Numerical Methods and Simulation Techniques for Scientists And Engineers

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Lecture 12
Simpson's 1_3rd rule, Gaussian integration

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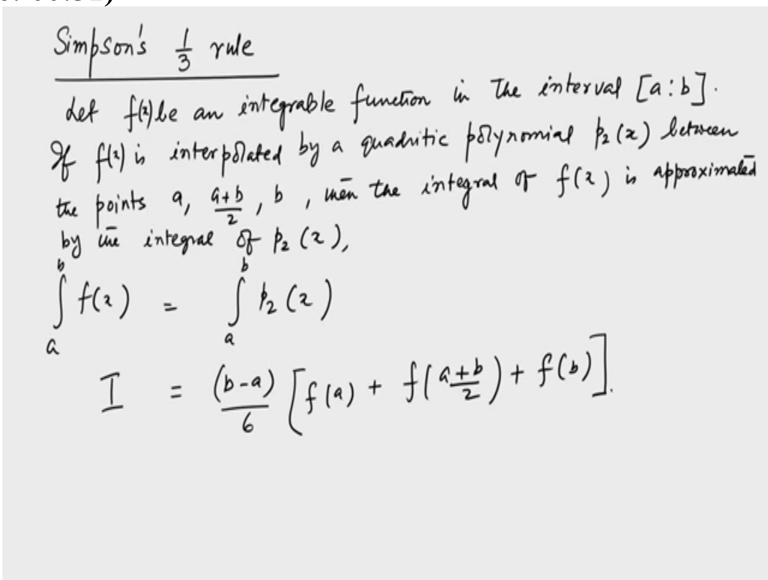

So, let me summarize Simpsons 1/3 rule it states that that let f be an integral function or integrable function rather it is an integrable function in the interval a and b that is its integral in the whole range a b. Now if f is interpolated by a quadratic polynomial p 2 x between the points a b and of course a + b by 2 that is a midpoint between a and b. Then the integral of f fx, so let us write fx and this is also fx the integral of fx is approximated by the integral of of p 2 x.

So, which is a to b f of x its equal to a to b p2 of x and which we have seen that has a form which is equal to f of a + f of a + b by 2 + f of b ok. Now 1thing is worth noting here is that we have used Newton's interpolation formula ok for arriving at this expression of p 1x or the p 2x we can as well use the Lagrange's interpolation or any other interpolation and even a Taylor series expansion of a function about certain a point is also going to give us the same formula.

I will try to address some of these issues in the tutorials but however let us at this moment keep it the derivation we kept only with the Newton's interpolation polynomial as we have done ok. But as I said that the Lagrange's interpolation or any other interpolation scheme would given the same result as it is written here. So, the I is equal to this so this is known as Simpsons 1/3 rule. So, let us see some more examples of this and how to use this.

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Example The distance covered by a rocket in meters from $t = 8s$ to $t = 30s$ is given by,

$$x = \int_{8}^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

a) Use Simpson's $\frac{1}{3}$ rule to find the approximate value of x.

b) find the error.

a) $x = \frac{b-a}{8} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$ $\qquad a = 8$, $b = 30$, $\frac{a+b}{2} = 19$

$$f(t) = 2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t$$

$$f(8) = 2000 \ln \left[\frac{140000}{140000 - 16800} \right] - (8)(9.8) = 177.27 \ ms^{-1}$$

So, example so the distance covered by rocket, so it is a physics problem or a aeronautical engineering problem if you like by a rocket in meters from t equal to 8 seconds to t equal to 30 seconds is given by x which is equal to 0 to 30 okay. And it is the integral of sorry not 0 to 30 it is between 8 and 30. So, it is 8 to 30 and so this is 2,000 log of 140,000 divided by 140000 - 2100 t - gt which is the g has a value.

So, let us write the value itself it is 9.8t and then a dt so this is a formula for the rocket motion of course this formula or this kind of motion you have not seen much but it goes as a log and then of course the time appears in the denominator of the argument of the log. And then of course there is also a gt term. In any case say this is given and now 1has to compute it or evaluate the integral using the Simpsons 1/3 rule.

