, h^3 , we will get. So, that shows us that the leading error term will be this and similarly we will find that the f''' term will get cancelled just like this part. And the next term similarly if you can if you calculate then you will find that you will get this now note that this is that term which we will get in the actual midpoint rule integration formula.

So, error will be the rest of it and in that series of the error it is this term which will dominate. So, the leading error will be of the third order and therefore, this is called third order accurate that is accuracy of the midpoint rule is of the third order which means that the error term will be error will be dependent upon the step size up to the cubic order, but then that is only for one sub interval as you try to sum up such components over all these sub intervals then the complete formula you get as from a to b . So, such terms added over all the sub intervals that is i equal to 1 to n ; n sub intervals.

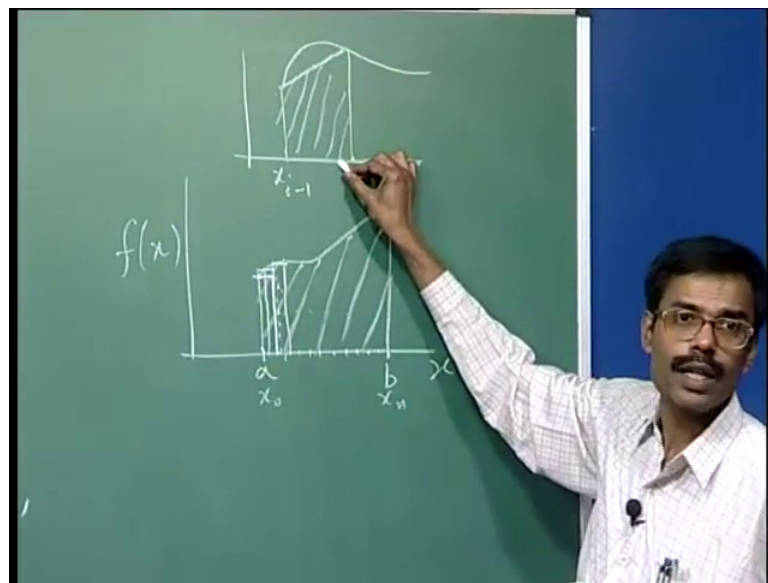
Now, this same thing when we add up now in this addition this term has been turn out this term has been neglected because the leading error term is this. So, when we add up this for i equal to 1 to n this is of course, this in which the; this is the midpoint rule formula result and this will be the error. So, when we try to sum it up, then we find that here the error will have this sum of the second derivative at these midpoint whatever is the second derivative. Now, if the second derivative is varying, then somewhere it is small somewhere it is large and so on then from the mean value theorem you will find that there will be some value of x between a and b where the second derivative value is the average over the complete interval.

If that value is this x_i , then you will you can say that the sum of the second derivatives over all the intervals is n times the second derivative value at that point whatever maybe that point. So, n times this. So, take that n from here and combine it with h . So, nh is the size of the interval n sub intervals of h size. So, nh is the size of the complete interval complete domain which is b minus a that is why you find that one power of h has got

reduced here and then; that means, that the error in the integral over the entire domain is proportional to h^2 that is it is proportional to the square of the step size so; that means, that the third order accuracy over each sub interval will mean that over the entire domain it will be second order accurate this is midpoint rule.

Now, this was the result of getting taking one function value in every sub interval if you decide to use 2 sub intervals then that will mean that for every a 2.

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Points or every sub interval then that will mean that over every sub interval, you will not approximate the function with a constant value, but you will approximate it with a say this is the interval shown accelerated. So, whatever is the function like this? So, if this is one interval, then the next rule is trapezoidal rule which makes a linear interpolation between these 2.

So, just over a constant value the next possible approximation next possible estimate is the linear interpolation between the 2 end points, in this case, the linear interpolation between 2 end points will basically try to work out the integration of this function which will be this area of this trapezium and that is why the corresponding rule is called that trapezoidal rule what is the area of this trapeze trapezium half into h into the sum of these 2, right. So, that is as if you are taking this area. So, the next step next higher rule will be by approximating the function with the linear interpolation.

