Computational Science and Engineering using Python
Prof. Mahendra K. Verma
Department of Physics
Indian Institute of Technology, Kanpur

Lecture - 11
Integration I: Newton Cotes

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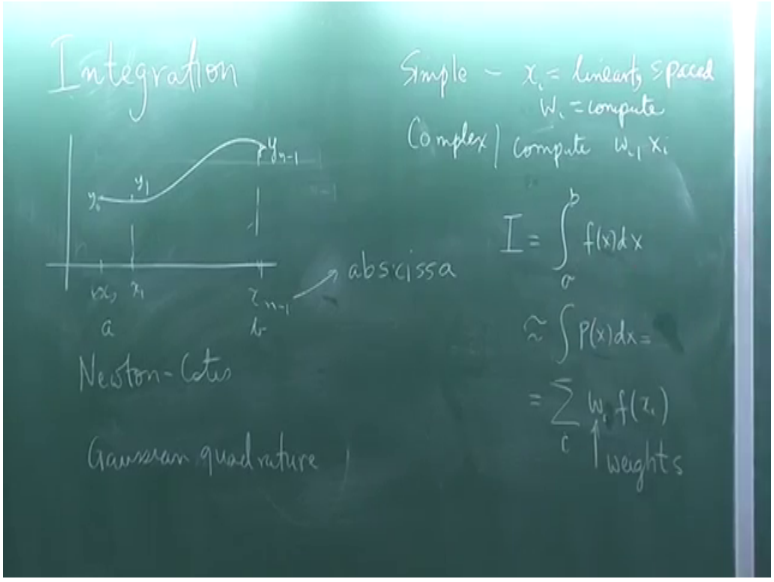

So, now we go to integration, so we will do numerical integration. So, we will be given n points; so, we have X axis. So, we have x 0 to x n minus 1 and values of the function at this point. So, this is common theme; interpolation we had n points given x i's and y i's and I try to fit a function. So, please note that interpolation I do not need to find the value at the given point; any point which is not given, but I can give the full function and using which you can find at any place you like.

So, there is a whole idea; so, I have give you a function; which will go through all those points. So, integration also we have all these y's; so, there is y 0, y 1; so, some curve will go through this. So, of course this curve I need interpolate and once I interpolate the curve, then I can find out integration; so if I have f of x, I can integrate.

So, well and if the technology is within several steps and there is many methods to integrate. So, I will cover two; so, this called Newton cotes; again these are same Newton; Newton cotes method and the second one will be Gaussian quadrature, in fact so this methods are classified into two class; called simple method, where it is simple method and complex method. So, a simple method; there are some notation here; so, x i's called abscissa. Now, I am going to approximate the integral, so we have finally, the formula whatever derivation you do; the formula for the integral. So, I go from recall this point from a and point b; so, n points are a and b. So, integral a b, f X; d X these are approximated by a polynomial P X; d X and this is going to be written for all the; these are notations. So, standard notation which you follow equal to W i; f x y. So, this x i's are abscissas and W i's are called weights.

So, this function is known to me these are all y i's; I just multiply by W i and that I getting it. Of course, our objective is to compute W i's, give W i's so in simple methods; x i's are linearly spaced, they are given to you and you compute W i's. So, that will be part of Newton cotes, but in complex method Gaussian quadrature; x i's are not known. In fact, if you get x i's so that your integral is accurate; best accurate possible.

So, here in this case; compute both W i and X i so that your error is least. So, they are more complicated that is why is complex method, but this really good it gives you very accurate results. This is not so accurate, so we will cover first which is simpler; Newton cotes. So, idea is quite simple; so, see I need to get this P x, which is the approximation of f x.

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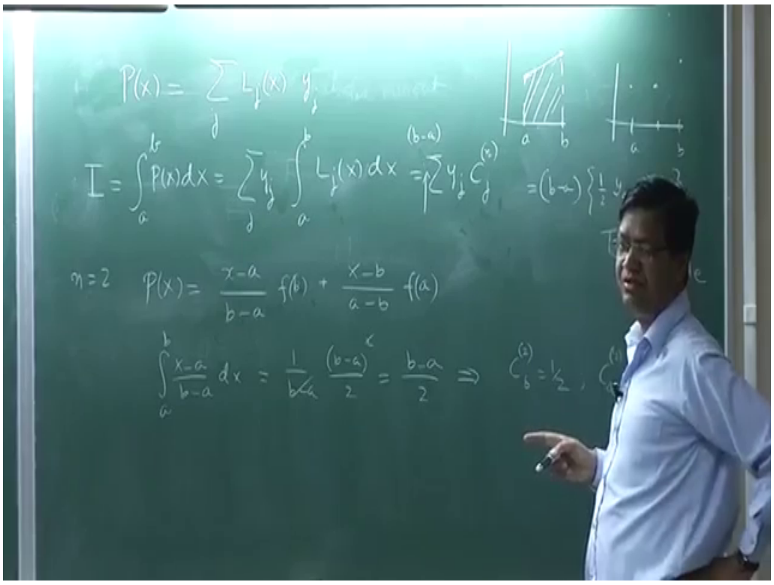