So, the questions are as follows a use Simpsons 1/3 rule to find the approximate value of x ok. Second is of course find the error or whatever you call it relative error or percentage error find the error in this. So, we will use a simple Simpsons 1/3 rule that is not use any segments in between. So, the formula is simply x is equal to b - a by 6 f at a just what it was written there excuse me I forgot a factor of 4 here okay this is very important this factor of 4 is very important.

So, this is not just f a + b it is 4 in times f a + b all right so this is 4 f a + b by 2 + f b and so this is the formula we have b equal to so let us write a equal to 8 seconds b equal to 30 seconds I am only writing it in terms of just numbers a by a + b by 2 is 30 + 8 is 38 and this is so this is 19 that is all in seconds and so f of t that is the integrand which you otherwise would have used a polynomial but that the integrand is given here is simply 2,000 log of 140,000 divided by 140000 - 2,100 t – 9.80.

So, we have to find 3 of them f at 8 f at 30 and f at 19, so let us calculate all those things so f at 8 it is a 2000 log and 140000 divided by 140000- 8 into 2100 is 008 and then 168 and so on and this is 9.8 into 9.8 okay and then if you simplify this, this becomes equal to 177.27 and if I am allowed to use a unit because it is you and multiplied dt that is which as a unit of time. So, this second will cancel and I will get a meter so the integrand has the dimension of meter per second which is velocity and which is known that x is vt + dt.

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$$f(30) = 2000 \ln\left[\frac{140000}{14000 - 2100(30)}\right] - (9.8)(30) = 901.67\ m s^{-1}$$

$$f(19) = 484.75\ m s^{-1}$$

$$x = \left(\frac{30-8}{6}\right)\left[f(8) + 4f(19) + f(30)\right]$$

$$= 11065.72\ m. \longrightarrow \text{distance traveled.}$$

(b) Error.

Exact value of the integral $= 11061.34\ m.$

$$E_t = 11061.34 - 11065.72 = -4.38\ m$$

Abs. p.c. relative error $\dfrac{4.38}{11061.34} \times 100\,\% = 0.0396\,\%$

Now let us calculate the other 2 so this is 1, so f of 30 that is at the end point it is 2,000 log of again 140000 divided by 140000 - 2130 and - 9.8 into 30 and this one has if you so it is 901.67 meters per second. So, the rocket travels in this interval from f 8 the integrand is actually the velocity rather the velocity increases from this value which is 177 meters per second to 901.67 meters per second. But what is important for us to get the other one which is f of 19 I will you can write down for these time as 19.

Finally what you get is that it is a 484.75 meter per second okay. So, now I got the value of the function at all the 3 points sampling points which are the end points and plus a point at the middle. So, now I am ready to put it there into the formula which is b - a by 6 which is 30 - 8 divided by 6 and we have a f of 8 and + a 4 f of 19 and + f of 30 ok. So, that is this and if you simplify this, this becomes equal to 11065.72 meter okay.

Now the exact value so this is part 1so this is the distance travelled you get it. And for Part b for calculating the error we need to know the exact value. So, the exact value of the integral and this I am not showing it but you can do it easily value of the integral it is equal to 11061.34

okay. So, you simply have to integrate this expression which is a log of this, so it is like a log of a by b which you can expand as log a - as log b.

So, the log a term will give a constant which when you integrate it over dt will give you just a t and the log x so to say log x dx can be integrated and between the limits t equal to 8 to t equal to 30 and finally what you get is this value the exact value of the integral. You see you have gotten pretty close in terms of the number excepting that it varies only at the 5th decimal place not the 5th decimal place fifth place that is in the you know the ones place as it says.

So, this is the value of the integral so in case you want to know the error, so the error the magnitude of the error or rather the error itself is like 11061.34 - 11065.72, so this is like a - 4.38 meters so this is very small right I mean 4.4 meters in some 11,000 meters is very small. So, the relative error is basically so the percentage relative error is so it is 4.38 and I will take the absolute value.

So take the absolute so it is 4.38 I will not take the sign here and 11061.34 into 100 and in percent and it gets only 0.0396%, so just one interval or rather the bare Simpsons 1/3 rule for this problem of rocket motion is gives you a value which is pretty close and it is only off by this 04% say for example okay. Now let us compare it with a multi segment or multiple segments Simpsons 1/3 rule which we have learned that if each of the you if you divide the entire interval into n such segments.

