Computational Science in Engineering

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Lecture - 36
Numerical Analysis

So, we have looked at the numerical differential procedure now how to get the differentiation. Now we will look at the numerical integration and this is what we come across different function where we need to integrate within some interval and how we can do that numerically that is what we are going to now discuss.

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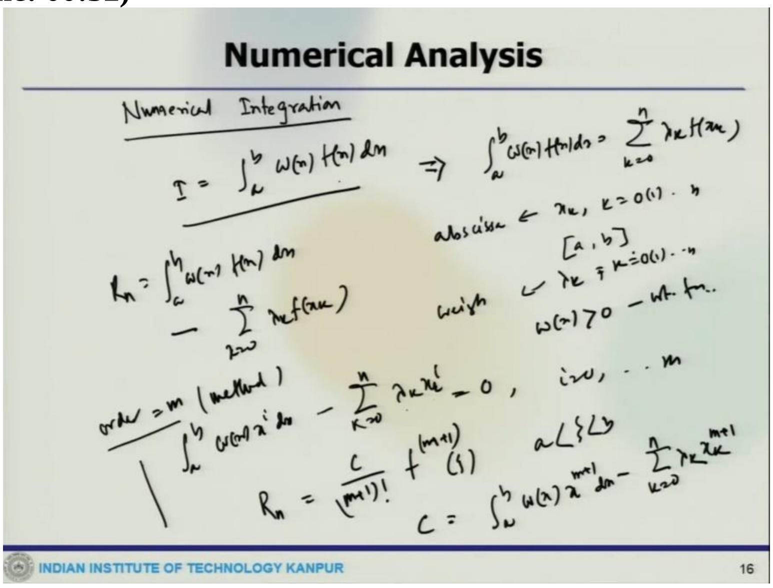

So let us start with the numerical integration part. So, let us say we have an integral, which is let us say function within that

$$I = \int_a^b w(x) f(x) dx$$

so, this is what we have to integrate. So, now this is what we have to get numerically. Now, by the finite linear combination of the values $f(x)$, this can be written as like this

$$\int_a^b w(x) f(x) dx = \sum_{k=0}^{n} \lambda_k f(x_k)$$

So, where x_k and k goes from 0 to n is called the abscissa or nodes which are distributed within the limit of integration between a and b.

And λ_k would be where k goes from 1 to n, which is called the weights. So, this is called abscissa and this is called the weight. The integration method of the quadrature rule where the $w(x) > 0$ this is called the weights function. So, the error of the integration is given us that

$$R_n = \int_a^b w(x)f(x)dx - \sum_{k=0}^{n} \lambda_k f(x_k)$$

An integration method of this is said to be order p, if it produces exact result, where $R_n = 0$. So, this is what we are going to get now, for a method of order m. Now, let us say we take an order m that is the method. So, in that case, what we get

$$\int_a^b w(x)x^i dx - \sum_{k=0}^{n} \lambda_k f\left({x_k}^i\right) = 0$$

for i goes from 0 to m. Now, here the weights are λ_k and the abscissas are x_k. And so, error would be

$$R_n = \frac{C}{(m+1)!} f^{(m+1)}(\xi)$$

where $a < \xi < b$ and C is nothing but

$$C = \int_a^b w(x)x^{m+1}dx - \sum_{k=0}^{n} \lambda_k f({x_k}^{m+1})$$

So, this is what you get for a method with the order of m, you get this kind of error and the integration values.

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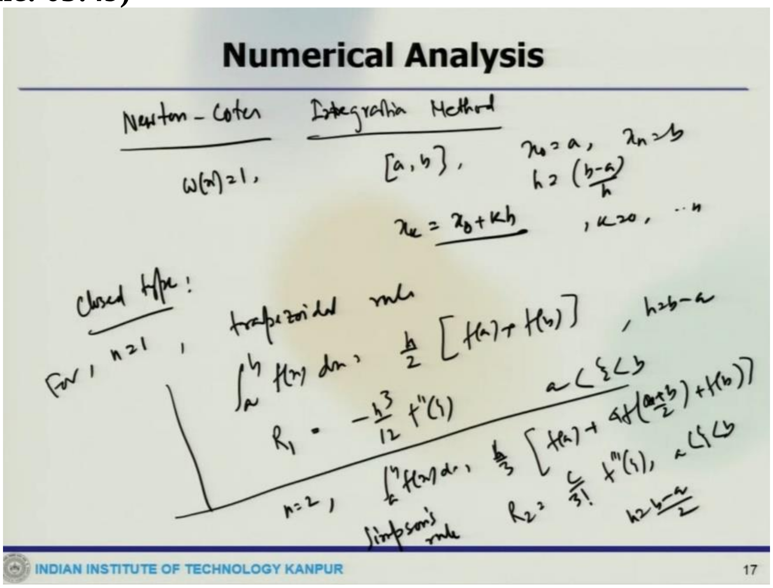

Now, the one first we are going to look at is the Newton cotes integration method. So, these are different ways one can do that Newton cotes integration method. So, now, in this case here

$w(x) = 1$ and the nodes x_k's are uniformly distributed between a and b. So, $x_0 = a$ and $x_n = b$ and the spacing is $h = \frac{b-a}{n}$. Since the nodes all these x_k's can be represented as

$$x_k = x_0 + kh$$

where k goes from 0 to n.

