Computational Science and Engineering using Python

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Lecture -12
Integration II: Gaussian Quadrature

So in the last class I did Newton cotes; so, the same Newton. So, they were all working on how to compute. So, one way I do want to remark that in research we do require computation. So, thinking that everything is in head; it does not work, even in theory we do require computation. And I think this nothing called theoretical physics and computation physics or external physics.

Finally, you need to compute and get the numbers; so, one should keep in mind that one should really restrict this guys no one what today I am going to tell you is the toughest algorithm I come across in computation physics. This gauss quadrature defined that is a very involved and is by gauss no lesser pressure; so, you have to pay attention this is quite difficult.

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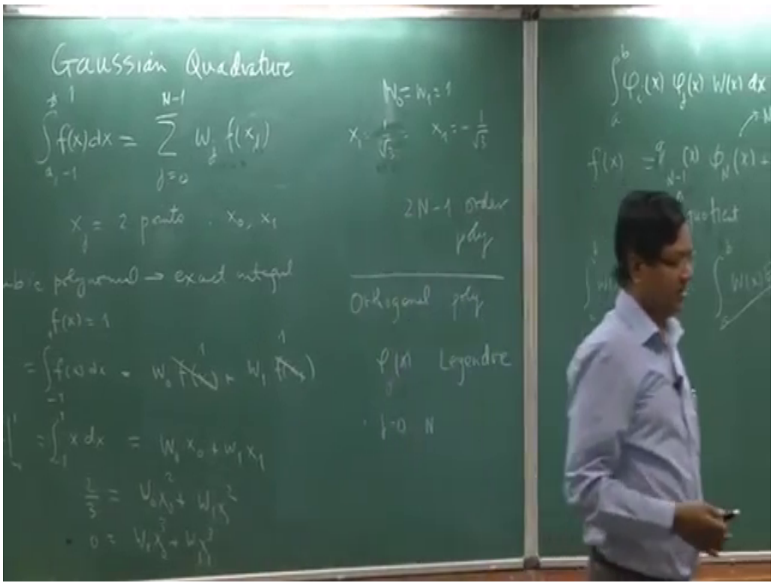

So, today we will do Gaussian quadrature; so, as I said complex method. So, in complex method; we approximate f x; d x a to b; as sum W j; f x j d equals to 0 to N points. So, for this method x j and W j both are unknowns. In the last class, when I did; I kept x j; x j was known. So, I only computed W j, but in today’s class I will keep both x j and W j are known. Now let us first think of the idea and with simple example; so before I go to the proof, I will work with simple example.

So, suppose I want to have; I have only two points. So, x j will be only two points my abscissas are two points; I have two weights W j. So, what is a function which I can integrate exactly; till what kind of function I can exact do it exactly? Linearly definitely and you can do better; integration I am asking integration within this formula. So, it turns out, I will prove show you that anything which is less in cubic order equal to less than equal to and less in cubic order it can be done; exactly that is the power; so, anything cubic there is a bit two point.

So, let us I mean this proof is not difficult; for this proof is very easy; we had to go there we are not started the main proof. So, I am imposing the condition that cubic polynomial; I should get exact integral. So, I have to just do it for 4 of them; so, f x equal to 1; it is a (Refer Time: 03:41) problem. So, for f x is equal to 1; a, b I actually choose my a, b. So, I think I chose my a b; so, if I am choosing integral minus 1 to 1 for this problem. So, I am going to choose this to a minus 1 and its b 1.

So, integral this is going to give you integral of f x; d x minus 1 to 1 and right hand side is this. So, that 2 W's and 2 x j's. So, I have to just write this as W 0; f x 0; x 1. Now, what is function f x 0 is 1, so this becomes 1 and this totally known this is 2. So, I can do the next one; so I just do next one after that I will not do it. So, next one is minus 1 to 1; now you choose f x, I will do it here f x is linear; do it for x, this is how the x act.

So, this going to be x t x; this is x square by 2 minus 1 to 1; so, one half; so this is 0; this is one function. So, this 0 and right hand side will be W 0; f x 0, so I have to put that; no no actually by the way is not at the N points; x is not known to me, abscissas are unknown. So, I do not know this x is; they not the N points. So, let us call them x 0 and x 1; so let me call them x 0 by just (Refer Time: 05:48). So, x 0 plus; so, I get two more equations; for one for x square and one for x cube.