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Newton-Cotes Integration Formulae

Trapezoidal rule
Approximating function $f(x)$ with a linear interpolation,

$$\int_{x_{i-1}}^{x_i} f(x) dx \approx \frac{h}{2} [f(x_{i-1}) + f(x_i)]$$

and

$$\int_a^b f(x) dx \approx h \left[\frac{1}{2} f(x_0) + \sum_{i=1}^{n-1} f(x_i) + \frac{1}{2} f(x_n) \right].$$

Taylor series expansions about the mid-point:

$$f(x_{i-1}) = f(\bar{x}_i) - \frac{h}{2} f'(\bar{x}_i) + \frac{h^2}{8} f''(\bar{x}_i) - \frac{h^3}{48} f'''(\bar{x}_i) + \frac{h^4}{384} f^{(iv)}(\bar{x}_i) - \dots$$

$$f(x_i) = f(\bar{x}_i) + \frac{h}{2} f'(\bar{x}_i) + \frac{h^2}{8} f''(\bar{x}_i) + \frac{h^3}{48} f'''(\bar{x}_i) + \frac{h^4}{384} f^{(iv)}(\bar{x}_i) + \dots$$

$$\Rightarrow \frac{h}{2} [f(x_{i-1}) + f(x_i)] = hf(\bar{x}_i) + \frac{h^3}{8} f''(\bar{x}_i) + \frac{h^5}{384} f^{(iv)}(\bar{x}_i) + \dots$$

Recall $\int_{x_{i-1}}^{x_i} f(x) dx = hf(\bar{x}_i) + \frac{h^3}{24} f''(\bar{x}_i) + \frac{h^5}{1920} f^{(iv)}(\bar{x}_i) + \dots$

Then you will find half into h into the sum of the functional values at the 2 points write 2 end points. So, that is the next rule now here again if you sum of over all the sub intervals then you will sum this for i equal to 1, 2, 3, 4, 5, 6, up to n , right as you do that you will find that the first sub interval gives you x_0 and x_1 , second one will be giving x_1 and x_2 , third one will be giving x_2 and x_3 . This is an advantage of trapezoidal rule that every internal point x_1, x_2, x_3 , up to x_{n-1} is actually used of in 2 places; that means, the function evaluation at that those points are use very efficiently.

So, then all the internal points turn out to appear twice and the initial point x_0 and the final point x_n appear only once and therefore, this half function value at the initial point half function value at the final point and every individual point x_1, x_2, x_3 , up to x_{n-1} , they get use twice in the entire sum therefore, half plus half they get full contribution here 1 to $n-1$. So, this is the complete trapezoidal rule for the full domain.

Now, similarly a similar to the case of midpoint rule if we try to conduct an error analysis in this case then again, we compare this result that we get this is compare over a single sub interval this result that we get if we try to compare that with the Taylor series we find this Taylor series expansion about the midpoint that same expansion we use for x_{i-1} which is there in the formula here and $f(x_i)$. There is starting point of the sub interval end point of the sub interval and then we get this you note that x_{i-1} is

midpoint minus h by 2. So, you get minus sign in the odd terms and xi is midpoint plus h by 2. So, you get all signs plus.

Now, if we try to see what do we get in this from this formula then we will sum of these 2 right and then a multiply that with h by 2. So, as you sum of these 2 we find that this comes twice and then multiplication with h by 2 gives us twice this into h by 2; that means, h into this; this what we got in midpoint rule and then this will cancel out, these fellows these 2 added together will give us h square by 4 multiplied with h by 2 we will get h cube by 8 and similarly these will cancel out these will give us 384 straight away and so on

Now, this turns out to be what we get from the trapezoidal rule and then we can recall this actual Taylor series of the integral of f x around the midpoint that was this. So, this same expression if we use here and then we find that this is what we got from the trapezoidal rule and this is what we get by the integration of Taylor series is tells term by term. So, the difference of these 2, we will give us the error estimate of the trapezoidal rule as we try to find out the error estimate this completely cancel out because this much is correct and the difference of these and difference of these will give you the third degree and fifth degree terms in the error estimate the leading term will be the third degree term.

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Mathematical Methods in Engineering and Science

Basic Methods of Numerical Integration

Newton-Cotes Integration Formulae

Error estimate of trapezoidal rule

$$\int_{x_{i-1}}^{x_i} f(x) dx = \frac{h}{2} [f(x_{i-1}) + f(x_i)] - \frac{h^3}{12} f''(\bar{x}_i) + \frac{h^5}{480} f^{(4)}(\bar{x}_i) + \dots$$

Over an extended domain,

$$\int_a^b f(x) dx = h \left[\frac{1}{2} (f(x_0) + f(x_n)) + \sum_{i=1}^{n-1} f(x_i) \right] - \frac{h^2}{12} (b-a) f''(\xi) + \dots$$

The same order of accuracy as the mid-point rule!