This method is called the Newton cotes integration method, where we can determine the weights of that λ case. Now, there are 2 types one could be close type. So, let us look at the close type and in the closed type what happens that n = 1 for n = 1 we get the trapezoidal rule which says

$$\int_a^b f(x)dx = \frac{h}{2}[f(a) + f(b)]$$

and where $h = b - a$ and the error term

$$R_1 = -\frac{h^3}{12}f''(\xi)$$

where $a < \xi < b$.

Now, similarly, you can have different order of n so, this is how for n = 2 you get it. Now, for example, you can also do it for n = 2 like if it is n = 2 then what you get like this

$$\int_a^b f(x)dx = \frac{h}{3}[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)]$$

and

$$R_2 = \frac{C}{3!}f'''(\xi)$$

where $a < \xi < b$ and $h = \frac{b-a}{2}$.

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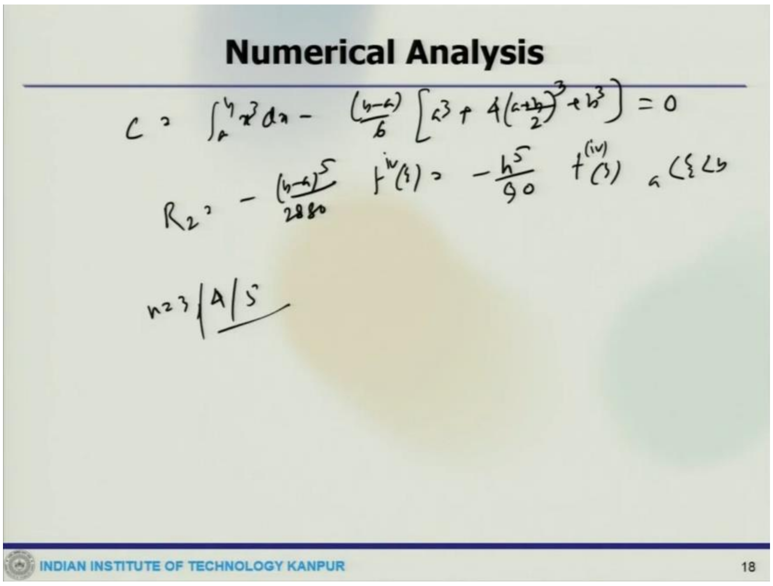

So, now the error term is given so, in this case the C would be

$$C = \int_a^b x^3 dx - \frac{(b-a)}{2}\left[a^3 + 4\left(\frac{a+b}{2}\right)^3 + b^3\right] = 0$$

So, we can see we can find out and finally, we get that

$$R_2 = -\frac{(b-a)^5}{2880} f''''(\xi) = -\frac{h^5}{90} f''''(\xi)$$

where $a < \xi < b$. Now, similarly, you can get for different order n like n could be 3, 4, 5 like that and you can get all these different terms.

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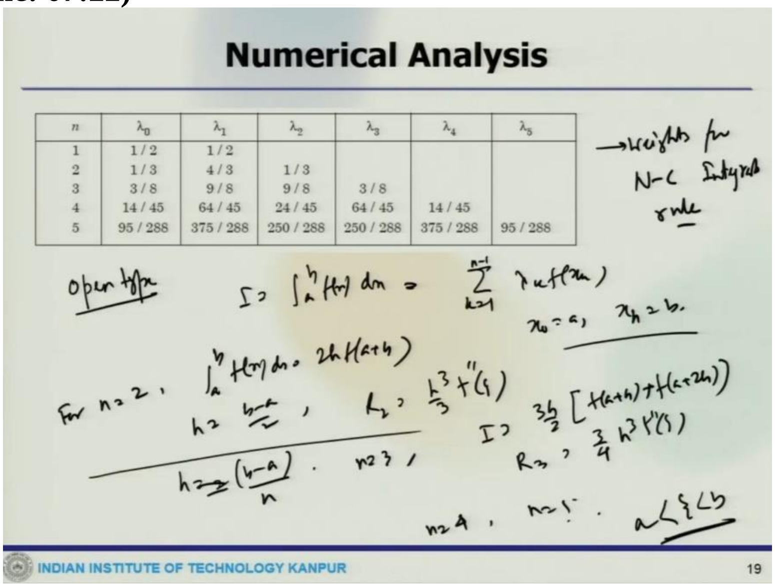

Like you can see here this is for weights for Newton cotes integration rule. So, what you get here is that different weights and for different order of accuracy of the method. So, there could be another option will be the open type method. Now, in open type method, your integral is

$$I = \int_a^b f(x)dx = \sum_{k=1}^{n-1} \lambda_k f(x_k)$$

So, here $x_0 = a$ and $x_n = b$ which are these are the 2 points which are actually excluded.

So, for example, for n = 2 you get this integral

$$\int_a^b f(x)dx = 2hf(a+b)$$

Where, $h = \frac{b-a}{2}$ and the error would be

$$R_1 = -\frac{h^3}{12} f''(\xi)$$

Similarly, for I mean so, that means, h is in generally it is $h = \frac{b-a}{n}$. And we can devise n = 3 where

$$I = \frac{3h}{2}[f(a+h) + f(a+2h)]$$

And

$$R_3 = \frac{3}{4} h^3 f''(\xi)$$

Similarly, n 4 or n 5 you can get where $a < \xi < b$. So, no matter what is the order of these things, you can always find out in those.