So, P x will apply Legendre polynomial, Legendre interpolation which goes through all the n points. So, we already done this so, that is why defined that interpolation using which can we derive lot of numerical schemes that is why it is called mother of; well I will not say all, but lot of numerical schemes.

So, we write this as j; L j; X and y; so this is function of x. Of course, a remorse also X i's, but is no y dependence. So, once affects axis; then this is independent of y's; now to get the interview. So, I (Refer Time: 05:58) approximate I; so, integral P X; d X. So, when notation is slightly changing I and j; so, please do not mind. So, I; j is running index, so the integral; so, I will put a to b; n points.

So, this will act only on L j; it cannot y is constant. So, I can say y j outside some more j's; integral L j; X, d X; a to b. Now this can be computed given X i's given abscissas you can compute this and so, this y j and notation is C j with; so, how many points are using for abscissas. So, minimum I need two points; so, there is no intermediate point, you just a and b. So, the minimum will be; so, let me just draw it here a and b, so value of the functions are given here. So, there is a lowest order; so, it will give a linear interpolating function.

So, next would be I give you 3 points; so, there will be a point in between a and b. So, the a b and there is something in between; linear spaces phases equal to midway. So, I give 3 points like this or 4 point; so, for all this point you need to give a C's; C i's is c j. So, I need to specify how many points are using; so, that is why there is a notation called n. So, for this n is 2, for this n is 3 and you can have n to 4, so more points you take; more accurate that will be. So, we need to integrate this; now let us do some trivial functions which n equal to 2.

So, n equal to 2; what is my L j? So, let us look at P X. So, P X will be; so in fact we did this before. So, x minus a; so, the next one b minus a; this will be f of a, f of b. So, if you put x equal to b; then I get f of b and then I get x minus b, a minus b. So, this is a formula of Legendre interpolation; now so these are L j's; two of them. So, I need to integrate this; so, that will give me two coefficients; which will multiply at f a and f b.

So, integral of this is x minus a, b minus a b x; a to b; so this is straight forward know. So, 1 by b minus a; so, b minus a whole square by 2; I made one mistake. So, this multiplied by b minus a; so, there is a multiplication of b minus a. So, C's are the dependence of c minus a is less on C's. So, there is a b minus a factor; so, this is b minus a by 2; implies what is c corresponding to this half. So, C corresponding to point b is half; similarly you can compute this is just algebra; C corresponding to a is also half for n equal to 2. So, what is answer for integral formula for n equal to 2?

So, it is b minus a; half y a plus half y. So, this what is it called? You might have heard this; the trapezoid rule; in fact, this area, so this is called trapezoid rule. We can also do for n equal to 3; there is a Sympy rule. So, n equal to 3 has 3 coefficients and n equal to 4 has 4 coefficients and so on. So, I am going to run the code actually I leave Sympy well I hope you want to learn it.

So, symbolic manipulation I can do integral exactly; you do not be numerically integration, but this integration can done exactly because a, b are symbols and I will get half; exact half. I will show you how to use Sympy, but less before going into that these are formula for arbitrary n; these called Newton cotes method. So, your objective is compute this, now what is the error? So, we should also be able to find out what is the error is; formula for the error. So, how do I estimate error? I am going to erase this part.