Different sources of merit

- ▶ **Mid-point rule:** Use of mid-point leads to symmetric error-cancellation.
- ▶ **Trapezoidal rule:** Use of end-points allows double utilization of boundary points in adjacent intervals.

How to use **both the merits?**

So, as we do that we find that this is the integral based on the Taylor series this is a integral which trapezoidal rule gives us and this is the these are the leading error term cubic term fifth the term and. So, on that is obtain just by subtracting these 2. So, you see 1 by 24 and 1 by 8. So, which is 3 by 24 difference will be 2 by 24 that is 1 by 12. So, that 1 by 12 is here in the cubic term and so on.

Similarly, over an extended domain if we sum up these for i equal to 1, 2, 3, 4, up to n then that sum will give us this formula for these which we have already got half contribution from the first term and the last term and full contribution of integer terms this will be obtained from the trapezoidal rule formula and the leading error will come from here right. So, the same evaluation again $f''(\xi)$ summed over all the intervals all the sub intervals will give us n times the average value and average value is this and nh is b minus a .

So, again we find that the leading error term over the entire interval is this now interestingly we find that here also the error order is same as the midpoint rule over a sub interval it was cubic order over an in over the entire domain it was a quadratic order even though in the midpoint rule in every sub interval only one function value was used. And in the trapezoidal rule over every sub interval 2 function values were used still there are the error order is the same the actual error magnitude may vary, but the order of the error is same.

Now, in this case midpoint rule has an advantage and trapezoidal rule has another advantage what is the advantage that midpoint rule has midpoint rule has the advantage that just by using one function value at the midpoint the leading error on this side and that side can 2 cancel out this is advantage of midpoint rule and the trapezoidal rule has the advantage that the boundary is use and so, every interior boundary is actually used in on both sides. So, that way over an extended interval the number of functions function evaluations function values that was used in this and this actually do not differ by much.

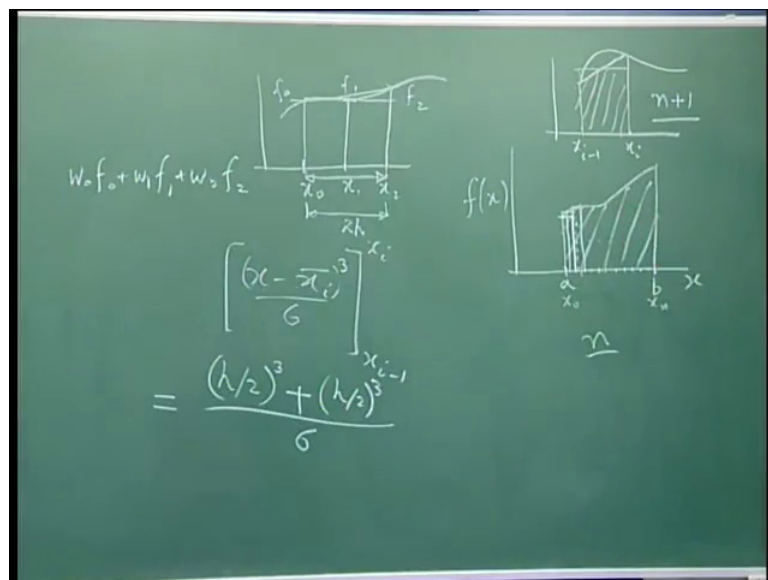
Even though it sounds as if the number of function values here is almost double, but actually it is not double it is very marginally more than these how here you find that in every sub interval one function value was used the midpoint, but that was used only in that sub interval because it was an internal point integer point midpoint. So, over n sub

intervals n function values where use here; here over n sub intervals; how many function values were used n plus 1 not much.

So, that way between n function values and n plus 1 function values if you get the same error order then it is not a very surprising situation and you do not; you do not miss much that is the combination resource that you has spent here is actually comparable to the computational resource that you have spent here another question is considering this. These 2 different sources of merit different sources of merit in midpoint rule and trapezoidal rule in the midpoint rule use of midpoint leads to symmetric error cancellation which will be an advantage of all those methods all those rules which use symmetric positioning of points in a sub interval or over a panel of sub intervals.

