

Numerical Methods and Computation

Prof. S.R.K. Iyengar

Department of Mathematics

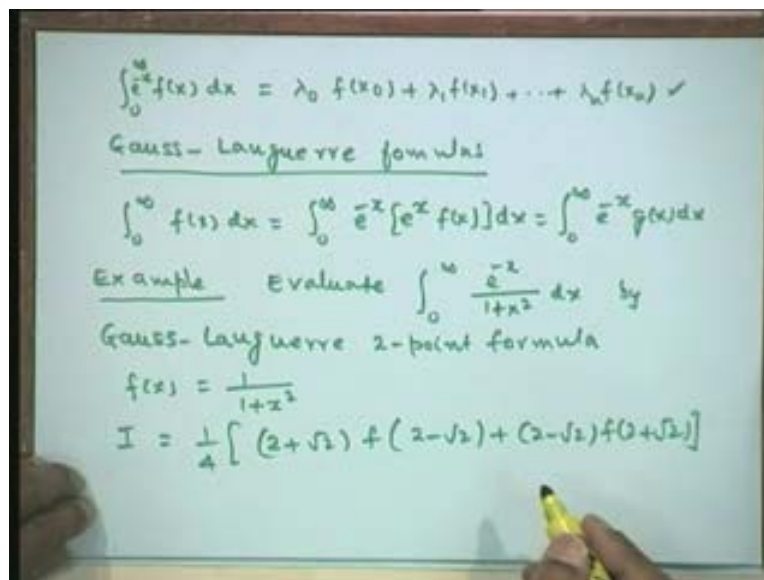
Indian Institute of Technology Delhi

Lecture No - 41

Numerical Differentiation and Integration (Continued)

Now in the previous lecture we have derived numerical integration formulas for evaluating an improper integral and the improper integral that we have considered was of the form 0 to infinity $F(x) dx$ and for evaluating this integral we have written a formula of the type $\lambda_0 f(x_0)$ plus $\lambda_1 f(x_1)$ plus so on plus $\lambda_n f(x_n)$.

(Refer Slide Time: 01:12)



$$\int_0^{\infty} f(x) dx = \lambda_0 f(x_0) + \lambda_1 f(x_1) + \dots + \lambda_n f(x_n) \checkmark$$

Gauss-Laguerre formula

$$\int_0^{\infty} f(x) dx = \int_0^{\infty} e^{-x} [e^x f(x)] dx = \int_0^{\infty} e^{-x} g(x) dx$$

Example Evaluate $\int_0^{\infty} \frac{e^{-x}}{1+x^2} dx$ by Gauss-Laguerre 2-point formula

$$f(x) = \frac{1}{1+x^2}$$
$$I = \frac{1}{4} [(2+\sqrt{2}) f(2-\sqrt{2}) + (2-\sqrt{2}) f(2+\sqrt{2})]$$

The formulas that we derived we call them as a Gauss Laguerre quadrature rules and these formulas depend on the Laguerre orthogonal polynomials. We have derived the 1 point 2 point formulas and we have use the weight function here as exponential of minus x. If the weight function is not available we said we shall supply the weight function so that we can use this formula so that we write it as exponential of minus x into exponential of x $f(x) dx$ and then we consider this as the new function as 0 to infinity exponential of minus x $g(x) dx$, then we can apply the formula that we have derived here on this new function. Now let us illustrate it by

taking an example on this, so let us take this example. Evaluate, let us take a simple example exponential of minus x upon 1 plus x square dx; let us take 1 plus x square by let us give the formula also Gauss Laguerre 2 point formula. Now here we have been provided in the suitable form therefore we simply have f(x) is equal to 1 upon 1 plus x square. Therefore I can evaluate the integral by using the 2 point formula, the 2 point formula we had written was 1 upon 4 [(2 plus root 2) f of (2 minus root 2) plus (2 minus root 2) into f of (2 plus root 2)]. Now would like to substitute this in the function and then simply evaluate them.

(Refer Slide Time: 03:51)

The whiteboard shows the following handwritten work:

$$= \frac{1}{4} \left[(2+\sqrt{2}) \frac{1}{[1+(2-\sqrt{2})^2]} + (2-\sqrt{2}) \frac{1}{[1+(2+\sqrt{2})^2]} \right]$$

$$= \frac{1}{4} [2.54195 + 0.04628] = 0.64706$$

Example Evaluate $\int_0^{\infty} \frac{1}{x^2+1} dx$ using 2-point Gauss-Laguerre formula

$$\int_0^{\infty} \frac{dx}{1+x^2} = \int_0^{\infty} e^{-x} \left(\frac{e^x}{1+x^2} \right) dx$$

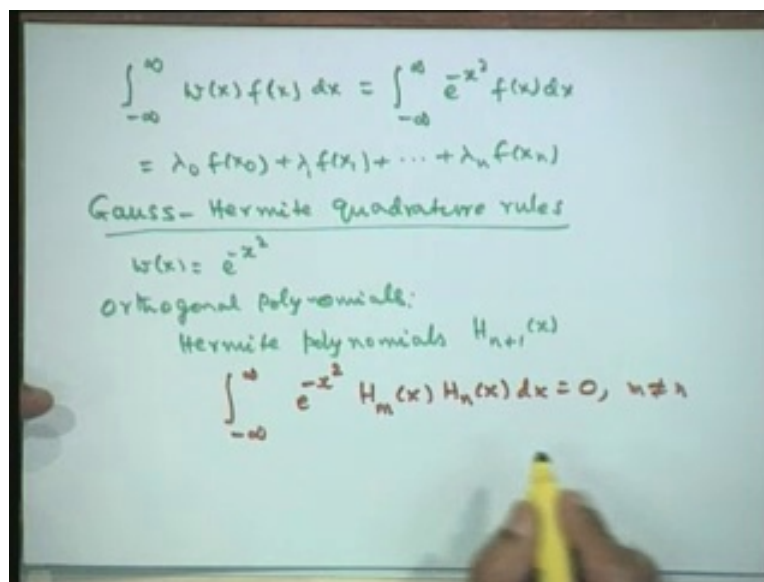
$$f(x) = \frac{e^x}{1+x^2}$$

$$I = \frac{1}{4} \left[(2+\sqrt{2}) \frac{e^{2-\sqrt{2}}}{1+(2-\sqrt{2})^2} + (2-\sqrt{2}) \frac{e^{2+\sqrt{2}}}{1+(2+\sqrt{2})^2} \right]$$