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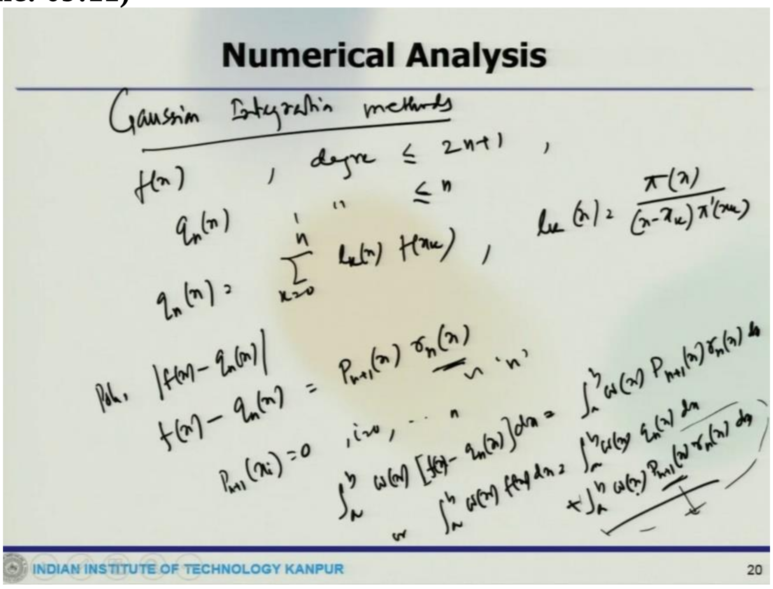

Now, we go to Gaussian integration methods. So, these are slightly different ways one can do a when both the nodes and the weights in the integration methods are to determine these are called the Gaussian integration method. So, in this case, like let us say $f(x)$ you have a polynomial of degree less than or equals to, so, degree is less than equals to (2n + 1). Then

$q_n(x)$ with a lag range interpolating polynomial of degree which is less than equals to n then what we can write that

$$q_n(x) = \sum_{k=0}^{n} l_k(x)\, f(x_k)$$

Where

$$l_k(x) = \frac{\pi(x)}{(x - x_k)\pi'(x_k)}$$

so, the polynomial $|f(x) - q_n(x)|$ has 0 at x_0, x_1 and x_n hence, we can write that

$$f(x) - q_n(x) = P_{n+1}(x) r_n(x)$$

and $r_n(x)$ is a polynomial of almost a degree almost n and

$$P_{n+1}(x^i) = 0$$

for i 0 to n. Now, when you integrate this what do we get

$$\int_a^b w(x)[f(x) - q_n(x)]dx = \int_a^b w(x) P_{n+1}(x) r_n(x) dx$$

or we can write

$$\int_a^b w(x) f(x) dx = \int_a^b w(x) q_n(x) dx + \int_a^b w(x) P_{n+1}(x) r_n(x) dx$$

So, this is what we can write the second integral this term here is 0 if $P_{n+1}(x)$ is an orthogonal polynomial. So, if this is orthogonal so, this goes to 0 and so, this is orthogonal means this is orthogonal with respect to the weight function w then this goes to essentially 0.

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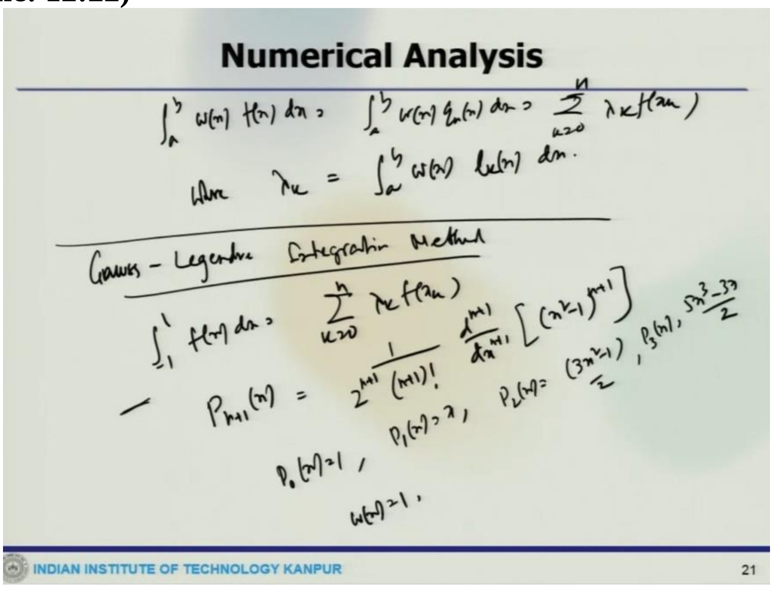

So, then what we have is that

$$\int_a^b w(x)f(x)dx = \int_a^b w(x)q_n(x)dx = \sum_{k=0}^{n} \lambda_k f(x_k)$$

Where

$$\lambda_k = \int_a^b w(x)l_k(x)dx$$

So, now, what you can have been that you can see how we can write all these things. Now, we can say some Gauss Legendre integration method. So, in this case, we will consider the integration rule

$$\int_{-1}^{1} f(x)dx = \sum_{k=0}^{n} \lambda_k f(x_k)$$

now, the nodes x case are 0 for Legendre polynomials.

So, here x_k's are 0 so, the polynomial we have is

$$P_{n+1}(x) = \frac{1}{2^{n+1}(n+1)!}\frac{d^{n+1}}{dx^{n+1}}[(x^2-1)^{n+1}]$$

The first few Legendre polynomials which are kind of given which is

$$P_0(x) = 0, P_1(x) = x, P_2(x) = \frac{(3x^2-1)}{2}, P_3(x) = \frac{(5x^3-3x)}{2}$$

and so on. So, the Legendre polynomials are orthogonal with respect to the weight function $w(x) = 1$. Now, the methods which we say it here are called the gauss Legendre integration method.