So, I have four equations and how many unknowns? I have four unknown's 2 weights and 2 x's; I can compute it. For the equation for x cube; so just let me write the equation. Next equation is two third W 0 x square and the last equation, I will just put it here 0 is equal to; now it turns you can solve it exactly you will not go this cubic, but you can do some simplification and it comes out; you know the answer and the answer which comes out to be; both the W's are 1 and my x 0; x 1 is 1 by root 3; x 1 x.

So, I should choose my Xs at that point; so, my function so any cubic order function. If you compute that function at these points x 0 and x 1 and I will choose these weights I will get exact integral; no error of course, fourth order will have error. We can also estimate error in this method; difficulty with this of course, I can continue this exercise and do it for Nth order polynomial.

So let us say N abscissas and N weights; I can get exact integral by this method up to unknown 2 N minus 1; N plus N are abscissas and N weights. So, I can get exact integral for 2 N minus 1; order polynomial. Problem; how where is at we will have very high order polynomial to solve that I mean this cubic already and fourth order fifth order there will be error in computing the X's. So, that should gauss comes in and this is where we can do it at better. So, I will just show you how to get it using one of the polynomials and we use first thing is; we use orthogonal polynomials, I mean this is this will use some of you knowledge of mathematics.

So, we will focus on orthogonal polynomials it has advantage which become apparent in the proof. So, I am going to again demand that I can do the exact integral up to 2 N minus 1. So, I am going to call this phi js is going polynomial; j polynomial, one example is legendre polynomial; I am going to use hermit polynomial, ligor polynomial all this polynomials are their advantages first one or (Refer Time: 09:21) but I focus right now legendre.

So, I am going to use legendre; so, we will use polynomials up to from j is going from 0 to N and because they are orthogonal legendre polynomial orthogonal.

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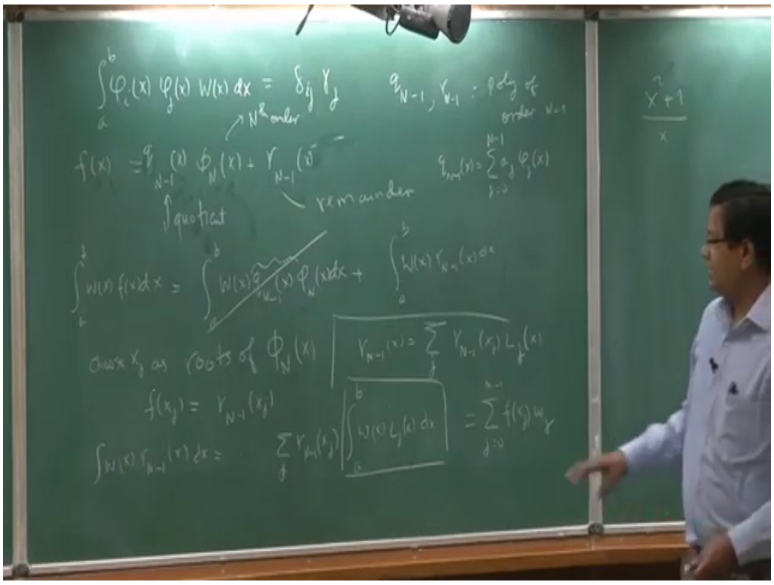

This satisfy the property phi I x; phi j x and this called weight function; weight function d x; a to b. So, this do not be equal to 1; they are not normalized orthogonal functions they are functions and this delta I j and gamma j. Gamma j is the number that is the properly orthogonal; everybody knows this.

Student: Sir

Yeah

Student: (Refer Time: 10:30)

Well polynomials; no W x we keep it separately, is convenient. Polynomials are; it is convenient not always W x is 1; you do not absorb in phi x; not true. So, this is a orthogonality; now I am going to start the proof. So, my function f x; since I demand that it is exact for this. So, assume that function of this order, so this function I will write. So, I divide this function by phi N x; phi capital N. So, divide this by phi N x; so, there will be reminder and the division. So, reminder is of what order. So, divide let us say function x square plus one by. So, this I divide by x.