So what we would therefore have this is equal to 1 upon 4 [2 plus root 2 and 1 upon [1 plus (2 minus root 2)] whole squared plus (2 minus root 2) into 1 upon [1 plus (2 plus root 2)] whole square]. We just simplify this and that is the required solution 1 upon 4, this actually comes out to be [2 point 5 4 1 4 5 plus 0 point 0 6 2 8] and this is point 6 4 7 0 6. This result may not be of the required accuracy, the computation can be done using the 3 point or the 4 point formulas. The computation can be stopped when the magnitude of the difference of 2 successive values of the integral is less than the given tolerance. Now let us take an example in which the weight function is not given to us, is not provided in the suitable form. Evaluate 0 to infinity 1 upon x square plus 1 dx, using the 2 point Gauss Laguerre formula. Now here I have not been provided the weight function so therefore we would write this given integral as dx upon 1 plus x square as equal to 0 to infinity exponential of minus x into exponential x upon 1 plus x square dx. Now we choose this as our function f(x), therefore f(x) is e to the power of x upon 1 upon 1 plus x square. Now we shall use f(x) as exponential x divided by 1 plus x square in the 2 point rule that we have derived earlier.

So the value of the integral I is 1 upon 4 [(2 plus root 2) into exponential of 2 minus root 2 by 1 plus (2 minus root 2) whole squared, (2 minus root 2) exponential of 2 plus root 2 by 1 plus (2 plus root 2) whole square]. This can be evaluated and I will give the result, you can compute it, this comes out to be 1 point 4 9 3 2 6. Now in this case you can actually compare your solution with the exact solution, we have taken it any way, this is simply tan inverse of x 1 upon 1 plus x square so I will have this, our exact result as tan inverse of x from 0 to infinity, tan inverse of infinity is pi by 2 and tan inverse of 0 is equal to 0, so pi by 2 is the exact solution in this problem, this is possibly 1 point 5 something, so we can compare the 2 results. Notice that the abscissas (2 plus root 2) and (2 minus root 2) are not covering the domain 0 to infinity sufficiently, here it is like approximating infinity at 2 plus root 2. To obtain more accurate results we should choose formulas with more abscissas; then the abscissas cover a larger domain. The largest value of the abscissa can be sufficiently big for a higher order formula for example if we have n is equal to 5 that is a 6 point formula, the largest abscissa is 15 point 9 8. The largest weight corresponds to the smallest abscissa, the values of the weights decrease with respect to the larger abscissas; the smallest weight is obtained corresponding to the largest abscissa.

(Refer Slide Time: 08:38)



Handwritten mathematical notes on a whiteboard:

$$\int_{-\infty}^{\infty} w(x) f(x) dx = \int_{-\infty}^{\infty} e^{-x^2} f(x) dx$$

$$= \lambda_0 f(x_0) + \lambda_1 f(x_1) + \dots + \lambda_n f(x_n)$$

Gauss-Hermite quadrature rules

$$w(x) = e^{-x^2}$$

Orthogonal Polynomials:

Hermite polynomials $H_{n+1}(x)$

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx = 0, \quad m \neq n$$

Now let us take the next improper integral that is evaluating minus infinity infinity of a particular form and we would consider the formulas of this particular type $w(x) f(x) dx$ and we shall choose $w(x)$ as exponential of minus x square, exponential of minus x squared $f(x) dx$ and this we would like to write again as $\lambda_0 f(x_0)$ plus $\lambda_1 f(x_1)$ plus so on $\lambda_n f(x_n)$. These groups of formulas are called the Gauss Hermite quadrature rules, these are called the Gauss Hermite quadrature rules, Gauss Hermite quadrature rules that means the weight function in this case is exponential of minus x square, the weight function is exponential of minus x square.

The orthogonal polynomials here are the Hermite polynomials, orthogonal polynomials or the Hermite polynomials which are denoted by $H_{n+1}(x)$. The orthogonal property of this Hermite polynomials is integral of minus infinity to infinity exponential of minus x square $H_m(x) H_n(x) dx$ is equal to 0 for m not equal to n, so this is the orthogonal property of the Hermite polynomials. Now let us define what is the Hermite polynomial, let us just a few of the Hermite polynomials.

(Refer Slide Time: 10:49)

$$\begin{aligned}
 &= \lambda_0 f(x_0) + \lambda_1 f(x_1) + \dots + \lambda_n f(x_n) \\
 &\text{Gauss-Hermite quadrature rules} \\
 &w(x) = e^{-x^2} \\
 &\text{Orthogonal polynomials:} \\
 &\text{Hermite polynomials } H_{n+1}(x) \\
 &\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx = 0, \quad m \neq n \\
 &H_{n+1}(x) = (-1)^{n+1} e^{x^2} \frac{d^{n+1}}{dx^{n+1}} (e^{-x^2}) \\
 &H_0 = 1
 \end{aligned}$$

The Hermite polynomial is defined as this, so $H_{n+1}(x)$ is given by minus 1 to the power of n plus 1 exponential of x square outside d^{n+1} upon dx^{n+1} of exponential of minus x square with H_0 is equal to 1. This is again similar to the Rodrigues formula for the Legendre polynomials which is also similar for the Laguerre polynomials, so all the Hermite polynomials can be generated just by using this particular formula. Let us take few of this and then construct our quadrature rules.

(Refer Slide Time: 11:35)

$$\begin{aligned}
 H_1(x) &= -e^{x^2} \frac{d}{dx} (e^{-x^2}) \\
 &= -e^{x^2} [e^{-x^2} (-2x)] = 2x \\
 H_2(x) &= +e^{x^2} \frac{d^2}{dx^2} (e^{-x^2}) \\
 &= e^{x^2} \frac{d}{dx} [e^{-x^2} (-2x)] \\
 &= -2e^{x^2} [e^{-x^2} \cdot 1 + x e^{-x^2} (-2x)] \\
 &= 2[2x^2 - 1] = 4x^2 - 2 = 2[2x^2 - 1] \\
 H_3(x) &= 4(2x^3 - 3x)
 \end{aligned}$$

So let us write down what is our $H_1(x)$, I have to take n is equal to 0 over here so I will have minus sign here, exponential of x square d upon dx (exponential of minus x square). So I have this as exponential of x square, I differentiate this [exponential of minus x square (minus $2x$)], so $H_1(x)$ is simply $2x$. Now let us take one more polynomial $H_2(x)$ is, n is equal to 1 therefore I have a plus sign here then I have a exponential of x square d square upon dx square (exponential of minus x square). So let us evaluate this exponential of x square d upon dx [exponential of minus x square into (minus $2x$)]. Let us take this minus 2 outside and then have exponential of x square then I have differentiate this as a product so [exponential of minus x square into 1 plus x into e to the power of minus x square (minus $2x$)]. I have taken it as a product of x into exponential of minus x square, exponential of minus x square into 1 plus x into this product. Now exponential of x square again cancels and let us retain this 2 outside, take the minus sign inside [$2x$ minus 1], [$2x$ square minus 1] or we can write it as $4x$ square minus 2. Now this 2 is outside so let us retain 2 as the quantity that is outside. Now I can similarly show, let me just give what is this $H_3(x)$, it is 4 into ($2x$ cubed minus $3x$).