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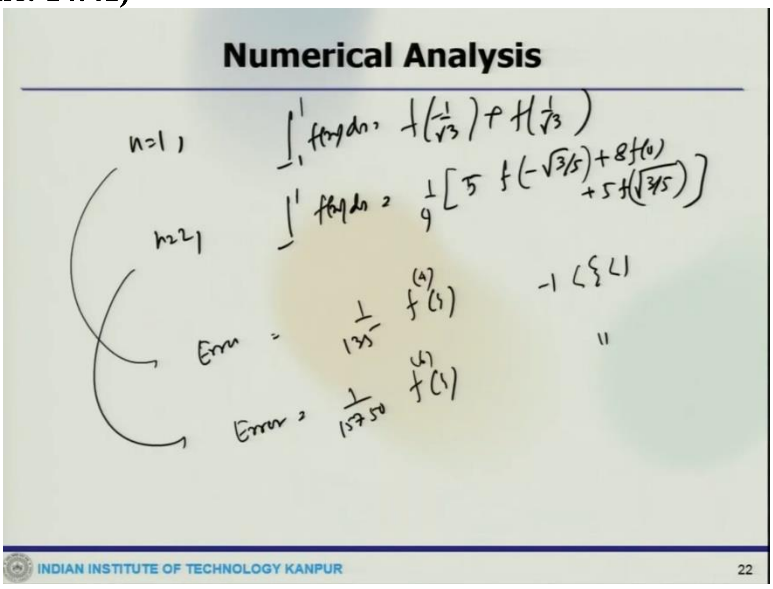

And we can get, for example, let us say we can write for n = 1 we get this is

$$\int_{-1}^{1} f(x)dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

for similarly, n = 2, we get

$$\int_{-1}^{1} f(x)dx = \frac{1}{9}\left[5f\left(-\frac{\sqrt{3}}{5}\right) + 8f(0) + 5f\left(\frac{\sqrt{3}}{5}\right)\right]$$

like this and there are also error terms which are associated with that for n = 1 the error would be

$$error = \frac{1}{135} f^{(4)}(\xi)$$

where $-1 < \xi < 1$ this case the error would be

$$error = \frac{1}{15750} f^{(6)}(\xi)$$

where $-1 < \xi < 1$.

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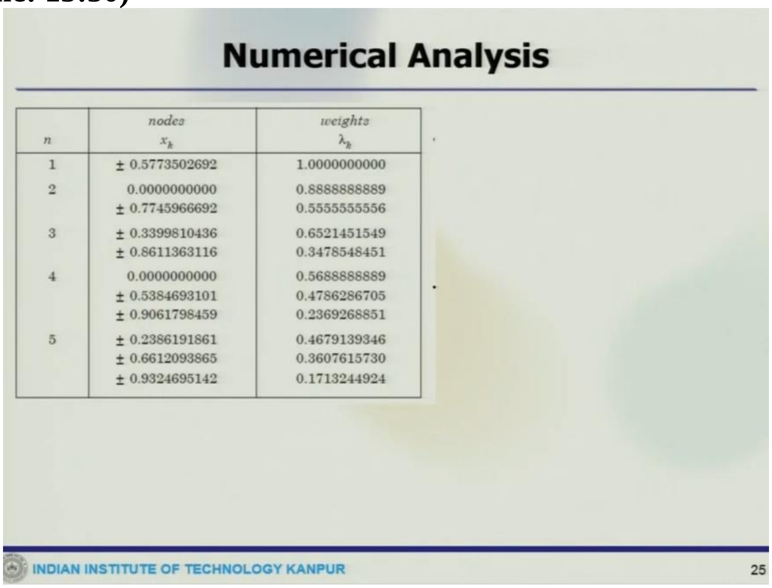

n	nodes x_k	weights λ_k
1	± 0.5773502692	1.0000000000
2	0.0000000000	0.8888888889
	± 0.7745966692	0.5555555556
3	± 0.3399810436	0.6521451549
	± 0.8611363116	0.3478548451
4	0.0000000000	0.5688888889
	± 0.5384693101	0.4786286705
	± 0.9061798459	0.2369268851
5	± 0.2386191861	0.4679139346
	± 0.6612093865	0.3607615730
	± 0.9324695142	0.1713244924

So, the nodes and the corresponding weight of this particular method which you can see it here. So, this is for different n 1, 2, 3, 4, 5 and like that and these are the weights what you find out and these are the nodes. So, this is what you can get for Gauss Legendre.