On the other hand trapezoidal rule has a merit that is use of end points allows double utilization of boundary points in adjacent intervals. Now how to use both the merits that is any method with uses symmetric positioning of sample points will have this advantage on the other hand any method that uses the boundary points of the sub intervals will have this advantage right you can think of using (Refer Time: 26:34).

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In which you use the boundary points as well as the midpoint say if this is a function and if you use the boundary this is a sub interval this is sub interval and if you use this function value this function value. And this function value then you see that over this sub domain over this sub domain the 3 points are used symmetrically midpoint is there and 2

other points are there which are equally disposed compare to the midpoint. So, this is symmetric positioning of point in putting the midpoint.

And the other advantage is that the boundary points are used; that means, in the next sub interval this boundary point will be used once more, right. So, if we use these kind of 3 points positioned, then the rule that you get is Simpson's one-third rule and that will have both of these advantages the Simpson's.

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Mathematical Methods in Engineering and Science

Basic Methods of Numerical Integration

Newton-Cotes Integration Formulae

Newton-Cotes Integration Formulae
Richardson Extrapolation and Romberg Integration
Further Issues

Simpson's rules
Divide $[a, b]$ into an even number ($n = 2m$) of intervals.
Fit a quadratic polynomial over a panel of two intervals.
For this panel of length $2h$, two estimates:

$$M(f) = 2hf(x_i) \quad \text{and} \quad T(f) = h[f(x_{i-1}) + f(x_{i+1})]$$

$$J = M(f) + \frac{h^3}{3}f''(x_i) + \frac{h^5}{60}f^{(iv)}(x_i) + \dots$$

$$J = T(f) - \frac{2h^3}{3}f''(x_i) - \frac{h^5}{15}f^{(iv)}(x_i) + \dots$$

Simpson's one-third rule (with error estimate):

$$\int_{x_{i-1}}^{x_{i+1}} f(x) dx = \frac{h}{3}[f(x_{i-1}) + 4f(x_i) + f(x_{i+1})] - \frac{h^5}{90}f^{(iv)}(x_i)$$

Fifth (not fourth) order accurate!

Here what we do is that we divide the overall interval overall domain into an even number of intervals why even because in every interval we will use double the size of the interval that is if we have $2n$ intervals then 2 interval here 2 interval 2 sub intervals here 2 sub intervals next 2 sub intervals next and so on.

So, if we divide the entire domain from a to b into an even number of sub intervals even number of intervals then over every such pair of sub intervals we evaluate the function at 3 points, one at this end one at the midpoint and one at this end right . And then we say that through these 3 function values we can fit a quadratic model in this local neighborhood and then consider the integration the exact integration of that quadratic model function note that in the single point formula we use the constant value in the 2 point formula that is trapezoidal rule we used a linear approximation in the 3 point formula in the same manner we will use a quadratic approximation.

So, now this is one way to arrive at Simpson's; one-third rule there is fit a quadratic through this 3 point; points through this 3 function values and consider the exact integration of that quadratic function this is one way another way to do the same thing is at suppose these are x_0, x_1, x_2 and the corresponding function values are say f_0, f_1 and f_2 . You can also say that till now, we have seen that the integral estimate that we get integral value that we get is a weighted some over weighted some of the function values in the trapezoidal rule we found that for every sub interval the weights were half half right of the both the function values.

Similarly, here we can say that we will consider some weight value this and then try to determines w_0, w_1, w_2 . So, there are several ways of a having a Simpson's one-third rule first is that through these 3 function values try to feed a quadratic and integrate that quadratic expression analytically you get Simpson's one-third rule formula the second possible way is to assume it in this manner. And then claim that the result of this sum must be correct with respect to the Taylor series up to such an such order that is first order second order third order errors should be 0. That means, you conduct the Taylor series approximation and integrate that and with that the error of this you subtract that with that with that you consider the error of this that is from that you subtract this you get the error estimate in terms of h and from that say that the h term h square term and h cube terms. These 3 terms must be 0 and from that equations on w_0, w_1, w_2 and then get the correct values of w_0, w_1 and w_2 and you will get the correct values this will be $1; 1$ by 3 this will be 4 by 3 this will be 1 by 3 . So, that will be another way to arrive at Simpson's one-third rule.

These 2 independent ways of arriving at Simpson's one-third rule you find in the exercises in the text book and here we try to find a third way to arrive at the same formula and that is based on what we were discussing just now; how to use both the merits. So, using this kind of a pair of sub intervals you say that over this double interval of size $2h$ we can use midpoint rule to find out an integral estimate or we can use trapezoidal rule over 2 of this and try to evaluate the integral like that.