(Refer Slide Time: 14:00)

$$\begin{aligned}
 &= -e^{x^2} \left[e^{-x^2} (-2x) \right] = 2x \\
 H_2(x) &= +e^{x^2} \frac{d^2}{dx^2} (e^{-x^2}) \\
 &= e^{x^2} \frac{d}{dx} \left[e^{-x^2} (-2x) \right] \\
 &= -2 e^{x^2} \left[e^{-x^2} \cdot 1 + x e^{-x^2} (-2x) \right] \\
 &= 2 [2x^2 - 1] = 4x^2 - 2 = 2[2x^2 - 1] \\
 H_3(x) &= 4(2x^3 - 3x) \\
 \text{Abscissas: } &\text{zeros of } H_{n+1}(x) = 0 \\
 \text{Weights: } &\lambda_k = \int_{-\infty}^{\infty} \frac{e^{-x^2} H_{n+1}(x)}{(x - x_k) H'_{n+1}(x_k)} dx
 \end{aligned}$$

Now when once we write down these Hermite polynomials, let us now write down what are the abscissas in our quadrature rule, the abscissas are zeros of $H_{n+1}(x)$, zeros of $H_{n+1}(x)$ is equal to 0. And the weights as we have done last time we have used the Lagrange fundamental polynomial form so λ_k will be minus infinity to infinity the weight function exponential of minus x square $H_{n+1}(x)$ divided by $(x - x_k)$ into derivative of $H_{n+1}(x_k)$ dx . So these will be the weights for the Gauss Hermite quadrature rule. We have been using all through whether is Legendre, Chebyshev polynomials or the Laguerre formulas we have been using this as p_{n+1} and this is p_{n+1} prime of x_k , now let us obtain few rules.

(Refer Slide Time: 15:07)

1-point rule $n=0$, $H_1(x) = 2x$; $x_0=0$

$$\lambda_0 = \int_{-\infty}^{\infty} \frac{e^{-x^2} \cdot 2x}{x(2)} dx = \int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

$$\int_{-\infty}^{\infty} e^{-x^2} f(x) dx = \sqrt{\pi} f(0) : \text{Order: 1}$$

2-point rule $n=1$, $H_2(x) = 2(2x^2-1)$

Abscissas: $H_2(x)=0$, $x = \pm \frac{1}{\sqrt{2}}$

$$x_0 = -\frac{1}{\sqrt{2}}, x_1 = \frac{1}{\sqrt{2}}$$

$$H_2(x) = 4(x-x_0)(x-x_1)$$

So let us use this and write down the 1 point rule, 2 point rule and 3 point rule. So let us take 1 point rule that means n is equal to 0, $H_1(x)$ is equal to $2x$ we have taken. Therefore let us substitute λ_0 is minus infinity to infinity exponential of minus x square $2x$ by x minus x_0 therefore this is x , the zeros of this are, if you put it as equal to 0 we will simply get x_0 is equal to 0, as the abscissa of this. Now this is x minus x_0 that is x and derivative of this is simply 2. So $2 \times 2 \times x$ cancels, I simply have this as minus infinity to infinity exponential of minus x square dx . This we know that this is equal to root of pi. Therefore our integration rule is exponential of minus x square $f(x) dx$, if the weight is root pi f of abscissa is 0, f of 0 and the order of the formula is 1, order of the formula is 1. Now you can see it looks like a midpoint formula, 0 is the midpoint minus infinity to infinity, so it is almost like a midpoint formula that we have, so let us take a 2 point rule. So we have here n is equal to 1 therefore $H_1(x)$, $H_2(x)$ is equal to, $H_2(x)$ we have derived as 2 times $(2x^2 - 1)$ therefore the abscissas, let us write down the abscissas by putting $H_2(x)$ is equal to 0, we get from here x is equal to plus minus 1 upon root 2. Therefore I can take x_0 is equal to minus 1 upon root 2 and x_1 is 1 upon root 2. Then as we done in the previous cases let us write down this leading coefficient as 1, so let us take 4 outside so that I can write this as $(x - x_0)(x - x_1)$.

(Refer Slide Time: 18:07)

$$\begin{aligned}
 \lambda_0 &= \int_{-\infty}^{\infty} \frac{e^{-x^2} 4(x-x_0)(x-x_1)}{(x-x_0)^2 8x_0} dx \\
 &= \frac{1}{2x_0} \int_{-\infty}^{\infty} (e^{-x^2} x - e^{-x^2} x_1) dx \\
 &= -\frac{x_1}{2x_0} \int_{-\infty}^{\infty} e^{-x^2} dx = -\frac{x_1}{2x_0} \cdot \sqrt{\pi} \\
 \lambda_1 &= \frac{1}{2x_1} \int_{-\infty}^{\infty} (e^{-x^2} x - e^{-x^2} x_0) dx \\
 &= -\frac{x_0}{2x_1} \int_{-\infty}^{\infty} e^{-x^2} dx = -\frac{x_0}{2x_1} \cdot \sqrt{\pi}
 \end{aligned}$$

Now let us write down our weights, let us also, we also need our derivative, let us write down the derivative also, H_2 prime of x is equal to, let us take from here, this is equal to 8 times x , this is simply 8 times x . So let us write down λ_{00} that is minus infinity to infinity exponential of minus x square into, $H_2(x)$ is $(x \text{ minus } x_0)(x \text{ minus } x_1)$ divided by $(x \text{ minus } x_0)$ and derivative is 8 x therefore 8 x_0 . Now $(x \text{ minus } x_0)$ cancels with the $(x \text{ minus } x_0)$, let us take this constant outside so I will have 1 upon 2 times x_0 coming from here, this is minus infinity to infinity exponential of minus x square, let us open it into 2 integrals, into x minus exponential of minus x square into x_1 dx , just multiplied exponential of minus x square into x minus exponential of minus x square into x_1 . Now this is an odd function in minus infinity to infinity therefore the value of this integral corresponding to this is equal to 0, so only this will contribute and let us take minus x_1 outside, so I will have minus x_1 upon 2 x_0 minus infinity to infinity exponential of minus x square dx .