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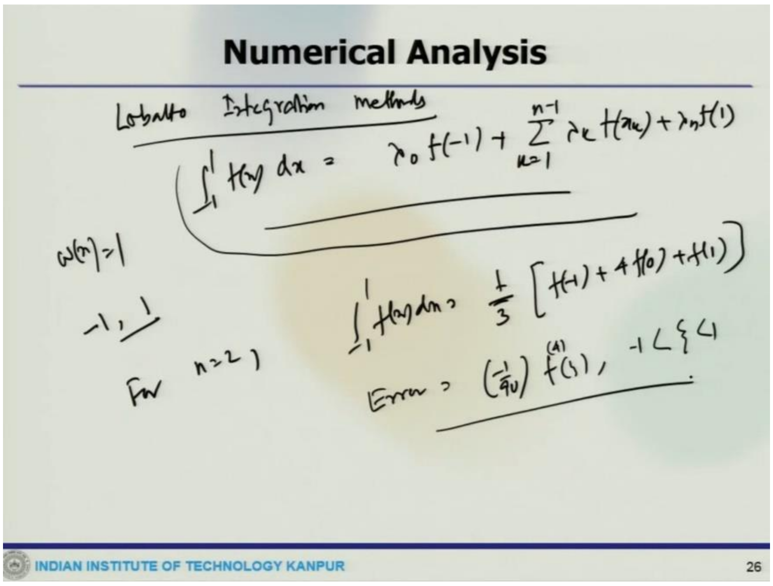

Now, there is another one which is also known as a Lobatto integration method. So, these are different methods which one can apply for doing the numerical integration and this case also weight can write the function

$$\int_{-1}^{1} f(x)dx = \lambda_0 f(-1) + \sum_{k=1}^{n-1} \lambda_k f(x_k) + \lambda_n f(1)$$

So, this is called Lobatto integration these things in this case also weight function $w(x) = 1$ and there are 2 endpoints, which is - 1 and 1 these are taken as nodes and then rest of the nodes which can be integrated like this.

So, for example, if n = 2, then we obtain a method like

$$\int_{-1}^{1} f(x)dx = \frac{1}{3}[f(-1) + 4f(0) + f(1)]$$

where error would be

$$Error = -\frac{1}{90} f^{(4)}(\xi)$$

where $-1 < \xi < 1$

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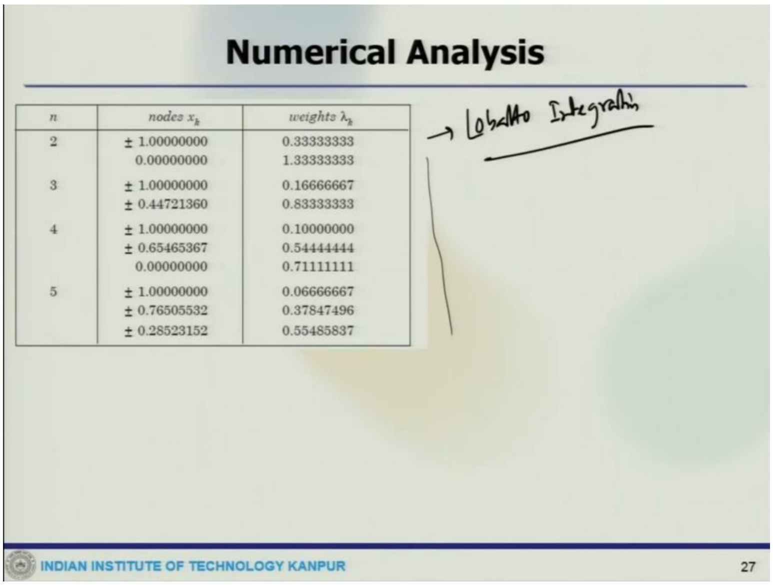

So, similarly, you can see these are the things for this is for Lobatto integration nodes and the weights in that integration. So, this is what you get for different nodes and integration points where you can have like.

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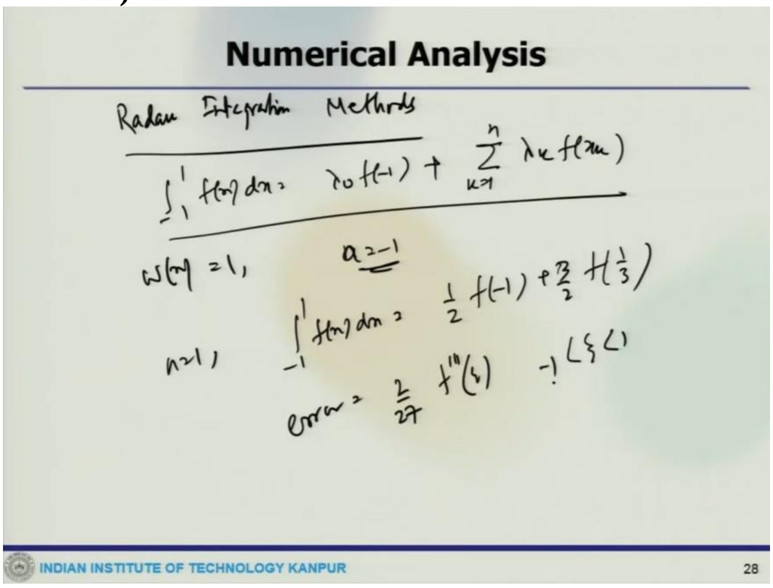

Now, similarly, you may have like Radau integration method these are different methods where the different weights are used. And one can always check where again this was again the

$$\int_{-1}^{1} f(x)dx = \lambda_0 f(-1) + \sum_{k=1}^{n-1} \lambda_k\, f(x_k)$$

this is how it is written here the weight function is 1 and the lower limit that a = - 1 taken as a node, the remaining end nodes are determined. So, this is called Radau here, if it is n = 1, then this guy becomes

$$\int_{-1}^{1} f(x)dx = \frac{1}{2} f(-1) + \frac{3}{2} f\left(\frac{1}{3}\right)$$

and where error could be

$$Error = \frac{2}{27} f'''(\xi)$$

where $-1 < \xi < 1$.