And then apply the rule the bear rule Simpsons 1/3 rule for each one of those segments and then add all the contributions up and there is certainly going to be a better approximation for the integral.

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Multiple Segment Simpson's $\frac{1}{3}$ rule.

$f(a) = f(x_0)$

$f(b) = f(x_n)$.

$h = \frac{b-a}{n}$

$$I = \frac{h}{3}\left[f(x_0) + 4\{f(x_1)+f(x_3)+\dots f(x_{n-1})\} + 2\{f(x_2)+f(x_4)+\dots f(x_{n-2})\} + f(x_n)\right]$$

$$= \left(\frac{b-a}{3n}\right)\left[f(x_0) + 4\sum_{\substack{i=1\\ i\in odd}}^{n-1} f(x_i) + 2\sum_{\substack{i=2\\ i\in even}}^{n-2} f(x_i) + f(x_n)\right]$$

a) use 4 Segment Simpson's $\frac{1}{3}$ rule to find the distance traveled, x.

b) Error.

So, we will solve the same problem okay using multiple segments. So, here of course we have to divide the interval into the entire interval by n and we have seen this formula earlier and if you want the I will again write down the value of the integral. So, it is h over 3 that is a value at a and then there are 4 times the value for the odd number. So, it is f of x 1 + f of x 3 + f of x n - 1 so these are all the odd-numbered intervals or rather the sampling points the values of the function at all these odd sampling points.

And twice for the values add those ah even number of sampling points it is f x 4 and so on all the way up to f x n – 2. And finally you know the f of x which is x n which is equal to b so let us just you know make that distinction so x 0 and x n. So, just to make sure that we know that f of x f of a equal to f of x 0 that is a value of the function at the initial for the left extremity of the interval and this is at the right extremity of the interval is they are called as x 0 and x n and the values are values of the function are like this.

So the important part is that for this multiple segments Simpsons 1/3 rule what you have to do is that you have to take all the sampling points odd number of sampling points such as 135 and so on and multiply it weighted by 4 the numbers will have to be weighted by 2 and for the leftmost point and the rightmost points are left al1with a weight 1 ok. So, if this is their so a this is what we had written earlier in a slightly compact notation.

So it is b - a by 3n and we have a f of x 0 so let us this + 4 and this is like i equal to 1 to n - 1 make sure i is odd and then I have a f of x i just the second term then I have i from 2 to n - 2 and I have f of x i with i being even + f of x n ok. So, this is this is that and then we want to solve the same problem, use so the question is use 4 segments Simpsons 1/3 rule to find x, find the distance travelled by the rocket. And find of course the error that goes with it and you will see that the error is negligibly small okay.

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Solution $n=4$, $a=8$, $b=30$, $h=\frac{b-a}{n}=\frac{22}{4}=5.5.$

$$f(t)=2000\ln\left[\frac{140000}{140000-2100t}\right]-9.8t.$$

$$\rightarrow f(t_0)=f(8) = 177.27\ ms^{-1}\ ✓$$

$$\rightarrow f(t_1)=f(t_0+h)=f(8+5.5)=f(13.5) = 320.25\ ms^{-1}\ ✓$$

$$f(t_2)=f(t_1+h)=f(13.5+5.5)=f(19). = 484.75\ ms^{-1}\ ✓$$

$$\rightarrow f(t_3)=f(t_2+h)=f(19+5.5)=f(24.5) = 676.05\ ms^{-1}\ ✓$$

$$901.67\ ms^{-1}\ ✓$$

$$\rightarrow f(t_4)=f(t_n)=f(30) =$$

$$x=\left(\frac{30-8}{3\times 4}\right)\left[f(8)+4\left(f(t_1)+f(t_3)\right)+2f(t_2)+f(30)\right]$$

$$=11061.64\ m.$$

So, let us try calculating all these things so what is this n is now 4 so we have a solution that needs to be done n equal to 4 for a equal to 8 b equal to 30 h which is the step size is equal to b - a divided by n which is 22 by 4 which is a 5.5 so and of course f of t for reminding ourselves it is a log of 140000 and 140000 - 2,100 t - 9.8t okay. So, if at t 0 we are calling it x 0 or t 0 which is f of 8 which we have already calculated earlier we can take that value which is 177.27.