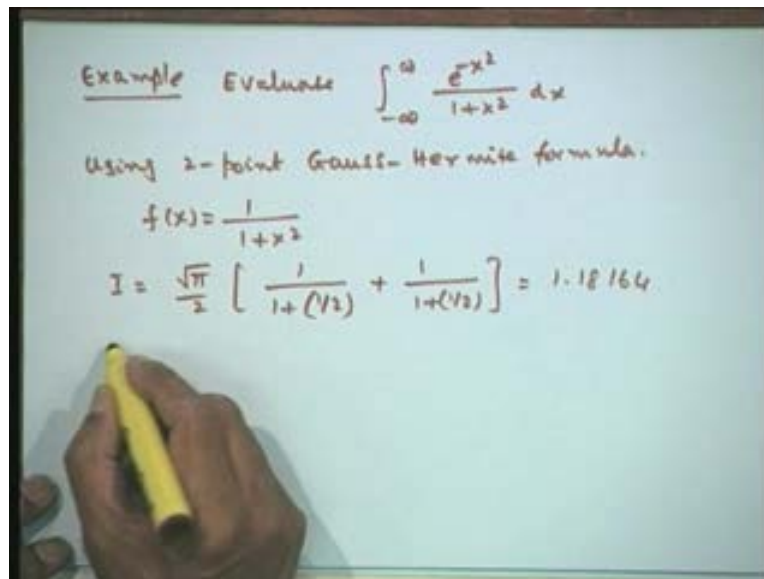
Now this is equal to, now let us take the ratio of x_1 and x_0 , these are in magnitude same, its ratio is minus 1, so the ratio is minus 1 so it will have plus half and this is root of π . Therefore we have λ_{00} is equal to root π by 2. Now λ_{01} , we can just look at this one, we have the numerator is same, denominator is $(x \text{ minus } x_1)$ and this is 8 x_1 therefore $(x \text{ minus } x_1)$ cancels and I will have x_1 here, so let us write down this particular step therefore this is 2 times x_1 minus infinity to infinity exponential of minus x square into x exponential of minus x square x_0 dx . So $(x \text{ minus } x_1)$ cancels with this, the numerator will be left out with the $(x \text{ minus } x_0)$, so that is $(x \text{ minus } x_0)$ denominator is equal to x_1 . Again for the same reason this is an odd function therefore the value of this first integral is again 0. I take minus x_0 out, so I will have x_0 upon 2 x_1 minus infinity to infinity exponential of minus x square dx and the ratio is minus 1 therefore again I get this as root π by 2.

(Refer Slide Time: 21:31)

$$\begin{aligned}
 &= -\frac{x_1}{2x_0} \int_{-\infty}^{\infty} e^{-x^2} dy = \frac{1}{2} \cdot \sqrt{\pi} \\
 \lambda_1 &= \frac{1}{2x_1} \int_{-\infty}^{\infty} (e^{-x^2} x - e^{-x^2} x_0) dy \\
 &= -\frac{x_0}{2x_1} \int_{-\infty}^{\infty} e^{-x^2} dy = \frac{\sqrt{\pi}}{2} \\
 \int_{-\infty}^{\infty} e^{-x^2} f(x) dx &= \frac{\sqrt{\pi}}{2} \left[f\left(-\frac{1}{\sqrt{2}}\right) + f\left(\frac{1}{\sqrt{2}}\right) \right] \\
 &\text{Order: 3}
 \end{aligned}$$

Therefore our formula is integral minus infinity to infinity exponential of minus x square f(x) dx, both the weights are same root pi by 2 [f of (minus 1 upon root 2) plus f of (1 upon root 2)] and the order of this formula is 3. Now you can see that these are evenly distributed symmetrically placed about the origin, this minus 1 upon root 2 and 1 upon root 2 are the two abscissas, now as you go to the 5 point formula or the odd ones if you take 9 point formula all of them would be symmetrically placed, 1 less than 0, 1 greater than 0, they are symmetrically placed about the origin and as we take the order of the formula higher and higher these value of this abscissa would grow larger and larger to more domain so that the result will be much more accurate.

(Refer Slide Time: 22:40)



The image shows a whiteboard with handwritten text and equations. At the top, it says 'Example Evaluate' followed by the integral $\int_{-\infty}^{\infty} \frac{e^{-x^2}}{1+x^2} dx$. Below this, it says 'using 2-point Gauss-Hermite formula.' Then, the function $f(x) = \frac{1}{1+x^2}$ is written. Finally, the integral is evaluated as $I = \frac{\sqrt{\pi}}{2} \left[\frac{1}{1+(1/2)} + \frac{1}{1+(1/2)} \right] = 1.18164$. A hand holding a yellow marker is visible at the bottom left of the whiteboard.

Example Evaluate $\int_{-\infty}^{\infty} \frac{e^{-x^2}}{1+x^2} dx$

using 2-point Gauss-Hermite formula.

$f(x) = \frac{1}{1+x^2}$

$I = \frac{\sqrt{\pi}}{2} \left[\frac{1}{1+(1/2)} + \frac{1}{1+(1/2)} \right] = 1.18164$

Let us take a simple example on this. Now in this case again if the weight function is not available, we shall provide the weight function for it. So let us take evaluate minus infinity to infinity exponential of minus x square upon 1 plus x square dx using 2 point Gauss Hermite formula. Now here it is given in the suitable form so we can straight away pick up what is our $f(x)$ that is one upon 1 plus x square. Therefore our given integral I is equal to, we shall use this particular formula that we have just written that is 2 point formula root pi by 2 f of minus 1 upon root 2 whole square that is simply 1 upon 2 plus 1 upon 1 plus (1 upon 2). I have taken 1 upon root 2 whole square written it as 1 upon 2 on this, so this comes out to be simply 1 point 1 8 1 6 4. Now so far we have derived number of formulas and then we said that these formulas have got precision $2n + 1$ or order $2n + 1$ which implies that these formulas would integrate exactly polynomials of degree less than or equal to $2n + 1$ that means if I set up the $f(x)$ is equal to 1, x, x square, x to the power of $2n + 1$, I will get the left hand side is equal to right hand side identity therefore it integrates exactly. Now **how is the**, how do we get the error terms for these equations, the error term is again **from first we shall** do it, let us just illustrate that as an example, how do we get the error term, in all these quadrature rules that we have derived.

(Refer Slide Time: 24:56)

using 2-point Gauss-Hermite formula.

$$f(x) = \frac{1}{1+x^2}$$
$$I = \frac{\sqrt{\pi}}{2} \left[\frac{1}{1+(1/\sqrt{2})} + \frac{1}{1+(1/\sqrt{2})} \right] = 1.18164$$

Error term?