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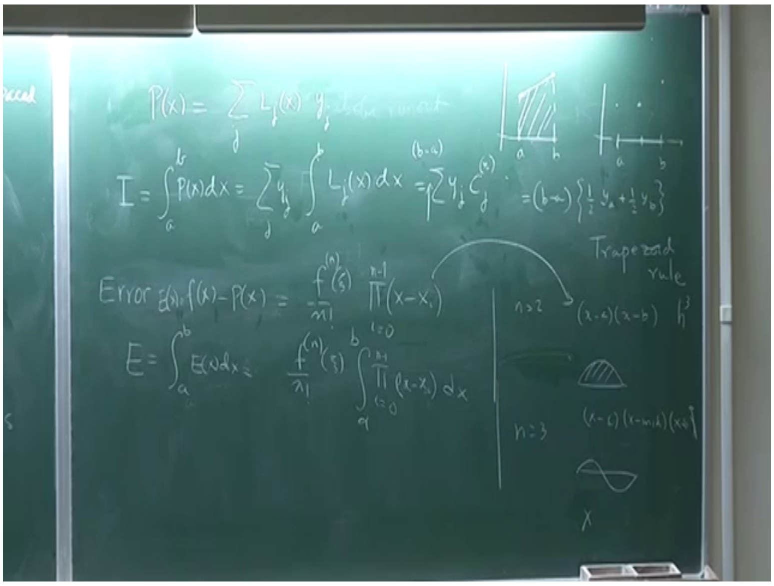

So, table I show you, so once I start the computer; I will show you the table where C's are nicely tabulated. You do not need to compute, you just take from the table; well you compute once; which are that you should compute once? But then after that take from the table how do I estimate error? So, you already done the error for Legendre polynomial; so, remove the error.

Student: (Refer Time: 12:46)

Yes.

Student: (Refer Time: 12:49)

This is analytically doable.

Student: But.

Well, which order do you want I mean computer will do for fiftieth orders; you will computer will do it will take longer time you can do 100 column.

Student: (Refer Time: 13:10)

Symbolic I will show you how to do it; that is not numerical, there is a mathematic symbolic manipulation.

Student: (Refer Time: 13:18)

Actually.

Student: (Refer Time: 13:25)

No look here polynomials can be integrated. So, these are polynomials; so, polynomials can be integrated analytically.

Student: Sir.

These are polynomials; so, integration possible. So, error I estimate by what is the error in Legendre polynomial itself. So, what is f x minus P x? Which is error E; f x, we said is one over n factorial, f n zeta; zeta lies between a and b, we do not know what zeta is but zeta is point in between. Product X minus X i's; i was from 0 to n minus 1; so, these are error in the function; we do not know zeta, but zeta lies in between.

So, how do I estimate the error? So, I want it f X; P X, but I computed P X; d X. So, error is basically interflow E X; d X. So, error is integral a to b E X; d X. So, this is a number; we do not know zeta, but we can make an estimate what is this number; upper bound on it. But this is duable; this integral again computer will do it. So, I can do over n factorial; f n zeta and integral of this. So, there is a error but there is a little bit of catch.

When once I do it I done this integral. So, if they only two points then error is finite this function will be. So, what is it function will be? For two points is product of for n equal 2; let us write n equal to two my function with this guy will be x minus a x minus b . So, this 0 at both ends when it is quadratic in between. So, this function look likes that; so, area under the curve is finite.

So, that is these non 0 value; but for n equal to 3, you get so in fact, this is the midpoint. So, x minus a, x minus mid, x minus b this will have behaviour like this and it does not because 0, which is good actually; Why is it good? So, my error at that order is 0, but I cannot see my error is 0; I have to go to higher order. So, error is higher order, so just to. So, I will give you the table; so this will computer will do all the computation. So, this error is of the order of h cube and h is b minus a; h cube. So, you can just do the algebra as h cube, but for this error is h 5 not h 4; so h 4 is 0 is goes higher order. So, it gives much better accuracy; so, you choose n odd points.

So, the one I will approximate; if this gives me 0; well as well affect you have to keep the polynomial of the next order in that computation and then that I will do is. So, I multiply this for taking a point outside and make a polynomial go through this, but integral only from here to here. So, E X is integrated from a to b from the polynomial is higher order polynomial and that gives you non zero error.

So, this error I am not going to do algebra here, but error is less for n odd. So, now let us; so is that clear? The idea is clear all of you? Now, I will show you two cotes; one how to compute this C i's and second just do Newton cotes by various orders; so, which one should we will do first?

Student: C.

C i?

Student: Yes.

Now, actually let us do the other one because C i have some new concepts. So, Newton cote give us C i's; I will show you how to compute within straight forward by just a code you should go through the code and how to compute the error. So, before we go there I will just show you the table.