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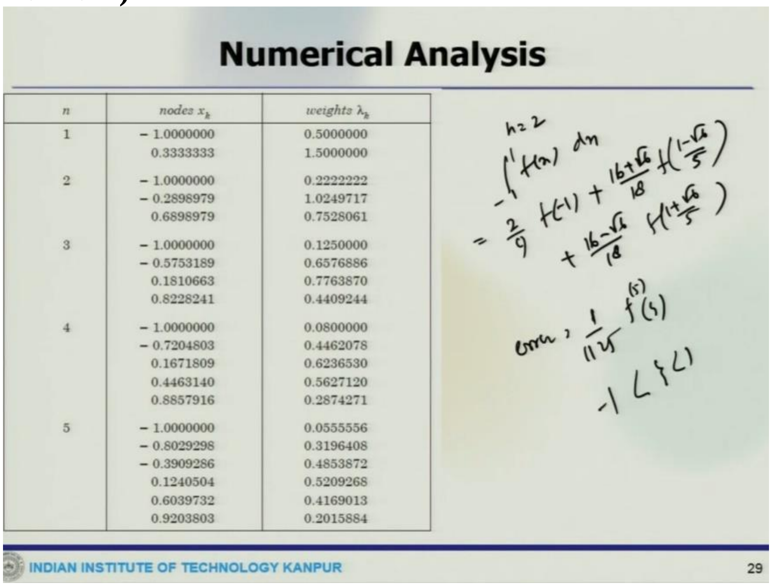

n	nodes x_k	weights λ_k
1	− 1.0000000	0.5000000
	0.3333333	1.5000000
2	− 1.0000000	0.2222222
	− 0.2898979	1.0249717
	0.6898979	0.7528061
3	− 1.0000000	0.1250000
	− 0.5753189	0.6576886
	0.1810663	0.7763870
	0.8228241	0.4409244
4	− 1.0000000	0.0800000
	− 0.7204803	0.4462078
	0.1671809	0.6236530
	0.4463140	0.5627120
	0.8857916	0.2874271
5	− 1.0000000	0.0555556
	− 0.8029298	0.3196408
	− 0.3909286	0.4853872
	0.1240504	0.5209268
	0.6039732	0.4169013
	0.9203803	0.2015884

So, these are the different. So, one can see what happens to n = 2 that this is written as

$$\int_{-1}^{1} f(x)dx = \frac{2}{9} f(-1) + \frac{16+\sqrt{6}}{18} f\left(\frac{1-\sqrt{6}}{5}\right) + \frac{16-\sqrt{6}}{18} f\left(\frac{1+\sqrt{6}}{5}\right)$$

and here the error will be

$$Error = \frac{1}{1125} f^{(5)}(\xi)$$

So, similarly, n could be 4 or 5 or 3 whatever it is and you can find out all the different weight functions for this kind of system.

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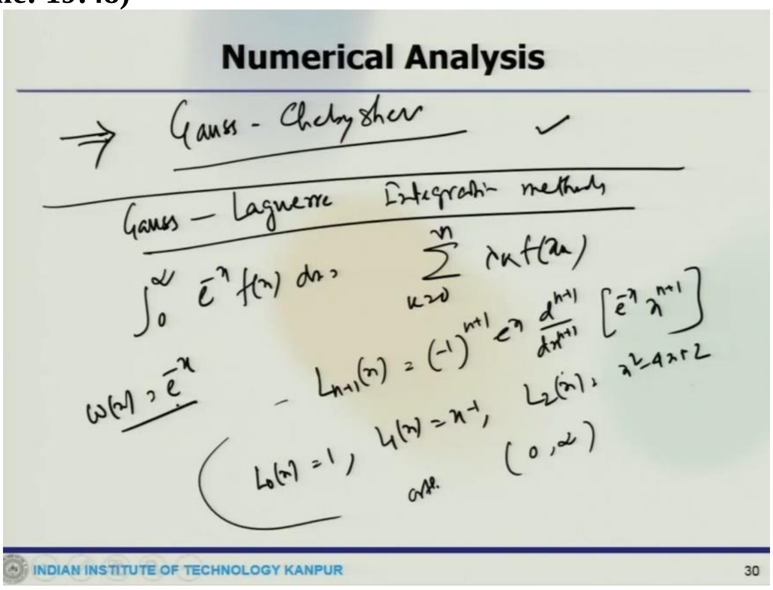

Now, there one can also look at I mean that we one can look at the textbook that Gauss Chebyshev. So, that is also one of the integration methods that one can look at but we can look at slightly another one to this you can check in textbook these are also another way of doing that, we look at Gauss Laguerre integration method. So, this is slightly different here, we consider the integral let us say

$$\int_0^{\infty} e^{-x} f(x)dx = \sum_{k=0}^{n} \lambda_k f(x_k)$$

here the weight function is given as e^{-x}, which is the weight function, and x_k's are the 0 for polynomial, which is

$$L_{n+1}(x) = (-1)^{n+1} e^x \frac{d^{n+1}}{dx^{n+1}} [e^{-x} x^{n+1}]$$

sum of the term like $L_0(x) = 1, L_1(x) = x^{-1}, L_2(x) = x^2 - 4x + 2$ and so on. Now, this is Laguerre polynomial is orthogonal on so this is orthogonal on $(0, \infty)$ with respect to the weight function e^{-x}.