So, I will get x plus 1 as the reminder. So, here this is nth order polynomial. So, reminder will be N minus 1 Nth order polynomial because overall is 2 N minus 1. So, these are reminder this while this called revision reminder; my English is poor this is a factor and reminder will be this notation; this not r, I have use my own notation q N; q N minus 1 this is factor and this r N minus 1; this reminds which remains is the factor and both of them are order. So, q N minus 1 is written here in fact, r N minus 1 polynomial of order N minus 1; is that ok? Just a division we do not need to figure out, but that is should be the case; in fact, this is called quotient.

Now, let us integrate this W x; f x; d x; a to b; W x the proof is definitely belongs. So, plus x; now what happens to this using orthogonality; this quotient is a N; s 1 N minus 1 order polynomial. So, it can be written this combination of; it can be written of polynomials in a series, but each of them will be order is less than equal to N minus 1. So, this is this 1; so, let me write here q minus 1; x is sum a j; phi j of x, but j goes from 0 to N minus 1 like polynomials that is what we do.

Now, if I integrate this here phi j and phi N; integral W x is 0 this integral gives 0. So, we need to only worry about this; so, the next step now I have to choose my x's please remember that I need to worry about that x j which x j I should choose and which weight I should well weight will be determined once you choose x j; so that is the whole idea.

Now, the next part; step two starts that which j should I choose. So, the x j you should choose; choose x j as roots of phi N of x. Since Nth order polynomial should we have N roots? Like x square minus one has two roots. So, it will have N root; so that is where I should choose and that simplifies. So, it in fact, it give me; so, no x j I am fixing. So, abscissa I am fixing and we need to find W; in as convenient form I do not want to I get some inconvenient integral, I should get a exact illustration. So, now if they are the roots then what happens to f x j; so, earlier the function add those points because this is 0. So, you will be see you will get r N minus 1 x j.

Now, let us look at this integral W x; r N minus 1; x d x, now I am going to expand this polynomial. So, this is j other r 1; so, I will expand this as the; so let me write this before I get here this part; r N minus 1 x. Actually not in terms of phi j; I am sorry I made a mistake, I want to do Lagrange interpolation not phi js.

So, do Lagrange interpolation; so, this r N minus 1 with the same points x j; l j of x, this Lagrange interpolation, so this guy; I am substituting this one here; so, this is a constant. So, you will come out the come out of the sum; so it comes happens to be r N minus 1 x j integral W x; l j x.

Now, I call this is the weight function; in fact, look r N minus x j is same as f x j. So, I can write this as f x j and there is a W j. If you compute this; this involves roots of phi N; So they involve x j; if you compute this I am done; in fact, that kind of; now only objective is to compute this. So, shall I just go through it once; so, we start from here. So, let us go through it once I mean this is there kind of very key steps which are taken. So, I expand my function; well actually this is I write my function after division with phi N x as this.

Now, I integrate this then I basically this becomes 0. So, I get a integral with r N minus 1 x; now choose x j's is the roots of phi N of this phi capital N of x and then this integral; this part, we want because this is the answer. This integral will happens come out to with this and this is my function value at x j's and this is my weight.

Student: (Refer Time: 20:07)

No, this will be all the polynomials which we leave with will have real roots like Lagrange has real roots hermit has a real roots. So in fact, use which are tabulated known those. Now, this bit of algebra for this I will just give the key steps; I have written on written them down in my notes. So, you can look at them in more detail how to solve this; how to simplify this not solve this.

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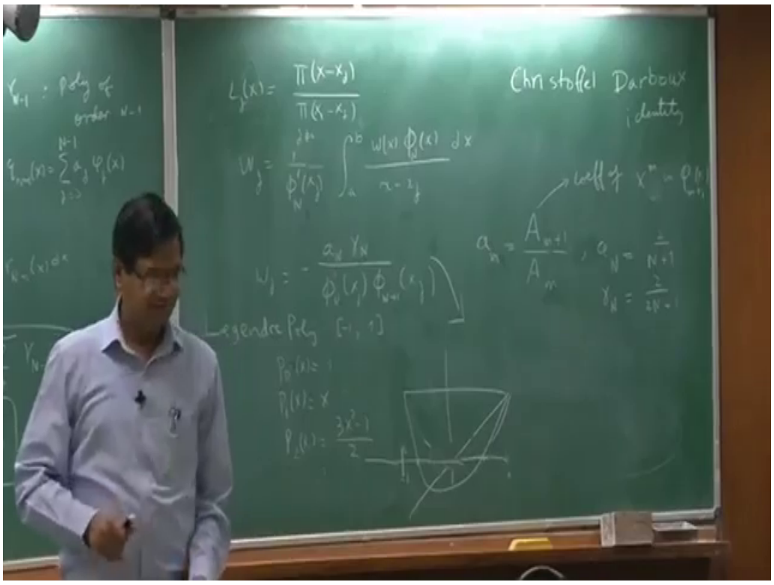