Formulas of order $2n+1$

\therefore They integrate exactly pol. of degree $\leq 2n+1$

$$f(x) = 1, x, x^2, \dots, x^{2n+1}$$

Now as I said these are formulas of order $2n+1$ therefore they integrate, they integrate exactly polynomials of degree less than or equal to $2n+1$ that means if I take $f(x)$ is equal to $1, x, x^2$, so on x to the power $2n+1$, then these formulas will integrate exactly.

(Refer Slide Time: 25:43)

Sub. $f(x) = x^{2n+2}$ and find the error constant

$$C = \left[\int_a^b w(x) f(x) dx \right] - [\lambda_0 f(x_0) + \dots + \lambda_n f(x_n)]$$
$$R_{2n+2} = \frac{C}{(2n+2)!} f^{(2n+2)}(\xi), \quad a < \xi < b$$

Example Find the error term in the Gauss-Laguerre 2-point rule

$$\int_0^\infty e^{-x} f(x) dx = \frac{1}{4} [(2+\sqrt{2})f(2-\sqrt{2}) + (2-\sqrt{2})f(2+\sqrt{2})]$$

It is given that the formula is of order 3.

Now if I want the error term therefore, I should take the next power of x that means to get the error term I would take $f(x)$ is equal to x to the power $2n + 2$, $2n + 2$ and find out the error constant, therefore we substitute this and find the error constant and error constant is c and what is this c ? This c is equal to whatever the formula that we have here $\int_a^b w(x) f(x) dx$. Now this is one of these formulas that we have now derived this one and bring the right hand side to this, so this is $\lambda_{a0} f(x_0)$, $\lambda_{an} f(x_n)$. Now I am substituting $f(x)$ is equal to x to the power of $2n + 2$ here so I am replacing $f(x)$ by x to the power of $2n + 2$ and I am replacing all these by x to the power of $2n + 2$. This is our error constant then the error is given by R_{2n+2} , it will be $2n + 2$, this is equal to c upon $(2n + 2)$ factorial and $2n + 2$ derivative of ϕ , ϕ is lying between the a and b . This is the general procedure for every method that we pick up this order of the formula and then find out the error constant and write down our final error formula here, so let us illustrate it through an example.

So let us take this as an example, find the error term in the, let us take Gauss Laguerre, let us take Gauss Laguerre 2 point rule that is 0 to infinity exponential of minus x $f(x) dx$ is 1 upon 4 $[(2 + \sqrt{2}) f(2 - \sqrt{2}) + (2 - \sqrt{2}) f(2 + \sqrt{2})]$. It is given that it is of order 3, it is given that the formula is of order 3. Now since the formula is given to us as order 3 it is going to integrate exactly $f(x)$ is equal to 1 , x , x square, x cubed, therefore the error term should come from the next power that is $f(x)$ is equal to x to the power of 4.

(Refer Slide Time: 28:58)

Since the formula integrates polynomials of degree ≤ 3 exactly, set $f(x) = x^4$

$$c = \int_0^\infty e^{-x} x^4 dx - \frac{1}{4} \left[(2+\sqrt{2})(2-\sqrt{2})^4 + (2-\sqrt{2})(2+\sqrt{2})^4 \right]$$

$$= \left[-(x^4 + 4x^3 + 12x^2 + 24x + 24) e^{-x} \right]_0^\infty$$

$$- \frac{1}{4} \left[2(2-\sqrt{2})^3 + 2(2+\sqrt{2})^3 \right]$$

$$= 24 - \frac{1}{4} \left[(40 - 28\sqrt{2}) + (40 + 28\sqrt{2}) \right]$$

$$= 4$$

Error: $R_4 = \frac{c}{4!} f^{(4)}(\xi) = \frac{1}{6} f^{(4)}(\xi), 0 < \xi < \infty$

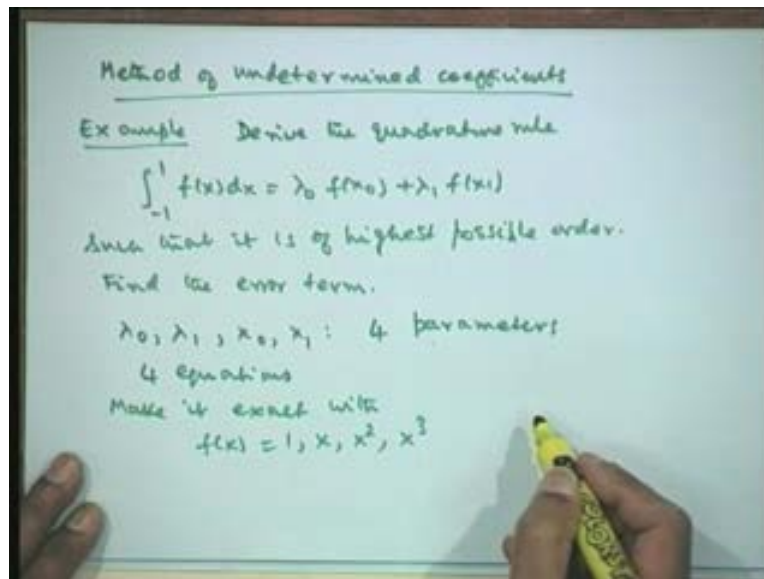
Therefore let us write down, since the formula integrates polynomials of degree less than or equal to 3 exactly that is n is equal to 3, let us take exactly set $f(x)$ is equal to x to the power of 4, so we will take $f(x)$ is equal to x to the power of 4. Therefore our error constant should be 0 to infinity exponential of minus x x to the power of 4 minus, we bring everything to left hand side 1

upon 4 (2 plus root 2) and f of x should be x to the power of 4 that is (2 minus root 2) to the power of 4 plus (2 minus root 2) into (2 plus root 2) to the power of 4. Now you can integrate this, let us, I will give you the value of this, if just integrate it this what you get, minus of x to the power of 4 of 4 x cubed, then you have 12 x squared, then you will have 24 x, then you will have 24, e to the power of minus x that is because you are integrating by parts so this will be, the first integral is minus x to the power of 4, then it is 4 times, 4 into x cube this is 12 x squared 24 x, 24 this one and this is evaluated between 0 to infinity. And the second term is 1 upon 4, let us take 2 at a time, let us take (2 plus root 2) into (2 minus root 2), combine them that will be 4 minus 2 that is 2, so what is left out is whole cubed and again I combine these 2 to give a 2 and (2 plus root 2) whole cubed, I am combining one factor each so that they get simplified.