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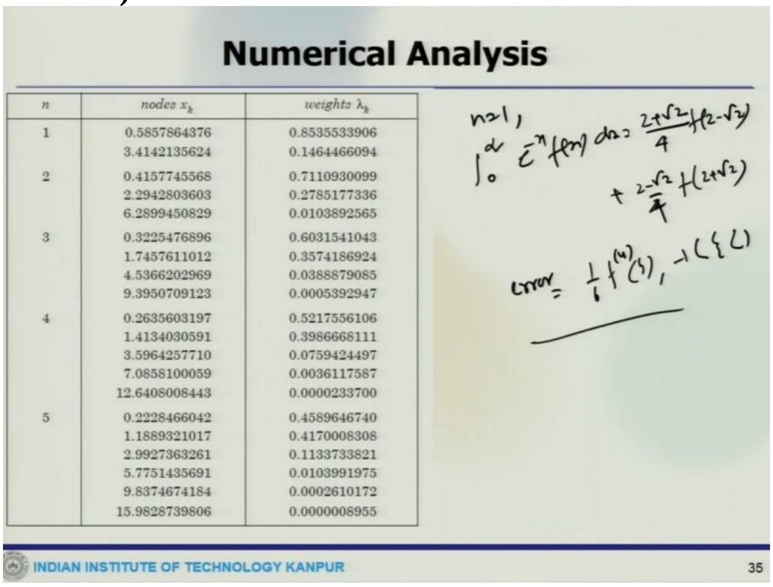

So, the integration method for let us say, for n = 1 what we can write that

$$\int_0^{\infty} e^{-x} f(x)dx = \frac{2+\sqrt{2}}{4} f\big(2-\sqrt{2}\big) + \frac{2-\sqrt{2}}{4} f(2+\sqrt{2})$$

and the error which is associated with that this would be

$$Error = \frac{1}{6} f^{(4)}(\xi)$$

where $-1 < \xi < 1$.

So, you can see for different n what could be the nodes and what do you even get that like different weight function for that kind of things.

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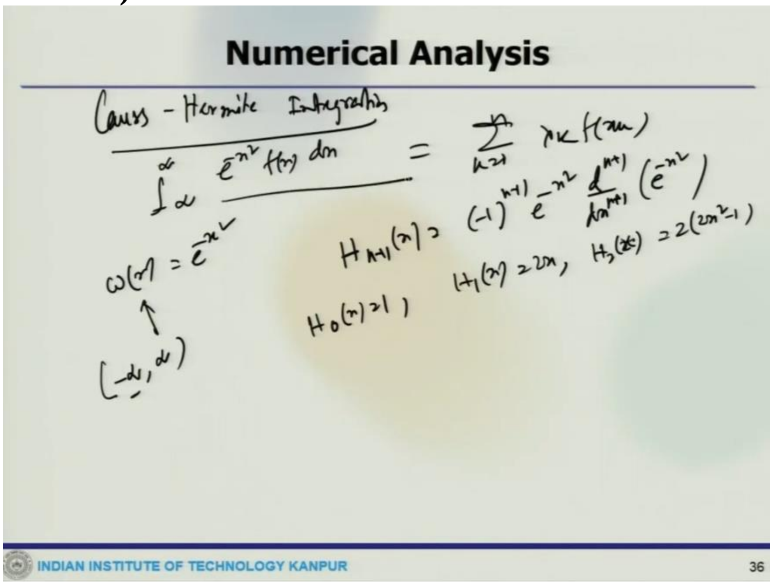

So, now, another is which we can quickly look is that Gauss Hermite integration. So, in that case, the function is integrated between

$$\int_{-\infty}^{\infty} e^{-x^2} f(x)dx = \sum_{k=1}^{n} \lambda_k f(x_k)$$

where the weight function here e^{-x^2} and the x_k are the nodes or the roots of the Hermite polynomial and which is given as

$$H_{n+1}(x) = (-1)^{n+1} e^{-x^2} \frac{d^{n+1}}{dx^{n+1}} \left[e^{-x^2}\right]$$

Some of the terms like $H_0(x) = 1, H_1(x) = 2x, H_2(x) = 2(2x^2 - 1)$ and so on. So, the Hermite polynomial is orthogonal to this weight function in between in the domain minus infinity to plus infinity. So, the Gauss Hermite integration method can be obtained like that.

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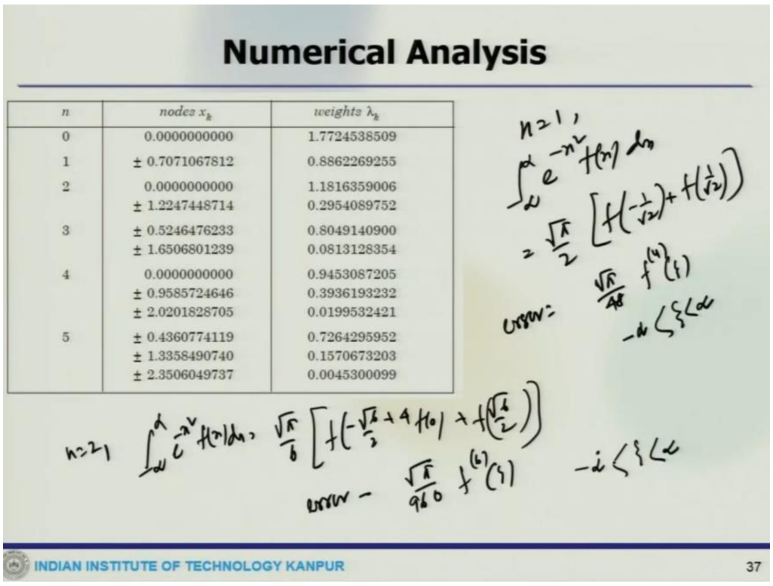

So, these are also the nodes for that, and for let us say n = 1. We can say

$$\int_{-\infty}^{\infty} e^{-x^2} f(x)dx = \frac{\sqrt{\pi}}{2}\left[f\left(-\frac{1}{\sqrt{2}}\right) + f\left(\frac{1}{\sqrt{2}}\right)\right]$$

where the error which is associated with that is

$$Error = \frac{\sqrt{\pi}}{48} f^{(4)}(\xi)$$

so, that is how you get it. And similarly, for n = 2, one can write like this as shown on the screen and these are the different integration rule.