So, over this entire interval $2h$ of $2h$ size if we use only trapezoidal rule over the entire interval together then we get this trapezoidal area right and that is this; so, trapezoidal rule over this entire double interval we will give us this that is half into $2h$ into some of f_0 and f_2 , right that is this. Similarly, if you use midpoint rule over this entire interval

then will find the value of this into $2h$ that will be this. So, estimate based on the midpoint rule is this estimate based on the trapezoidal rule is this and error estimates we have found earlier already in that same error estimate formulas if we put $2h$ in place of h because now the interval size is twice h then we will get these, then we say can we find out a linear combination of these 2. So, as to get a better estimate of j ; that means, so as to eliminate the leading error from here.

As you can see twice the first equation plus once the second expression if we add then you will get $2h^3$ by 3 positive and $2h^3$ by 3 negative and they will cancel out. So, twice this will be $2j$ and ones this will be $1j$ some of that will be $3j$, right. So, in that this will be missing and that expression then if you can divide by 3 you get another value of j which is a better value in the sense that the cubic error term will be missing. So, what we do? We multiply this with 2 this with one add up and then divide by 3. So, thereby you will get divide by 3. So, one-third of twice this plus this if we do that then you will get this which is the Simpson's one-third rule, one-third rule it is called because of this one-third factor coming here and the leading the error term is fifth order.

Now, notice that we expected up to fourth order error, but because of the symmetry we certainly find that we have got an advantage. So, these a fifth order formula and over a complete domain you will find that a corresponding error will be only fourth order now if we use $3n$ number of intervals like this rather than $2n$ and then we fit a cubic through 4 points x_0, x_1, x_2, x_3 over the 3 intervals and then conduct the integral then similarly we get another rule which will be a 4 point rule and that is Simpson's 3/8 rule.

But beyond this and in the case of Simpson's 3/8 rule also, we will find that the error will be only fifth order fifth order fourth order only just like Simpson's one-third rule because does not have the use of midpoint that does not have that advantage of the midpoint still higher order rules. I am not very advisable because they tend to give high oscillation binomials which are not true representations of the function rather in such situations we tend to use the trapezoidal rule or Simpson's rule themselves in 2 different strategies whereas, to improve the integral estimate rather than going for rules with more number of points.

One very good method for finding very accurate integral with very less computational cost is through Richardson extrapolation. Now note that Richardson extrapolation is a

methodology which is applicable not only for the numerical integration problem, but for any problem in which we try to determine a quantity f through computations over a step size h now if using a step size h , we make an estimate f of h . So, depending upon the step size the estimate will depend.

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Richardson Extrapolation and Romberg Integration

To determine quantity F

- ▶ using a step size h , estimate $F(h)$
- ▶ error terms: h^p, h^q, h^r etc ($p < q < r$)
- ▶ $F = \lim_{h \rightarrow 0} F(h)$?
- ▶ plot $F(h), F(\alpha h), F(\alpha^2 h)$ (with $\alpha < 1$) and extrapolate?

- $F(h) = F + ch^p + \mathcal{O}(h^q)$
- $F(\alpha h) = F + c(\alpha h)^p + \mathcal{O}(h^q)$
- $F(\alpha^2 h) = F + c(\alpha^2 h)^p + \mathcal{O}(h^q)$

Eliminate c and determine (better estimates of) F :