Now at infinity this entirely this is 0, at 0 all of them 0 except 24 so what is left out is simply 24 into 1 that is simply 24 that is what we get from the first bracket here. And the second bracket is 1 upon 4, **now these are**, this is odd power 3 so all these odd ones will cancel off that root 2 one will cancel and what I get here is I will the value of this, this gives you (40 minus 28 root 2) and this will give me (40 plus 28 root 2), this is the expansion of this, the expansion of this. Therefore 28 root 2 cancels of so will have 80 by 4 that is 20, 24 minus 20 that is simply equal to 4. Therefore I have the error term given as R_4 is c by factorial 4 $f^{(4)}$ of zhi that is 4 4 cancels so I will have 1 upon 6 f 4 of zhi, zhi lying between 0 and infinity. Therefore this is how the error can be obtained for any particular formula, so the main thing is when once you have to find the order of the formula correctly then I can immediately use the next power of x as the required function of x, find the error constant and then write finally the error of this formula.

If the integral that is given to you does not fit into anyone of this forms that we have considered then we have to construct some special formulas, for example we have integral a to b w(x) f(x) dx where the weight function w(x) is not 1 of the forms that we have considered. The integration rule should contain only f(x) not the weight function then one has to construct one's own formula, it is always done in many of the practical applications by just applying the fundamental principle. The fundamental principle is if there are 2 n plus 2 parameters we just have to make it exact with f(x) is equal to 1, x, x square, x to the power of 2 n plus 1 to get the required number of equations for required number of parameters, solve them and that will be our formula. Therefore it is possible for us to construct our own formula for any given w(x) irrespective of whether orthogonal polynomial exist or not, in that case orthogonal polynomials may not exist at all.

(Refer Slide Time: 34:08)



So we will call this as method of undetermined coefficients, method of undetermined, method of undetermined coefficients. Now let me first, I will take 2 examples, let me first take an example which we know already, the formula which we know already. So derive the quadrature rule, let us take the one that we know very well minus 1 to 1 $f(x) dx$ is $\lambda_0 f(x_0) + \lambda_1 f(x_1)$ such that it is of highest possible order, highest possible order, find the error term. In all these cases the error term is very important because that will really tell you the, not only order it gives you and what is the error constant that is the constant that is multiplying the actual error term. Now we first look at the formula, how many unknowns are there, there are, we have got λ_0 to be found, λ_1 to be found, x_0 to be found, x_1 to be found, therefore there are 4 parameters, therefore there are 4 parameters, therefore we need 4 equations, 4 equations. Now since we need 4 equations I must make it exact with $f(x)$ is equal to 1, x , x square, x cubed so each one will give us an equation so I will get 4 equations in 4 unknowns. If anyone of them turns out to be 0 is equal to 0 so we do not have an equation, so I will go to the next one x to the power of 4. Now let us do this.

(Refer Slide Time: 36:29)

$$\begin{aligned}
 f(x) &= 1: \int_{-1}^1 dx = 2 = \lambda_0 + \lambda_1 \quad \text{--- (1)} \\
 f(x) &= x: \int_{-1}^1 x dx = 0 = \lambda_0 x_0 + \lambda_1 x_1 \quad \text{--- (2)} \\
 f(x) &= x^2: \int_{-1}^1 x^2 dx = \frac{2}{3} = \lambda_0 x_0^2 + \lambda_1 x_1^2 \quad \text{--- (3)} \\
 f(x) &= x^3: \int_{-1}^1 x^3 dx = 0 = \lambda_0 x_0^3 + \lambda_1 x_1^3 \quad \text{--- (4)} \\
 (4) - (2) \times x_0^2: & \lambda_1 x_1^3 - \lambda_1 x_1 x_0^2 = 0 \\
 \lambda_1 x_1 (x_1^2 - x_0^2) &= \lambda_1 x_1 (x_1 - x_0)(x_1 + x_0) = 0 \\
 x_0 \neq x_1; \lambda_0 \neq 0, \lambda_1 \neq 0 \\
 x_1 (x_1 + x_0) &= 0 \\
 x_1 = 0 \text{ or } x_1 = -x_0 &\checkmark \\
 \text{✓ (2): } \lambda_0 - \lambda_1 &= 0, \lambda_0 = \lambda_1
 \end{aligned}$$

So let us put $f(x)$ is equal to 1 then the left hand side is minus 1 to 1 dx. Now left hand side is minus 1 to 1 dx that is equal to 2, we evaluate it, integral is equal to 2. $f(x)$ is taken as 1 so this is λ_0 plus λ_1 . Let us take $f(x)$ is equal to x , this gives us minus 1 to 1 x dx, odd function minus 1 to 1 0 and this is equal to $\lambda_0 x_0$ plus $\lambda_1 x_1$. Now let us take $f(x)$ is equal to x square, so I will have minus 1 to 1 x squared dx, now this is x cubed by 3 so I will have here 2 by 3, $\lambda_0 x_0$ square plus $\lambda_1 x_1$ square. Then I take $f(x)$ is equal to x cubed, therefore minus 1 to 1 x cubed dx, this is again an odd function in minus 1 to 1 so I will have a 0 here and this is $\lambda_0 x_0$ cubed plus $\lambda_1 x_1$ cubed. Now these equations at the phase of it they look very difficult to solve because they are non-linear equations but because of the way that the right hand sides are there and the coefficients here the solution of this can be done very easily in a very systematic way.

Now first let us consider **these** where you have got zeros that means equation 2 and 4, let us eliminate x_0 from here so what I would do is I will take the equation 4 and then multiply by x_0 square to eliminate the first coefficient. So I will multiply 2 into x_0 square, 4 minus 2 into x_0 square and that gives me $\lambda_0 x_0$ cubed $\lambda_0 x_0$ cubed cancels, so what I have here is $\lambda_1 x_1$ cube minus $\lambda_1 x_1 x_0$ square is equal to 0, the right hand sides are 0 both are 0, so this will be simply $\lambda_1 x_1$ cube minus $\lambda_1 x_1 x_0$ square. Let us simplify this, this is $\lambda_1 x_1 (x_1$ square minus x_0 square) so let us write down one more step and put it equal to 0, $(x_1$ minus $x_0)(x_1$ plus $x_0)$ is equal to 0. Now in the method that is given to us, this is method that we have been asked to derive, λ_0 λ_1 they are not equal to 0, these are distinct abscissa so x_0 is equal to, not equal to x_1 . Therefore we need to consider that here that x_0 is not equal to x_1 that is given in the problem, the weights are not equal to 0 so λ_0 is not equal to 0, λ_1 is not equal to 0, so these are all the properties of the given quadrature rule.