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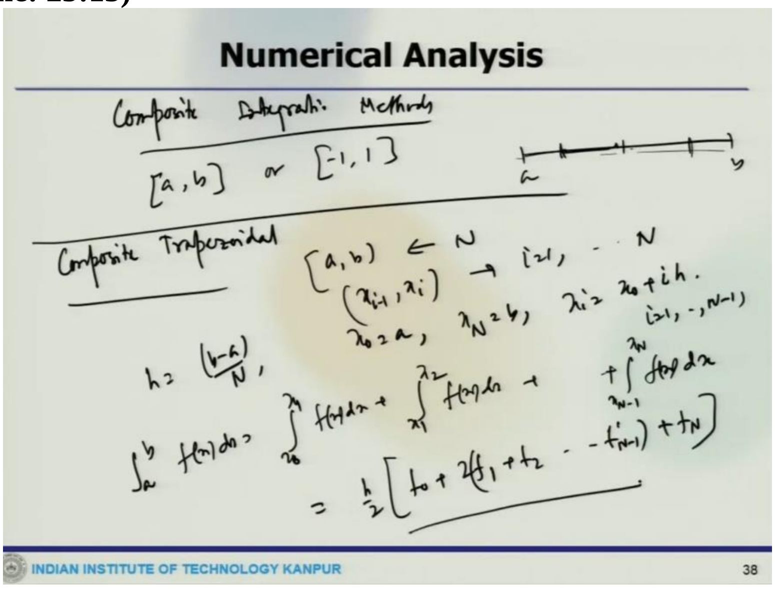

So, now, we can see one quicker thing which is called composite integration method. So, which is like that to avoid the use of higher order methods and still obtain accurate result. We can use composite integration methods. So, let us say we divide the interval $[a, b]$ or $[-1,1]$,into number of sub interval and evaluate the integral in each sub interval. So, for example, we can have similarly composite trapezoidal method.

So, that means, the whole interval between (a, b) are divided into multiple intervals and every interval you get the rule. So, for example, (a, b) which is divided by N sub interval. So, we get the sub intervals are (x_{i-1}, x_i) which are i goes to 1 to n and h would be $h = \frac{b-a}{N}$ where $x_0 = a$ $x_N = b$ and $x_i = x_0 + ih$, i from 1 to n - 1. So, what we can get is that

$$\int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{N-1}}^{x_N} f(x)dx$$

So, evaluating each integral and using the trapezoidal rule and this side will give you

$$= \frac{h}{2}\left[f_0 + 2\left(f_1 + f_2 + \cdots + f'_{N-1}\right) + f_N\right]$$

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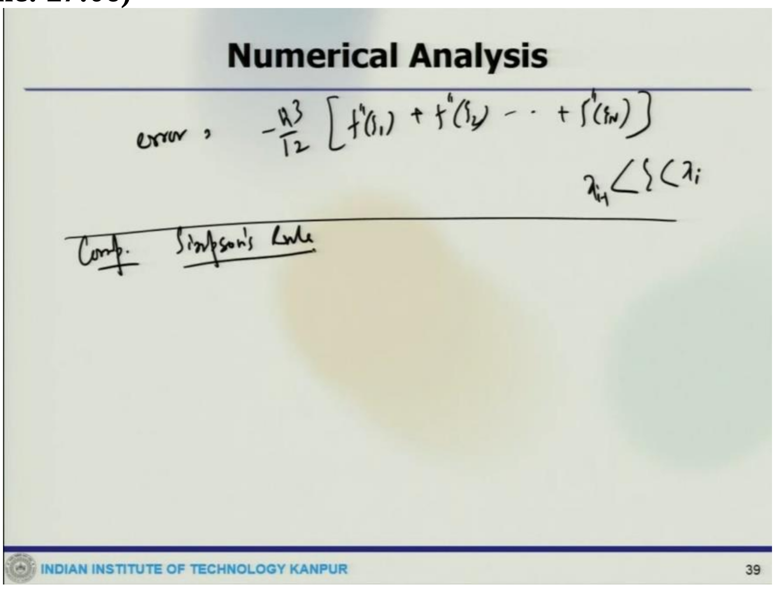

So, this is what you get and the error which would be associated with that

$$error = -\frac{h^3}{12}[f''(\xi_1) + f''(\xi_2) + \cdots + f''(\xi_N)]$$

where $x_{i-1} < \xi < x_i$. So, this is what you get and similarly, you can have composite Simpson's rule. So, this case also so we can have similarly the composite Simpson’s rule and where we can get this integration done.

So, you see that when you have this whole thing just instead of going for, I mean there are different order methods. And you can see instead of going for higher order methods, you can divide into multiple sub interval like this and get the integration done. So, we will stop here and this composite Simpson rule and another small portion like double integration we will look at in the next session before continuing with the other discussion.