Now f of t 1 is simply f of t 0 + h which is equal to f of t 0 is 8 + h is 5.5 which is equal to 13.5 so if you calculate f at 13.5 this comes out to be equal to 320.25 meters per second. So, you are taking more terms in the interval and what is f 2, f 2 is a further you know f of t 1 + h which is f of 13.5 + 5.5 which is nothing but f of 19 and we know f of 19 f of 19 is nothing but we have calculated it earlier 0.75 meter per second.

And similarly the f of t 3 which is nothing but equal to f of t 2 + h which is equal to f of 19 + 5.5 which is equal to f of 24.5 which is nothing but equal to which if you calculate it, it becomes 676.05 meter per second. So, that is ft 3 and then of course the final one is unknown f of t for it is equal to f of t n so to say which is 30 equal to f of 30 and whose value also we know because we have calculated it earlier 0.67 meter per second.

So, this is that okay so, we have all these things we have 1 here 1 here 1 here 1 here 1 here I see that these 2 will have to be left alone because in our formula they appear with rates one that is the first one and the last one now the odd ones will appear with weight 4. So, there is one odd and one odd here, so they appear with weight 4 that is this has to be multiplied by 4 let me show you. So, this has to be multiplied by 4 and this has to be multiplied by 4.

This will have to be multiplied because it is a second one which is an even it has to be multiplied by 2 and of course as I said the first and the last will have to be left alone in order to so fit into the formula okay. So, if we put in everything so my x will become 30 - 8 divided by 3 into 4 so that is 22 by 12 and then I have f of 8 + 4 times f of t 1 + 4 or let me write it in a bracket so that things become more you know they look same as a way we have written 2 f of 2 t 2 and then finally f of 30.

So, if you put all of them and then simplify this, this comes out to be 11061.64 meter the exact value we have already said.

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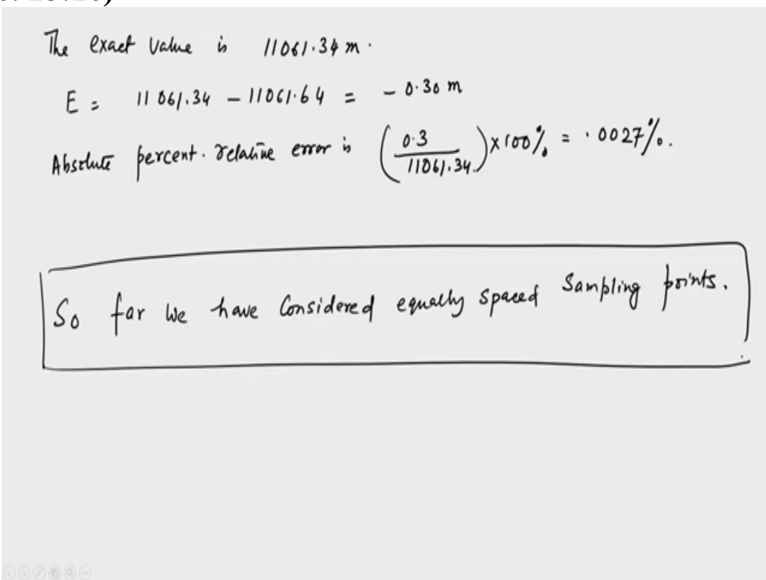

But let me write it here the exact value is 11061.34 meter, so this really, really close the so the error is 11061.34 - 11061.64 so it is actually in the second decimal place or rather the first decimal place it is differing and then this becomes as a .30 meter remember this was about 4 meters whereas this is less than a meter less than even half a meter is 0.3 meters. So, the absolute percent related to relative error is this .3 divided by 11061.34 and multiplied by 100 in percent and this becomes as .002727% okay that is a really small error and you can are pretty much approximated to be the exact just by using n equal to 4.

So, if you continue it to n equal to 6 and n equal to 8 and so on you will see that the error is reducing and it becomes vanishingly small for say n equal to maybe 8 or maybe n equal to 10 okay. So, this tells you that the Simpsons 1/3 rule is very powerful especially if you can if you take the composite or the multiple segment Simpsons 1/3 rule it really works very well. In this particular problem it we got for n equal to 4 we got error which is you know 10 to the power - 3% in percent.