If that is so you can see that x_1 is not equal to x_0 so this factor can be cancelled, λ_{a1} is not equal to 0 so it not to be cancelled so what is left out is simply x_1 into $(x_1 \text{ plus } x_0)$ is 0. Now **we can**, we shall exclude this gives you x_1 is equal to 0 or that is 0, so x_1 is equal to 0 or x_1 is equal to minus x_0 . Now we shall exclude x_1 is 0 because just look at 2 here, when x_1 is equal to 0 this goes off and hence λ_{a0} is equal to 0 that is not possible λ not equal to 0 or x_0 is equal to 0, if x_0 is 0 again x_0 is 0 x_0 , x_1 is equal to 0, both are equal, therefore this is also not possible. Therefore the only is x_1 must be equal to minus x_0 that is a only solution that comes from here. Let us substitute in 2, x_1 is equal to minus x_0 therefore that gives you λ_{a0} minus λ_{a1} is equal to 0 or λ_{a0} is equal to λ_{a1} . I substituted in 2 so x_1 is equal to minus x_0 , x_0 is common, cancel of x_0 , so we have λ_{a0} is λ_{a1} . When once we get this value I can substitute in 1, λ_{a0} is equal to λ_{a1} so I will get from 1 they are equal and 1, therefore from 1 it gives you λ_{a0} is equal to 1, λ_{a1} is equal to 1.

(Refer Slide Time: 41:48)

$$\begin{aligned}
 \textcircled{1}: \quad \lambda_0 &= 1 = \lambda_1 \\
 \textcircled{2}: \quad 2x_0^2 &= \frac{2}{3}, \quad x_0^2 = \frac{1}{3}, \quad x_0 = \pm \frac{1}{\sqrt{3}} \\
 x_0 &= -\frac{1}{\sqrt{3}}, \quad x_1 = \frac{1}{\sqrt{3}} \\
 \int_{-1}^1 f(x) dx &= f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \\
 f(x) &= x^4 \\
 C &= \int_{-1}^1 x^4 dx - \left[2 \left(\frac{1}{\sqrt{3}} \right)^4 \right] \\
 &= \frac{2}{5} - \frac{2}{9} = \frac{8}{45} \\
 R_4 &= \frac{C}{4!} f^{(4)}(\xi) = \frac{8}{45(24)} f^{(4)}(\xi) = \frac{1}{135} f^{(4)}(\xi) \\
 &\quad -1 < \xi < 1
 \end{aligned}$$

Now we can use the equation 3, since λ_{a0} is equal to λ_{a1} is equal to 1 and x_0 is minus x_1 , I have simply twice x_0 square is 2 by 3. So I am just substituting in this, so this gives you x_0 square is 1 by 3, x_0 is plus minus 1 upon root 3 and x_1 is equal to minus x_0 so I will have the opposite sign, so I choose x_0 as 1 of them either plus 1 by 3 or minus 1 by 3. So if I take x_0 is minus 1 by 3 I would get this as 1 by 3 or conversely I will get the reverse one but the formula will be same because λ_{a0} is equal to λ_{a1} . Therefore we have derived the formula minus 1 to 1 $f(x) dx$, λ_{a0} is equal to λ_{a1} that is equal to 1 so simply f of minus 1 by 3 plus f of 1 by 3, which is nothing but the our Gauss Legendre 2 point rule which we have already proved this one. Now let us take the error term, so I have to take $f(x)$ is equal to the next power that is x to the power of 4 and therefore the error constant c would be minus 1 to 1 x to the power of 4 dx minus, when x to the power of 4 it is even so both will be equal, $(1 \text{ upon root } 3)$ to the power of 4.

This is x to the power of 5 by 5 therefore 2 by 5 minus 2 by this gives you 9, this gives you 9 that is equal to 18 minus 10 that is 8 upon 45. Therefore we have the error term R_4 is c by factorial 4 fourth derivative at a point ξ that is 8 upon 45 into $24 f^{(4)}$ of ξ or 1 upon 135 $f^{(4)}$ of ξ , ξ lying between 1 and minus 1. So this is how we can get the error constant and using the error constant I can now get the error term for the given formula as this and then write down this one. So this completes the error term also and will see that the multiplicative factor of $f^{(4)}$ is 1 upon 135 which is quite small so that is how we can say how the error would now decay as we go along and we can use here also as we have done in the, earlier also we have shown we can break this up into given interval a to b , we can break it into a to c , c to b and then use a composite rule also so that the error would much smaller.

(Refer Slide Time: 45:06)

Example Calculate the weights, abscissas and remainder term in the Gaussian quadrature formula

$$\frac{1}{\sqrt{\pi}} \int_0^{\infty} \frac{e^{-t}}{\sqrt{t}} f(t) dt = A_1 f(x_1) + A_2 f(x_2)$$

4 parameters A_1, A_2, x_1, x_2
 Make it exact with $f(t) = 1, t, t^2, t^3$

$f(t) = 1: \frac{1}{\sqrt{\pi}} \int_0^{\infty} e^{-t} \cdot t^{-1/2} dt = A_1 + A_2$

$$\Gamma(\alpha) = \int_0^{\infty} x^{\alpha-1} e^{-x} dx$$

$$\Gamma(\alpha+1) = \alpha \Gamma(\alpha) : \Gamma(1/2) = \sqrt{\pi}$$

Now let us give one last example. 3, the order is 3 therefore the error term should get from $f(x)$ is equal to x to the power of 4, 4. So let us take one more example, so will say this is, calculate the weights, abscissas and remainder term in the Gaussian quadrature formula 1 upon root pi 0 to infinity e to the power of minus t by root t $f(t)$ is $A_1 f(x_1) A_2 f(x_2)$. Now this does not belong to any of the classes that we have described earlier even though 0 to infinity but this is not the e to the power of minus t form therefore it is not Gauss Laguerre. Therefore for this the only way is that we have go through this undetermined coefficient procedure. Again we have 4 constants therefore we have 4 parameters here A_1, A_2, x_1, x_2 . Therefore we make it exact, make it exact with $f(t)$ is 1, t , t square, t cubed, t , t square, t cubed. There are 4 parameters so we get 4 equations. So let us substitute them, so $f(t)$ is equal to 1, this is 1 upon root pi 0 to infinity e to power of minus t , I will take this up and write it that is t to the power of minus half into dt , I just take it off in this one and this is equal to A_1 plus A_2 , $f(x)$, f of x_1 is equal to 1, this is also equal to 1.