So, I will just write key; so, this l j’s; so, I will just write only few steps I will not write all the steps. So, l j how to (Refer Time: 20:54) l j of x is product, it involves a product x minus x a divided by product x I minus x j; j not equal to I all (Refer Time: 21:12) So, we did this in the past; now I think I will skip all the algebra because this is it I mean it is bit tedious to write on the board. So, I substituted; so W weight W j; 1 by x j integral a to be x, x, x. So, now I am getting back to phi’s because roots are sitting near the x j’s. So, I will skip the proofs, but now phi’s are appearing polynomial we started with.

Now, this can be further simplified by a theorem called Christoffeldarboux identity the proof is not difficult, but I will not do it on the board Christoffel. So, if you use it with quite few steps is one page W j; is minus a N gamma N and what is gamma N I defined already is a gamma; corresponding to j equal to capital N. And a N is defined as a N plus 1 divided by N and these are the coefficients.

In fact, let me define orbitry m. So, coefficients of X m; X per m a in phi m plus 1. So, there is a first coefficient; so, the x two per m write for phi m plus 1. So, this is first coefficient; so, these are the definition. So, polynomial need not be one first coefficient need not be 1. We will do an example show you how to compute for Lagrange; around is a proof clear; the key step there is algebra in any proof and there are key ideas in their group given proof.

So, the key ideas are like this function is key idea choosing roots is a key idea; this is really key idea and then as of is Brestal algebras; this is the key idea. So, you choose abscissas after that weight is automatically decrement. So, in any idea so if is the idea is key after that lot of algebra. So, instant theory; so what is key idea I mean you know for special duty and general duty today the big news. So, what the key idea of special relativity?

Student: (Refer Time: 24:52)

That is not the key idea all (Refer Time: 25:00) equal at. In fact, speed of light being same; according to me follows from the first that for relativity what is key idea?

Student: (Refer Time: 25:15)

General relativity.

Student: (Refer Time: 25:23)

Equivalence (Refer Time: 25:25) for the key idea. So, one can accelerate; accelerated frame is related to gravitation of frame. So, there is a key idea and algebra which of course, you have to good at, but you can refer here and there can well I survive with this key idea; but you the (Refer Time: 25:42). So, now let us work with Lagrange polynomial and try to get a formula working formula.

And in fact, you can use different formulas, different polynomials to get different quadrature formula this called quadrature this integration is same as quadrature. So, Lagrange polynomial; so, I have few of them. In fact, I have this plot nice plot, but I will just listed; so, p 0 of x is 1; typically they are constant. So, all polynomial first one is constant and it for this is 1; p 1 of x is x and so these are defined from minus 1 to 1. In fact, you encounter Lagrange know; where you encounter Lagrange?

Student: (Refer Time: 26:56)

Squaring harmonics it comes at cosign theta. So, cosign theta will give you minus 1 to 1, p 2 x is 3 x square minus 1 by 2 and so on p 3 x, p 4 x there all. So, you see factor is not 1; the first one a; m is not 1; here a means 1, but not here and so on. So, for Lagrange polynomial you can simplify this further because now I should tell you what that is N what is gamma N; so, this can be made simpler.

Now for Lagrange polynomial; so, this one actually let me just write this a capital N; a is divided by 2 N plus 1 N gamma N minus 1 and this bit more algebra which is again here in the notes. So, this is further simplified within this plus it turns out you can also rewrite this at terms of derivatives or you can write this terms of this. I will skip this; this algebra is not; so, exciting. So, if I substitute all this term the formula which is coded in text book is this; phi.