And it is only in some 11,000 + meters you get error of 0.3 meter which is less than a meter and this is the strength of this method for evaluating an integral. So, what it does is that once again just to remind you that you replace the integrand by a polynomial and then for a problem that is unknown so when you have x0 f x0 x1 f x1 x2 f x2 and all that so when you have a series of or rather a set of data points then you need to have a polynomial and you could as I said that you could have a polynomial going by the Newton's interpolation formula.

Or by the Lagrange's interpolation formula or by any other formula it is not going to make a difference to the result that we have obtained that is just quoting the result for the single segment that the value of the function at the left interval value of the function and the right interval and multiplied by the plus the value of the function at the midpoint of these 2 intervals multiplied by 4 that is this comes with a weight of 4 alright.

So, far we have discussed with equally spaced points as if because these x 0 x 1 x 2 x 3 they all differ from each other by some step size uniform step size h, so let us just write that so far we have considered equally spaced sampling points ok. And it could happen that in a particular experiment you do not have these equally spaced sampling points and then these Newton's interpolation formula cannot be used.

But as we have said that the Lagrange's interpolation formula can still be used which really doesn't require equally spaced point. But here we will discuss another method to you know to handle points which are not equally spaced let us see these are called Gaussian integration.

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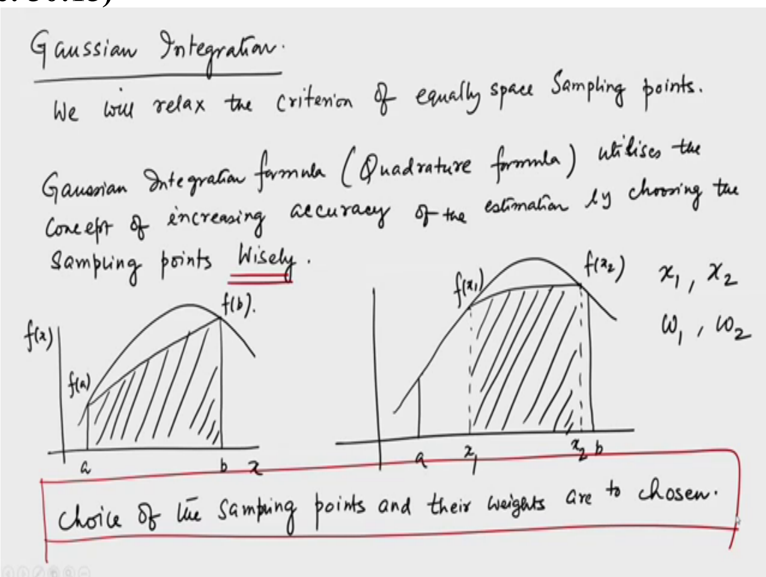

We will relax the criterion of equally spaced sampling points okay. So, in order to go about doing that let us give you an example of this particular thing of this trapezoidal rule. But before that let us say that what is this Gaussian integral, so this Gaussian integral or this integration formula which is also called as quadrature formula. So, if you see in literature a quadrature written it means the same as this the Gaussian integration formula.

So it utilizes the concept of increasing accuracy of the estimation of the integral of course by choosing the sampling points wisely. Let me underline this and try to say that what I mean okay so what is meant by wisely. So, what I want to say is that that we do not want to blindly choose the extreme points and the points which are half of that and so on. But in case we can make a distinction of the sampling points in such a manner that it gives me the best estimation of these for the interval in for the integration.

Then I think our job is done as an example let us look at this so this is a f of x versus x plot and when we have a to be like this and b to be like this then a simple trapezoidal rule uses a straight line between f of a to f of b and the width that is b - a is simply multiplied by the values of the function or this you know the average of the heights and things like that okay. But instead so these are we use these sampling points as the points of integration the lower and upper limits of the integration and find the values of the function at the extreme points that is fa and fb.

But instead if we do that the following that is we have the same curve okay and we simply use the fact that we do not take these points. So, we take instead of this points the; a point here we take a point x and instead of taking a point b here we take the point x2 ok. So, this is my x2 point and then what I say is that I will use this trapezoid and calculate the area of the trapezoid. Now there is a question the question is that that whether this trapezoid that we get by calculating the area.