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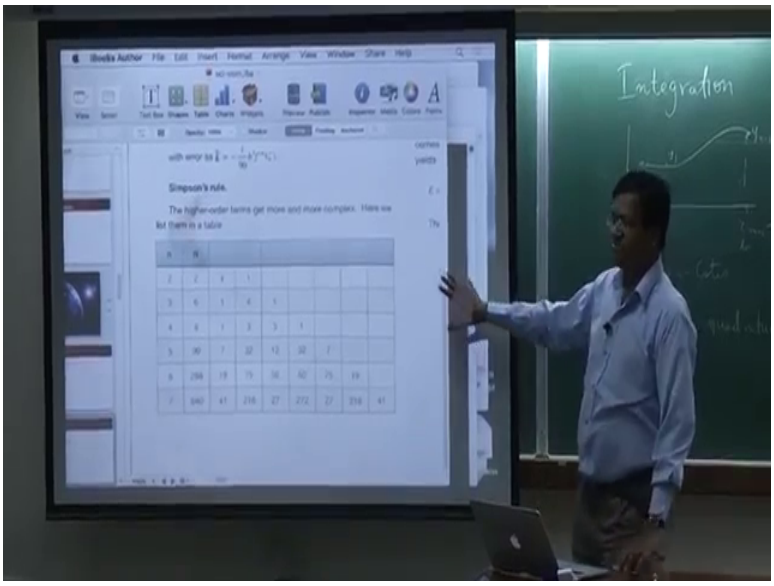

So, this table is given in any book; so, how do I get the coefficient. So, coefficient is obtained by; so, divide each of this numbers by N capital N. So, it is going to 1 by 2 and 1 by 2; for n equal to 2, number of points. If number points is 3 is going to 1 by 6, 4 by 6, 1 by 6.

Student: Is this computed?

Is computed. In fact, I will show you how to compute them by Sympy. So, for n equal to 4; the left most point is 1 by 8; the 2 midpoints are 3 by 8; 3 by 8, each and the last point is 1 by 8; this symmetric you see that is symmetric. So, these are the table we will not use; so, do not need to compute from scratch and what is the error? So, is that clear? So, these have to seventh order; you can compute higher order; this will; not a problem.

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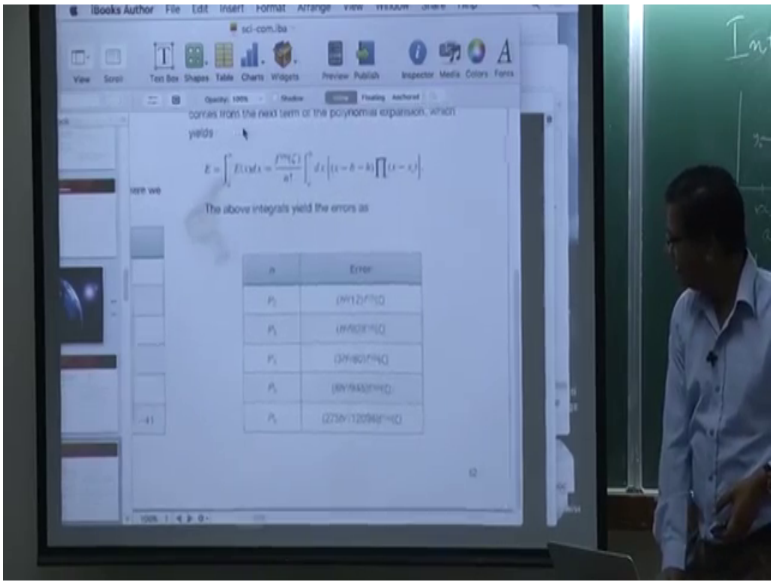

So, error for 2 points; error is h cube and the zeta, f 3 zeta; third derivative of zeta, but this fields always put a bound; lower and upper bound, I did that for exponential. So, these always we do not compute zeta that is insane, you do not want to compute zeta and is order as h cube; P 3 is order h 5; I am not sure you can see this order h 5. So, it jumped by 2; so, 3 I should exporate 4, but fourth order is 0; order higher. So, h is small; h is suppose small, so this more accurate P 4 gives the h 5. So, P 3, P 4 have same accuracy in terms of h P factor is different, but same accuracy.

P 5 is again h 7 and P 6 is again h 7, so these are formulas; we can also compute using (Refer Time: 20:40) like the factors 112, 190 is all comes. So, let us see the code this is coefficient alright; so, this is computing in different orders.