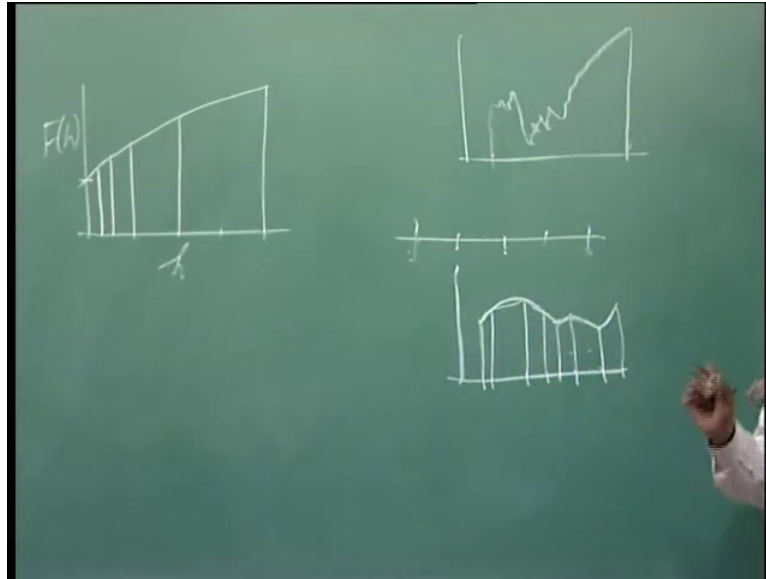
- $F_1(h) = \frac{F(\alpha h) - \alpha^p F(h)}{1 - \alpha^p} = F + c_1 h^q + \mathcal{O}(h^r)$
- $F_1(\alpha h) = \frac{F(\alpha^2 h) - \alpha^p F_1(h)}{1 - \alpha^p} = F + c_1 (\alpha h)^q + \mathcal{O}(h^r)$

Still better estimate: $F_2(h) = \frac{F_1(\alpha h) - \alpha^q F_1(h)}{1 - \alpha^q} = \frac{F}{1 - \alpha^q} + \mathcal{O}(h^r)$

Estimate will vary now finer and finer step that we take better and better estimate that will get and if the error terms are h to the power p h to the power q h to the power r etcetera with this arrangement and if $p < q < r$ have significant gaps then if we have way to improve the estimates by leaps and bounds through every next calculation.

For example suppose F is a quantity to which we are trying to estimate with the computation being carried out with the step size h now with the step size h suppose this is the value of F_h with.

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A half size of the step size suppose this is the evaluation this is the estimate one fourth size this is the estimate one 8 this is the estimate one 16, this is the estimate and can we what say that with very small step size the result should be something like this that is the extrapolated results based on the estimates which have been made over various different step size h . So, this is the idea of Richardson estimation.

So, if the correct value of f is the limit of f of Δ as Δ tends to 0, then plotting this with the plot extrapolating to h equal to 0 will get the correct value and very very accurate estimate. Now this will work when the leading errors have certain gaps now for example, suppose the in the evaluation of f of h through the numerical process here the leading error term is h to the power p . And next is h to the power q next the h to the power r and so on with gap then with α h α less than one in this example i have mention taken α equal to half which will be using in the f of numerical integration also.

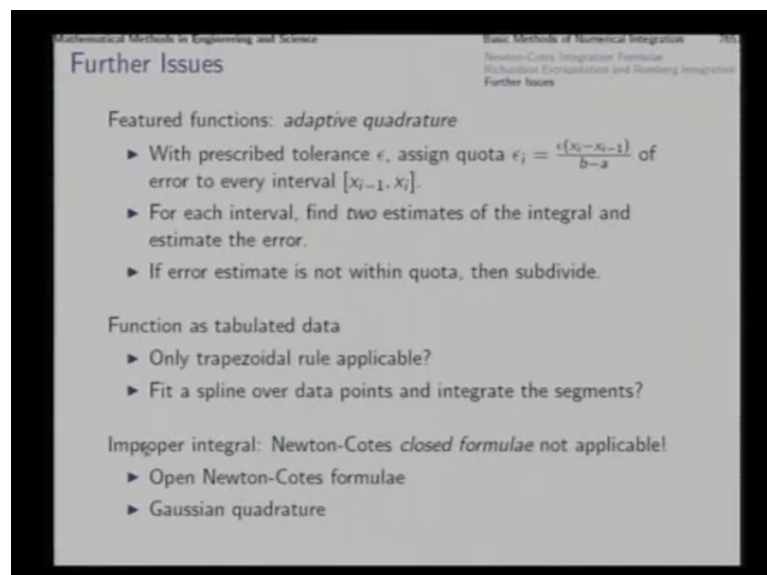
Now, with αh step size the estimate is this similarly for f a square h estimate is this now if you take the 2 higher equations from here and multiply the upper one with α to the power p and subtract then this c unknown, c will get cancelled and you will get 1 minus α to the power p into f right. And from there in between these 2 we will get a better estimate that is between these 2 this minus α to the power p times this will be this minus α to the power p times this right that is here and this one get cancelled and

1 minus alpha to the power p with that we divide and we get a better estimate of f that is f 1 in that the leading term of error h to the power p will be missing. Now the leading term will be h to the power q.