I mean calculating this integral value of the integral by using x 1 and x 2 as a sampling points is any better than that obtained by a and b as the sampling points that is not clear and whatever visual even if it looks that it is better or it is worse it does not have a meaning unless we wisely choose that is why we have you know underline this word wisely. So, if you wisely choose f I mean x 1 and calculate the value of the function at x1 and wisely choose x 2 by calculating the point I mean calculating f x 2.

Then we might get a much better estimate than what we would have gotten without with the simple trapezoidal rule by taking the endpoints as the only sampling points okay. Now for that to happen this wise choice should be accompanied by 2 things not by that is not only by x 1 and x 2 but the weights of these points that are associated with x 1 and x 2. So, what I mean is that when there is a lot of undulations of a function some region could be actually more important than other regions in a trapezoidal formula blindly neglects those you know inflection points.

And how it is varying and so on it simply takes 2 points and then does a you know area estimation of the area of the trapezoid and which gives the integral of the function. But here we are saying that not only x 1 and x 2 will be chosen wisely a corresponding weights w1 and w2 will have to be chosen wisely as well. So, choice of the sampling points and their weights are to be chosen let me box this because there is a central idea of this.

So there is no guarantee that by choosing the weights arbitrarily you would be able to you know generate better estimation than what is given by the Kappa sidle rule but there is every chance if you properly choose w1 and w2 it will give you a better estimation. Let us see how it can be done by an example.

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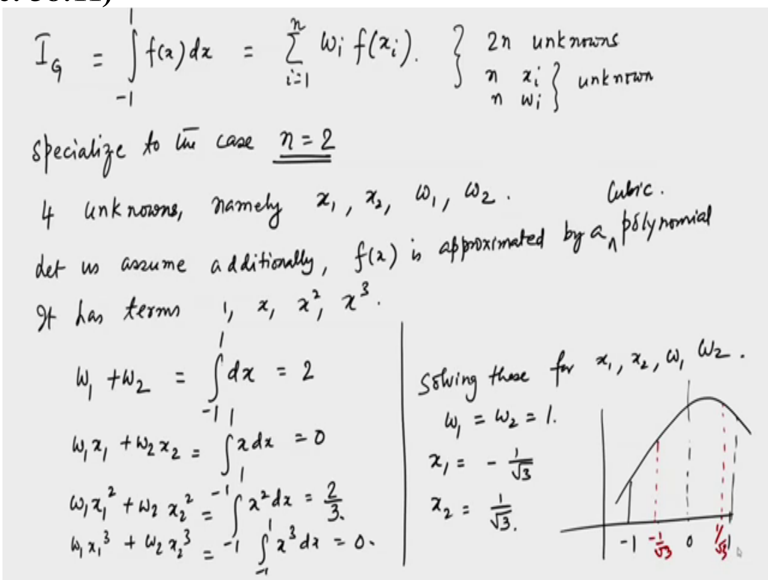

So, let us just write this integral as I G so I G stands for the Gaussian integral or the quadrature integral. And let us just take a simple example to begin with where we say that it is the integral is from - 1 to + 1 this will have to be so I equal to 1 to n and there is a w i f of x I okay where the i goes from 1 to n so we have how many unknowns we have to n unknowns in this equation, n size either unknown because those sampling points back to pick them is not known to me or known to us and also n wi those are also unknown that is the corresponding weight that had to be assigned to each 1of the sampling points is not known all right.

If it is not known then we have to find out a way to know these things and we cannot do it for large n so let us you know do it for n equal to 2, so specialized to the case okay n equal to 2. So, we have 4 unknowns in that case because it is 2n namely x 1 x 2 w 1 w 2 the weights associated with that. Now in addition let us assume additionally which means that independent of this above choice f x is approximated by a polynomial of I mean a cubic polynomial.

Let us say and it could be anything so this f of x is a cubic polynomial which means that it has terms which are 1 x x square x cube and you can actually consider any order but let us just assume that this is approximated by a cubic polynomial. And if it is a cubic polynomial then of course by this formula your w 1 + w 2 this is so for the 1of if f of x is equal to 1 then this is equal to a – 1 to + 1 dx ok which is of course equal to 2 then you have a w 1 x 1 + w 2 x 2 okay so this is like – 1 to + 1 dx which is equal to 0.