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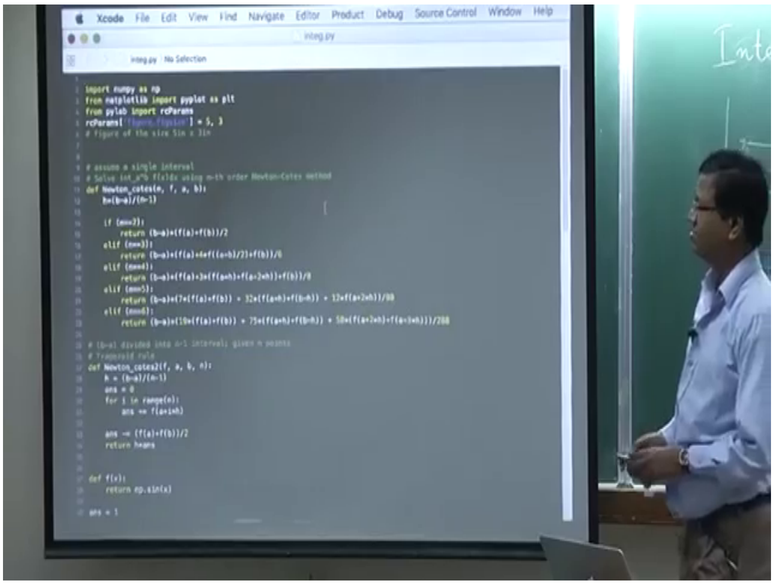

So, this is slightly tiny fonts; so, Newton cotes the number of points, the function I can pass a function as argument which I am not sure you may not have done it; you can pass the function as argument to (Refer Time: 21:32) So, we will define f; like f is defined here is sign X. Now, this by definition these a lower point and this is the minimum x and this max X. So, for second order this is just a b; for third order I have to insert a intermediate point.

So, h is half of b minus a by 2 well b half of b minus a. So, these are formula for 2 points; this step is are rolled. For 3 points; these again coming straight from the table one sixth of the first point, four sixth of the second point and one sixth of the sorry not 4 sixth; 4 sixth third is one sixth again and multiply by b minus a always. So, these all multiply b minus a and these are all taken from the table; is that clear how to write the formula? So, every point you multiply C i's and multiply by b minus a at the end.

So, this will give me function give me the n point and give me the number of points you will not use. So, you give me a and b; you do not give me intermediate points, I will compute it is linear linearly spaced. So, if you done it; so, this part is running the code; so max order is 6. So, I go up to sixth order I integrate it, so put the value and take and error is here from j going to 2 to 6 range. Actually we will go up to 2 to 5 in fact if you will not note range will take up to only 5; the range is last minus 1.

So, Newton cotes I know the formula; the function and error is computed as this is absolute you just take the absolute of this and I printed as a plot it. So, (Refer Time: 23:49) I need at least two points; so, I should not plot for 0.1 or 0.0 because they all 0's and they are plot in log scale because things are error is falling can have exponentially. So, I am putting log scale and this is the 2 to max order.

So, we will go to backs for minus 1; is range I am using range and this error up to this again is max order minus 1; last point is max order minus 1. These are standard; you understand where X are minus 1; so, if I say array of size array 5; then the last one is has index 4. So, that is the last index is 4; so, I put the label. So, if you just run this; so, shall I run it or I can show you the figure plot. So, let us run it.

It will give two plots, but first let me just run this.

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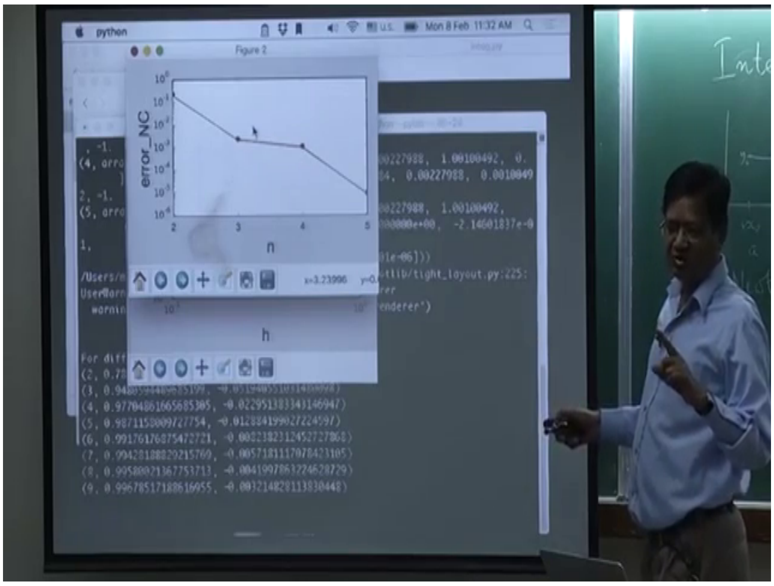