Now you would like to use the gamma function, definition of gamma function and evaluate as a gamma function. If you remember the gamma function, gamma of alpha is 0 to infinity $x^{\alpha-1} e^{-x} dx$ but gamma (alpha plus 1) is equal to alpha gamma alpha. We need here in particular what is the value of gamma half that is equal to root of pi, so I would like to use this particular property to evaluate this completely that is gamma half is equal to root of pi, gamma of (alpha plus 1) is alpha gamma alpha. Now if you see this definition of this, this is $x^{\alpha-1}$ therefore I need to have here gamma of, you have minus half here so if I take alpha is equal to half here, then I will get minus half so alpha is equal to half it gives me gamma half.

(Refer Slide Time: 48:42)

Handwritten mathematical derivation on a whiteboard:

$$\frac{1}{\sqrt{\pi}} \Gamma(1/2) = A_1 + A_2 \quad A_1 + A_2 = 1 \quad \text{--- (1)}$$

$$f(t) = \frac{1}{\sqrt{\pi}}: \frac{1}{\sqrt{\pi}} \int_0^\infty e^{-t} t^{1/2} dt = A_1 x_1 + A_2 x_2$$

$$\frac{1}{\sqrt{\pi}} \cdot \Gamma(3/2) = \frac{1}{\sqrt{\pi}} \cdot \frac{1}{2} \cdot \sqrt{\pi} = \frac{1}{2}$$

$$A_1 x_1 + A_2 x_2 = \frac{1}{2} \quad \text{--- (2)}$$

$$A_1 x_1^2 + A_2 x_2^2 = \frac{3}{4} \quad \text{--- (3)}$$

$$A_1 x_1^3 + A_2 x_2^3 = \frac{15}{8} \quad \text{--- (4)}$$

Therefore the left hand side is 1 upon root pi gamma of half and the right hand side is A_1 plus A_2 and gamma half is root pi therefore root pi root pi cancels, the first equation as A_1 plus A_2 is equal to 1, A_1 plus A_2 is equal to 1. Now the remaining equations are easy for us to do it, $f(t)$ is equal to t therefore root t cancels I will have t to the power of half in the numerator, t to the power of half dt and the right hand side is $A_1 x_1$ plus $A_2 x_2$. Now let us evaluate the left hand side here, this is 1 upon root of pi, this is gamma of 3 by 2, this is 3 by 2 minus 1 that is half therefore this is gamma 3 by 2 that is 1 upon root pi and we will use the property that gamma 3 by 2 is half gamma half, this gives you half gamma half that is equal to half, gamma half is equal to root pi, therefore this is equal to half. Therefore the second equation is $A_1 x_1 + A_2 x_2$ is equal to half and I will similarly give the remaining equations, you will get $A_1 x_1^2 + A_2 x_2^2$ is equal to 3 by 4 that is equation 3, $A_1 x_1^3 + A_2 x_2^3$ is equal to 15 by 8. You will have to follow exactly the previous method that we have done here that we take the first and third equation eliminate x_1 , second and fourth eliminate x_1 , then eliminate $A_2 x_2$ it will get a single equation in x_1 or x_2 and that will give the solution of the problem.

(Refer Slide Time: 51:01)

$$\begin{aligned}
 f(t) &= \frac{1}{2} : \frac{1}{\sqrt{\pi}} \int_0^{\infty} e^{-t} t^{1/2} dt = A_1 x_1 + A_2 x_2 \\
 &\quad \downarrow \\
 \frac{1}{\sqrt{\pi}} \cdot \Gamma(3/2) &= \frac{1}{\sqrt{\pi}} \cdot \frac{1}{2} \cdot \sqrt{\pi} = \frac{1}{2} \\
 A_1 x_1 + A_2 x_2 &= \frac{1}{2} \quad - (2) \\
 A_1 x_1^2 + A_2 x_2^2 &= \frac{3}{4} \quad - (3) \\
 A_1 x_1^3 + A_2 x_2^3 &= \frac{15}{8} \quad - (4) \\
 4x_1^2 - 12x_1 + 3 &= 0 \\
 4x_2^2 - 12x_2 + 3 &= 0
 \end{aligned}$$

And the equation for your verification the equation comes out to be same. And because of the symmetry you will get the same equation for x_2 also. Both the equations will be the same, obviously because of the structure of the formula the 1 will be one of the roots the other will be x_1 .

(Refer Slide Time: 51:23)

$$\begin{aligned}
 x_1 &= \frac{3-\sqrt{6}}{2}, \quad x_2 = \frac{3+\sqrt{6}}{2} \\
 A_1 &= \frac{3+\sqrt{6}}{6}, \quad A_2 = \frac{3-\sqrt{6}}{6} \\
 \frac{1}{\sqrt{\pi}} \int_0^{\infty} \frac{e^{-t}}{\sqrt{t}} dt &= \frac{1}{6} \left[(3+\sqrt{6}) f\left(\frac{3-\sqrt{6}}{2}\right) \right. \\
 &\quad \left. + (3-\sqrt{6}) f\left(\frac{3+\sqrt{6}}{2}\right) \right] \\
 \text{only 3.} \\
 C &= \frac{24}{16} \\
 R_4 &= \frac{1}{4!} \cdot \frac{24}{16} f^{(4)}(s) = \frac{1}{16} f^{(4)}(s), \quad 0 \leq s < \infty.
 \end{aligned}$$

Therefore the 2 roots are x_1 is 3, I am solving this and writing it $3 - \sqrt{6}$ by 2 and x_2 is equal to $3 + \sqrt{6}$ by 2 and I can find out the, then substitute back the values and then get my values of A_1 , A_2 , A_1 is $3 + \sqrt{6}$ by 6 A_2 is $3 - \sqrt{6}$ by 6. So let us just finally write down the formula $\int_0^\infty e^{-t} t^3 dt$ is 1 upon 6 because A_1 A_2 it has a minus 1 by 6 ($3 + \sqrt{6}$) that is this coefficient and f of x_1 that is ($3 - \sqrt{6}$ by 2) and the second one is plus ($3 - \sqrt{6}$) that is from A_2 , this is f of x_2 that is ($3 + \sqrt{6}$ by 2) and of course order we made it as 3, order is 3. And find out the error constant by taking the next term that is t to the power of 4 and what I would get here is simply c is 24 upon 16, 24, so that the remainder is 1 upon factorial 4 24 by 16 $f^{(4)}$ of zhi that is simply 1 upon 16 $f^{(4)}$ of zhi . Therefore what we are trying to say here is that if any practical application, if the weight function is not of the suitable form one can construct with own quadrature rule that fits that particular application problem and then follow the procedure the fundamental definition of what is the quadrature rule that **it would**, it should integrate polynomials of degree less than or equal to some $2n + 1$, then we will be able **to any** integration rule you want for any application. So we would now close with this. Thank you.