Similarly, if you use these 2, then in a similar manner we will get this minus alpha to the power p into this part will be cancelled and then 1 minus alpha to the power p with that we divide and get another better estimate there is even better that this within these 2 now consider in these 2 the evaluation has been done at one more steps further in which the leading error is now of qth ordered. Here again you can see that if we subtract alpha to the power q times this from the lower one then suddenly yet another better estimate we will get in which the q ordered error term also will get cancelled and that we get like this that is even better estimate.

So, now between 1 and 2 we will get this estimate between 2 and 4 we get this estimate and then between 3 and 5 we get yet another estimate which is even better. This is one way of improving the estimate of a true way limited number of actual evaluation and when we apply this Richardson extrapolation through the numerical integration problem with trapezoidal rule itself we get what is called the Romberg integral.

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That is we take the trapezoidal rule which is like this over finer interval from a to b and then here pqr are 2 4 6 called even term which are to half we have the advantage that in the first round we evaluated at these 2 point in the second round when we subdivided the

interval by 2 sub interval. Then we need evaluate here, here, here, but in these location is the function values are already there only the here we have to evaluate first and then next round at these 3 point we already have the function value at these 2 point, we have evaluate and so on.

So, if we use the same formula then trapezoidal rule will with h equal to capital H , we find you have estimate, then which h equal to capital H by 2 we find another estimate between these 2 estimates we will get a much better estimate. Similarly, which h equal to capital H by 4 will get another estimate I_3 ; now between I_2 and I_3 , we will get another much better estimate and between these 2 better estimates I_2 and I_3 we will get yet another estimate which will be extremely good.

Now, at every step we can check whether the difference between last 2 best estimates is extremely small if. So, then we can stop or we can continue. So, this process of integration is called Romberg integration and these gives very accurate results in a very efficient manner another way of using efficient means is through adoptive steps size, now why that is important because it may happen that there is a function with over a complete interval changes like this. Now, you will find that in this part of the domain large step sizes will give quite accurate results on the other hand here or here you will need small step sizes right. So, in that kind of a situation adoptive step size helps you to get a very accurate re estimate of the integral with less number of function evaluations.

So, what you can do is that in the beginning you have a tolerance value ϵ which is your statement about accuracy then you can say that for every sub interval of size x_i minus x_{i-1} you can assign a quota of error ϵ divided by b minus a into this sub intervals size. So, every sub interval we will have this much quota called error right. Then what you do for each interval find 2 estimates of the integral I over the full and I over the half now if the difference you find between the 2 estimates and from that you estimate the error. Now, if this error estimate is within this quota then you accept it or you sub divide the interval further this is the process of adoptive quadrature or adoptive step size in numerical integration this is quite often found very effective.

Another situation that arises is if you have the function as tabulated data and tabulated data is not necessarily over equal number of intervals for example, for this function suppose you have got the tabulated data at these x value then all at you can do is use

these function values only you cannot evaluate the function anywhere else suppose these are the function values and from that you have to integrate. Now, for this kind of a situation you can do 2 things one over every interval with unequal sizes now you use trapezoidal rule and sum of 1, 2, 3, 4, 5, 6, 7; 7. Such integrals you just take the sum this is one way to do it the other way to do it is through these function values to these data points you fit a spline the way we discuss in the previous lesson if it a spline and then conduct the integral of that plain this is another way either spline or any such other continuous representation of the function.

So, these are 2 different ways of handling the integral problem when all that you can use is function values given at certain data points and you cannot evaluate the function at any other point. So, they are either you use trapezoidal rule over single sub interval and at or you fit a continuous representation through function interpolation methods and then use that composite function to evaluate the integral.

Now, sometimes you find that the integral when you try to develop then the function value at the end of the interval is not appropriately define such integrals are improper integral and in that case these rules trapezoidal rule or Simpson's one-third rules etcetera. You cannot use and these formulas which are called Newton quotes close formulas they are not applicable in such situations where the end point of the interval is improper where the at the end point of the interval function is not defined.

For example for this point of a function where the end points of the interval have do not have the function define at those points. So, in such situations these rules these close formulae which will required you to provide the end point function values will failed in such cases you can reserved to similar open Newton quotes formulas which do not need the end point value or you can use Gaussian quadrature. Now, in the next chapter of the book we discuss Gaussian quadrature, but for the purpose of the course, we will omit that, but from the next; next lesson, next chapter of the book, we will take one very simple, but very powerful formulation and that is in multiple integral.