So, it is giving you this is a; this is figure this deriving two of them; these are error. So, this for n equal to 2, error is of the 0.1. So, this sign function is equal to phi by 2; answer is 1; integral sign X; T X and the error is 0.1, which is 10 percent; which is significant, but then it has come down to just taking 3 points; error is distance minus 3; so, it is 0.1 percent and 3 to 4 error then decrease much.

So, every odd points the error decreases rapidly. So, it should be odd number of points and at 5 error again decreases; 6 it do not be decrease much and it 7 will decrease again.

So, we can compute the error; now suppose I have function a and b are far apart; a and b are not close by they far apart. So, my function may be reasonably like this; if you use trapezoidal rule is bad. You should not use, we will had order it my capture intermediate it may capture in actually you should do? What should I do here? I should not use this 2 points.

The idea is two meet further divisions and each of this part; I apply Newton cotes. So, that is the idea, you should apply Newton cotes at each of this small slices. So, I made many slices; so, I have one example where I can just apply trapezoidal rule for with many slices. So, suppose you have m slices; so I am going to apply only trapezoidal rule which is simple and illustrate, you can also use the higher order.

Of course, I am assuming that the function can computed at all this points; is that clear? So, I am going to do trapezoidal here, trapezoidal here, trapezoidal here. So, this is point a and b, but I have intermediate points. So, actually if you call this is b; then this is again a; b like this. This is what I am trying to do; so, these are 0 and this X n minus 1.

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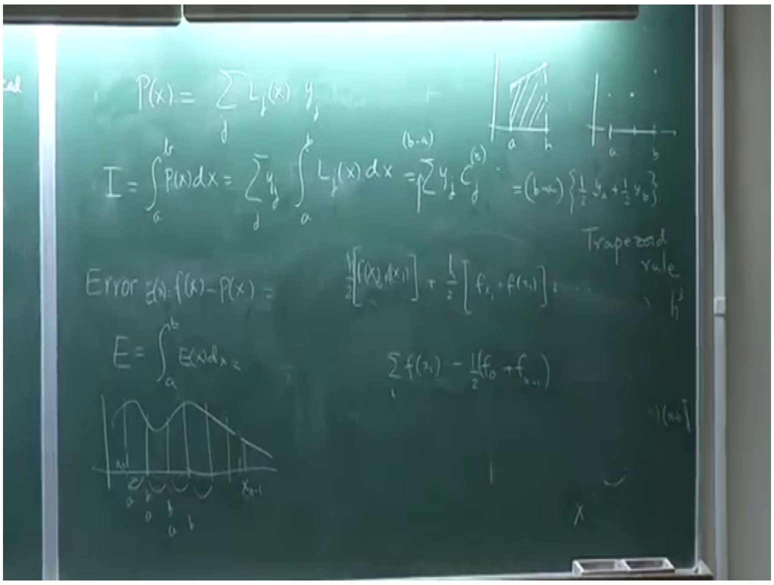

So, trapezoidal rule give what? The first integral give you X 0 plus X 1 by 2; non function not 0; half multiplied by this h, not b minus a. So, h then same thing I will get for f x 1; I am going to make a short n f x 2 like this. So, it is a sum of trapezoidal sums of each segment; each slice.

But if you see f x 1 can be added from here and here. So, all the intermediate points; you can add half plus half. So, this will know how many multiplication and addition; it involves 2 addition for each slice. I can decrease order; I can write this as sum f x i’s. So, sum more all because all of them are one because there is half contribution from the left and half contribution from the right.

But n point factor is half, right? So, what I should do? I just sum it of minus half at f 0 plus f n minus 1; this is cheaper, I do not have to do n sums; I just sorry 2 n sums, I just 1 n sums and subtract one number here. So, these kind of tricks one can use and one should use. So, that is a part shown here as well; so, if these quite common that you are do trapezoidal rules from minus slices or Sympy rule from minus slices. So, this integration part is given here.