Now, is you find this in table this is a derivative of the polynomial and you have to compute at the roots and x j is theta which is in fact, 0s of phi N; not phi prime. So, this can be computed and that will give U weights. So, let us compute it for second order before that I want give the formula for the error. The error formula is also the derivation is not trivial, the error formula derivation. So, error in this scheme will be 2 N right; so, is like I finish everything up to N; 2 N minus 1; so, error has polynomial order 2 N.

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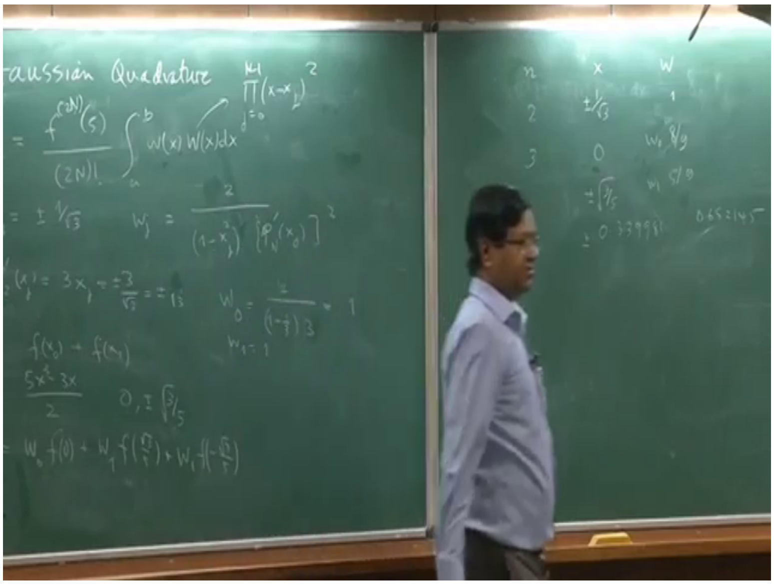

The formula for error is so, I am not proving it. In fact, that involves hermit polynomial which I skipped in class. So, I told you that you can write the Lagrange interpolation; this also hermits interpolation which involves interpolation; not on in the class from that one can derive the error formula and the error formula is 2 capital N and this one is product X minus X whole square . So, x j's are the roots, but squared; so, this is higher order polynomial 2 N minus 1 order polynomial; 2 N minus 2; 2 N minus 2. So, this is very accurate error is higher the order accurate in that series.

Now, let us work out the weights now is an example; so, I written down Lagrange interpolation polynomial. So, let me just get W N x; so, I am going to make this capital N equal to 2. So, capital N equal to 2; so, my integral will be exact up to 2 N minus 1; which is cubic. So, what is the abscissas x j? So, it should be root of p 2 or phi 2; I should have written phi 2 or p 2. So, what is the root of that one plus minus 1 by root 3; first take make it 0 and I will get plus minus 1 by root 3. So, these are root; so, you can also visualize them how they look like.

So, let us do it here; so flat very useful function in computation method. They are the most useful this one (Refer Time: 32:44) polynomial; they are the most useful not hermit hermit is not so useful, leggier is not useful. Lagrange and (Refer Time: 32:52) if you do computation; these are really very important. So, minus 1 to 1; so, well I am going to put; let us put the access here minus 1 to 1; flat x 1 is this one; third one is three x.

So, at x equal to 1; what happens? It is 1. So, it comes down like this is even know; this, this. So, all even ones a even and odd ones are odd; I mean odd n's are odd; even n's are odd even n's are even. So, you draw like this, so I am using this one. So, my abscissas will lie between minus 1; N 1; sorry I did a mistake it has two roots; it is 0's at this point.

So W's; how do I compute W's? W j? So, W j formula is where did I write? I erased it; I think erased that one. So, let us write W j formula.

Student: There is a W j there is a.

No 1 minus x square.

Student: (Refer Time: 34:22)

One with I just erase it; so, there is for Lagrange polynomial. So, this is general these two for any polynomial; in fact, we need to use other polynomials where limits are minus infinity to plus infinity that is why hermit is useful, but for finite Lagrange is useful for box and all that is Lagrange. And the formula for Lagrange I am using P let us use P N prime these uses a property of Lysander. So, this specific to Lagrange; so, what is P prime 2 of X, take the derivative of P2. So, it give me 3 X; so, 2 will cancels. So, now, I have to compute them at the abscissas points. So, the values of P X j will x j in fact, they are plus minus. So, 3 plus minus by root 3; so, this become plus minus 1 root.