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Mathematical Methods in Engineering and Science
Advanced Topics in Numerical Integration*
Gaussian Quadrature
Multiple Integrals

Multiple Integrals

$$S = \int_a^b \int_{g_1(x)}^{g_2(x)} f(x, y) dy dx$$
$$\Rightarrow F(x) = \int_{g_1(x)}^{g_2(x)} f(x, y) dy \text{ and } S = \int_a^b F(x) dx$$

with complete flexibility of individual quadrature methods.

Double integral on rectangular domain

Two-dimensional version of Simpson's one-third rule:

$$\int_{-1}^1 \int_{-1}^1 f(x, y) dx dy$$
$$= w_0 f(0, 0) + w_1 [f(-1, 0) + f(1, 0) + f(0, -1) + f(0, 1)]$$
$$+ w_2 [f(-1, -1) + f(-1, 1) + f(1, -1) + f(1, 1)]$$

Now, just like ordinary single integral you have such Simpson's rules etcetera for multiple integrals also and for examples over a rectangular domain square domain minus 1 to 1 minus 1 to 1 over xy you get this as the 2 dimension version of the Simpson's one-third rule which will be accurate for a bicubic up to a bicubic function the way a single variable function f x for that the Simpson's one-third rule is correct up to a cubic function. So, this will be exact up to bicubic, but this is not what we want to discuss, I will discuss here quickly a very powerful integration method called Monte Carlo integration which is a stochastic method and it is very useful for evaluating multiple; multiple integrals over very complicated domains.

For example over these domain a function is defined and this is the domain of integration and you want to integrate function f x over this domain now the description on the domain itself makes the thing quite complicated and over that the development of the integral is difficult. Now, in such situations Monte Carlo method of integration gives you a very quick and handy way to get the integral and for that requirements are very simple you want a simple volume in the case of a 2 variable problem, it is an area a simple volume enclosing the domain omega that is suppose this is the domain omega and what you need is a straight forward simple volume simple region geometrically simple region which encloses this completely for our purposes this rectangle can be that domain this is easy.

Now, suppose this is x_i this is x_f that is initial f final f similarly this is y_i and this is y_f initial y final y . So, this is the selected domain now it is very easy to find points which are in this rectangular domain it was extremely difficult to find points which are there in the domain Ω because of the shape of the domain, but it is extremely easy to find points which are inside this. Now, this is one requirement you have to have a description of a straight forward geometrically simple region which completely encloses the domain and you must have a point classification scheme that is after a point has been through inside this rectangular domain you should be able to tell whether that point is also inside the domain Ω or not whether it is here or here.

With these 2 things in hand we can generate random points in this big volume V in the domain V and then if the point is within Ω also then we count $f(x)$ and if it is not within Ω , then we count 0 and then.

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The slide contains the following text and formulas:

Mathematical Methods in Engineering and Science
Advanced Topics in Numerical Integration*

Multiple Integrals
Gaussian Quadrature
Multiple Integrals

Monte Carlo integration

$$I = \int_{\Omega} f(\mathbf{x}) dV$$

Requirements:

- ▶ a simple volume V enclosing the domain Ω
- ▶ a point classification scheme

Generating random points in V ,

$$F(\mathbf{x}) = \begin{cases} f(\mathbf{x}) & \text{if } \mathbf{x} \in \Omega, \\ 0 & \text{otherwise.} \end{cases}$$

$$I \approx \frac{V}{N} \sum_{i=1}^N F(\mathbf{x}_i)$$

Estimate of I (usually) improves with increasing N .

We go on adding and as we add up all these $f(x)$ values taking the actual function value if it fall within our domain 0 otherwise, then the sum of all these function values divided by n into the volume of these gives as the Monte Carlo indication value now you know that larger N more accurate will be the result.

Now, the practical implementation practical use of this Monte Carlo method Monte Carlo integration will require you to first make an estimate based on sum value of n say n equal to 100 make that estimate then in a fresh mid make the same estimate with n equal to 500

and then n equal to 1000, then n equal to 5000 and as you increase n after the point, you will find that this estimate does not change much; that means, that number of points that number of random points is enough for this problem and this gives you a very good estimate of the integral.

So, other issues in the chapter are related to Gauss quadrature and that you can covered at your lecture for the purposes of our course we are omitting that and in the next lecture we will go into the very important topic of numerical solution of ordinary differential equations.

Thank you.