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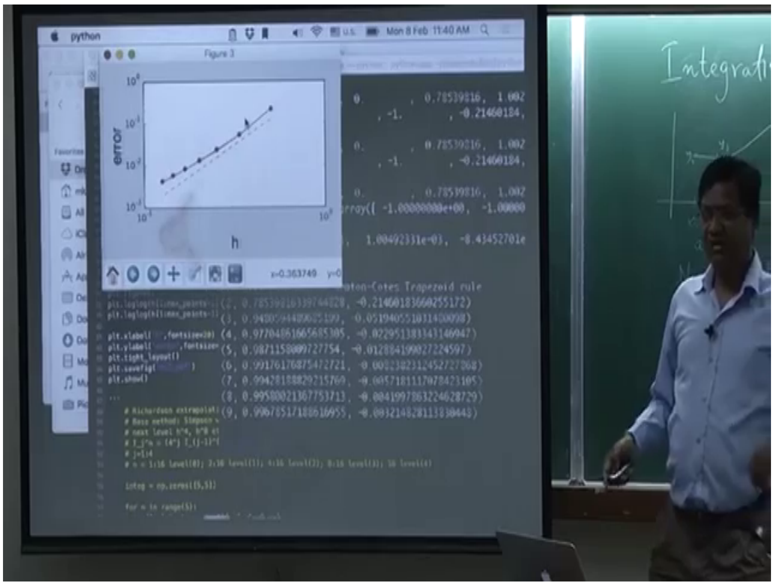

So, Newton cotes 2, but for 2 but I do for n points. So, I have to compute h which is b minus a. So, I am n minus 1 slices and then I do this sum; so, I just doing this sum; finally, subtract half of the n points. So, this will give me the answer for different h; so, this is what is done here; max number point is 10; then this sum is straight forward.

So, I get for different h; so, first time h is beat, which is phi by 2 and next time is h is phi by 2; phi by 4. Then phi by 8; not phi by 8; phi by 6; so I just keep dividing 1 by 2, 1 by 3, 1 by 4; so, that was other plot which we saw. So, question is how does error decrease with h? I am making small small slices.

So, we know the answer; I told you the answer. How does error decease? With h who said h cube error decrease h cube and so this is h cube. So, this for h which is largest h this one, then decrease h by 2; this h by 3, h by 4, h by 5 like this and this line is h cube. So, I am going to finer and finer h and my error is decreasing 10 phi minus; well somewhere like; so, you know how to read this of?

What is this value? This value; so you see the ticks? So, what is the value? Tell me. This value is how much? y axis 0.001; what is this take corresponds to this one 0.002 you should know how to read the log scale. Next is 0.003 this 0.004; they are not linearly space because it is log scale and when you plotting them. So, this is 0.2, 0.3, 0.4 like this; so this is h cube. So, it is going like h cube you can say; so I had 10 minutes to briefly introduce sympy. So, simple let us do one or two functions; so I will just do one this will quick I have 10 minutes. So, first import sympy or form sympy import; f i impose symbolic. Now, here I have to define which are symbols and which are numbers; well we do not define which are numbers. Numbers are already known; symbols you have to define which are symbols.

And is defined as; so, let us a I will not use X is a symbol. So, X equal to symbols and what I will going to use in your code; in your program. So, I am going to say I am going to use X itself, but X will not be evaluated; computer knowns that it is symbol. So, I put in single codes, this tells that X is symbol. So, I enter; so actually no; let us do one thing I have to say sympy dot symbol. So, that is what I; so I will not avoid that. So, X is symbol now you want to.

Student: (Refer Time: 35:24)

Sorry.

Student: (Refer Time: 35:26)

Start means all; so, you will not integrate. So, actually sympy has very good documentation; then there is download PDFI. So, sympy documentation if I say we will get the full documentation, but I want to do integration. So, integrate X; so, let us say X square; so, I will not integrate with X itself. So, it will do the symbolic integration X cube by 3.

So, this assumes that X is symbol and we will do it. I want to do within a bound; so, if you will not do within a bound. So, say X lower bound and upper bound; it give exact number, it not going to numerical integration; it gives this exact integration and one third. So, we will use this feature to do our computation of C X. So, is this clear? I mean quite simple you just try to which are the symbols and try to do it that is. So, it can do lot of stuff; this really fancy and this differentiate, we can do vector calculus derivative radiant all of it. So you have to see this.