Then it is a w 1 x 1 square + w 2 x 2 square which is – 1 to + 1 x square dx which is equal to 2/3. And finally w1 x1 cube + w2 x2 cube this is equal to a – 1 to + 1 x cubed dx which is again equal to 0 ok. So, if you solve these for x 1 x 2 w 1 w 2 we get w 1 equal to w 2 equal to 1 so the weights are 1, however x 1 equal to - 1 over root 3 and x 2 equal to + 1 over root 3 so you see the sampling points now change from - 1 to + from - 1 to + 1 to - 1 by root 3 to + 1 by root 3.

So, if you have a function like this and then your integration is from - 1 to + 1 say here I mean of course your 0 is now here now 1 by root 3 root 3 is like the square root of 3 is 1.73 and so on so this is my 1 divided by 1.73 is somewhere here, here and somewhere here. So, let me write it with a different colour maybe so these are the - 1 over root 3 and this - + 1 over root 3 ok.

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

Example.
$$\int_{-1}^{1} e^{x}\,dx = f(x_1) + f(x_2)$$
$$= f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$
$$= e^{-1/\sqrt{3}} + e^{1/\sqrt{3}}.$$
$$= 2.3426961$$

Exact value
$$e^{x}\Big|_{-1}^{1} = \left(e - \frac{1}{e}\right)$$

And if you do this then of course the formula becomes equal to so this I G for the Gaussian G for the Gaussian it is f of x dx from - 1 to + 1 it is equal to f of 1 by root 3 - 1 by root 3 + f of 1 by root 3, so if you add both of them at these sampling points then you get this you get this result which is more accurate and one can test it, I mean take an example of you know exponential x dx -1 to +1 so this is your so it is f of x 1 + f of x 2 this of course given for a -1 and +1 so we got these sampling points as 1 over root 3 + and -.

But if you take other values you will get appropriate sampling points for this so this is like f of a - 1 over root 3 + f of + 1 over root 3 and this is like exponential - 1 by root 3 and an exponential + 1 over root 3 and this is equal to some 2.3426961 that is that is the value numerical value for that. And exact value you can you can check by calculating the integral which is just this and so on.

So, this is like e - 1 over e and so on and you can find out the error and see that error is lesser than what you would have gotten using the trapezoidal rule by taking the value of the functions at this point, so if you take it at f 1 and f - f 1 and f - 1 you would have had a value which is you know not as close as this compared to the exact value. So, this is one example where we have never said that these x 1 and x 2 or if you talk about a multiple segment this of this rule then these x 1 x 2 x 3 x 4 or the intermediate points they do not have to be equally-spaced.

They can be spaced anywhere with appropriate weights which would appear for the interval. Now this particular problem the weights actually became one actually had to assign equal weights to both these but it may not be the case when you take this integral to be you know having different limits and so on. And maybe you can take a different polynomial that is not a cubic polynomial and maybe 4th order of 5th order polynomial this would definitely affect the results.

We show a very simple example one the important constraint is relaxed that your sampling points do not have to be equally spaced and then your; the ones that are given that is the endpoints that are given or the midpoint of 2 such intervals they do not need to be taken rather you can take any point and can use them as a sampling points provided they have weights such that your estimation of the integral becomes best.

So, we want to you know end this chapter or conclude the integration numerical integration part just summarizing that we have done this method of using I mean the Newton's interpolation polynomial and have seen a distinctly 2 types of integral to begin with when we are using the Newton Cotes formula. And where we have talked about you know trapezoidal rule and Simpsons one-third rule.

Majorly and Simpson’s 3-8th rule which is a slight variant of the 1-3rd rule by using you know 1order higher polynomial and showed that this Simpson’s 1-3rd rule is an excellent tool for doing the integration. In fact a large number of these numerical tools for integration they use the Simpsons one-third rule. And then finally we have shown through an example that how this Gaussian integral we done by choosing sampling points with appropriate weights by you know through certain criterion and the integral can be estimated to give better accuracy for the integral that we are looking for.