So, these are the; in fact, this happens be equal which is nice with since I do always squares. So, I will be safe I do not need to worry about this. So, what are the W's corresponding to this so. In fact, both let us say both 0 1 minus x j; I made a mistake square is inside. So, 1 minus square of this will one third square this one third and 2. So, this is 2 by 3; I made a mistake I think this root 3 above; 3 by root 3. So, this above; so, this is 3; so, this becomes 1.

So both; in fact, both W 1 is also 1 let just check. So, my formula what should I write for with N equal to 2. So, my integral is W 0; f x 0; so, f x of 0 W 0 is 1 and W 1 is also 1. So, f x 1 that is it this is straight forward know; I will give you cubic order accuracy. Now let us do the next one N equal to 3; so, 3 I have to write down on the polynomial third or polynomial.

So, p 3 of x is phi x cube minus three x by 2; by the way. the gamma is not want for this know I wrote the gamma is that. So, now you can just derive it, so I will not go through derivation. In fact, this can be done by hand. So, some of this you should do by hand. So, you can compute that derivative of this one what is the root. So, this should be 3; 3 roots 0 plus minus root 3 by 5. So, I should compute the functions at this values that is it; you do not need to compute elsewhere is compute this.

Now, weights so in fact, people give in terms of table. So, let me just write the table; so, you can compute W's so, but is written since is a odd or even. So, it turns of something weights are equal as some abscissas are plus minus. So, is written down table this is the following n, x, W.

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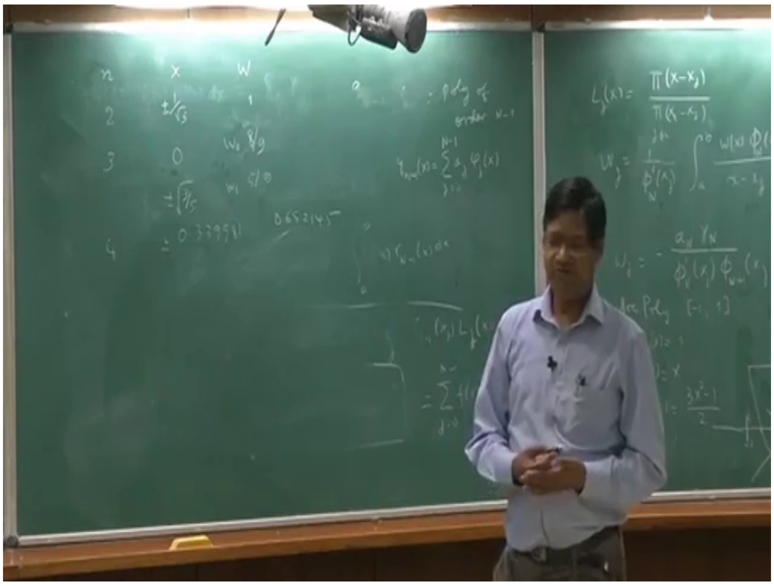

So, for N equal to 2; xs are 1 by root 3 plus minus and weights are equal 1. For 3 by roots are 0 plus minus root 3 by 5 and here it is now comes from some from 8 by 9; and this is 5 by 9. So, we write like this then for N equal to 4; now I written in terms of number; you can take a long 16 digit number.

In fact, you can just keep in your file 6 digits numbers; I have written only for 6 digits. So, there are four roots there plus minus only two of them; plus minus I just write one of them; 339981 and this is 0.652145; so, you can read of from the table.

And so, for p 3; my integral will be W 0 coming from here. So, I read of this one and well the function is computed 0; no sorry actually this one function computed 0 is fine f 0 plus W 1. So, W 1 actually 0; you should not mistake with this is x equal to 0; this is not j equal to 0; j equal to 0 will with really start from miligator. So, my function is computed at root 3 by 5. In fact, this weight is same as I am going to call this as W 1 and this computed at. So, this will give you accuracy up to fifth order x 2 or 5. So, that is why it is very powerful; in fact, if you compute the function at any given point Gaussian quadrature is the best for integration; not Newton cotes.