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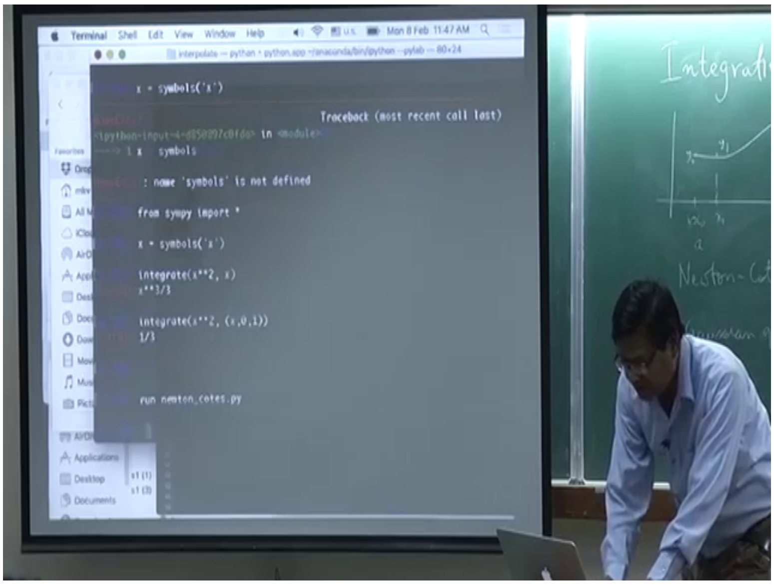

This code quite carefully; so, first start I want to declare what are my symbols. So, I have quite a few symbols we can do in one short. So, symbol within argument you have to put within a small bracket argument document; small brackets. So, X; a b and h these are my symbols; so, n is 3. So, I am just choosing three points; so, my h will be b minus a by n minus 1. So, this n is a integral, so computer knows that part and I am going to create X arrays where which will give me the coordinate of the abscissas; X array contain abscissas.

So, what are they I just do in a loop a plus I h straight forward, so it will be containing symbols will be a, a plus h, a plus 2 h, dot dot a plus 1 minus 2 h symbols. Now, this is the loop if you read my code about Legendre polynomial is exactly a copied from there. So, copy paste; so there is no shame in copy paste. So, n is size of the array; so, coefficient I am going to create.

So, I will be see clubbed together in array; so, coefficient is in array. So, you go in a loop. So, I had to how many elements are there? Coefficients are there? So, I have 0 to n minus 1; n of them and so, numerator this part is common from our earlier code. So, j not equal to y; so, this is a that L j; this L j, I get L j symbolic. Then I just integrated from a to b is the I have to factor b minus a; so I have to numerate this b minus a factor; I told that b minus a I have to divide b minus a, and do you simplify.

If you do simplify big expression and compute also compact; it does intelligently compacts it and it gives a number and I append it to in the loop. So, after all this computation I will get all the C i's for given n.

I can also compute error. So, for this factor is X minus X i for all i's, but recall I said for even n that will work for odd; I have to use a point after b's. So, this is that condition. So, if it is odd; even you have to do separately. So, this part of I am just multiplying by one factor; so, this works. So, is that clear to everybody? So, just do the symbol and only thing is difference in our earlier coding of python is this symbol and I have to do integration here like this.

So, let us run it; we have 3 minutes; is that ok? So, I will share the code I just have a look and study it. So, run Newton cotes; so I had to run this function. So, let us see it has defined the function; so, I need to run it. So, you can see what is X; X is a symbol, what is h? h is; so I am choosing n equal to 3; so 3 minus (Refer Time: 41:13) that is h.

Student: Sir (Refer Time: 41:15).

Simplify. So, without simplification the function is long one; it has a cube, b cube all that. So, what is a minus b square? So, a square plus b square minus 2 a; b; so, it will compact it, will divide it. So, it will do some more simplification. So, there h for 3 point; so, basically I need the midpoint when this is the midpoint; so, this h so I need the answer; so, Newton cotes coefficients. So, later what it written both coefficient as well as error factor. So, X array is already there; so, you just need to call X array is these for 3 points; so Newton cotes.

So, these are the answers. So, my coefficients are 1, 6, two third which is 4, 6 and one 6 and error is minus 1 by 90. So, I divide by already h 5; we look at the error part. So, there is a division; so, it works. So, you look at the table is exactly same number; you can increase n or decrease n plus decrease n and error is minus 1 where 12 h cube. So, I need to run again; so this is my answer. So, half coefficient and error is minus 1 by 12 h cube. So, you can put n equal to 4; so, it will work for all of them; so, you just then create this. So, we get it; so, you work play around with this sympy; slightly in order to just be use to it.

Thanks.