SCIENTIFIC COMPUTING USING PYTHON

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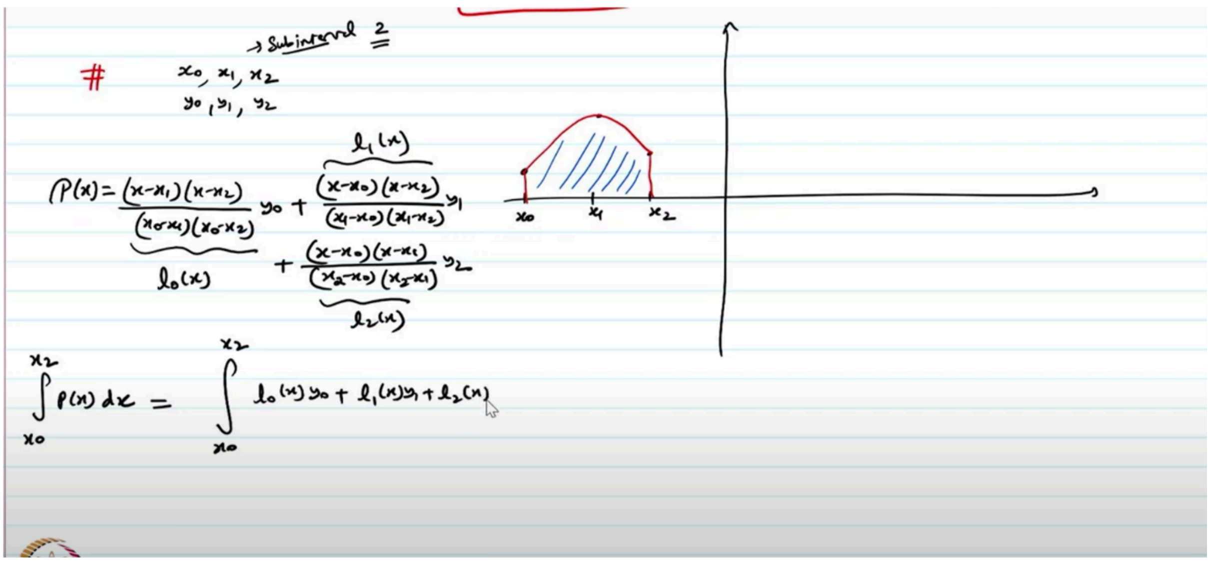
Lecture No. 31

Welcome to Scientific Computing in Python. In our last lecture, we started with numerical integration. So, today we will continue with it. So, let's get started. In our last lecture, we saw how we can calculate the area that we need to find or solve in integration using the rectangle rule. So, we also saw on the basis of the Python code how we can calculate it. Then we showed that we should make a trapezoidal rule. If we don't go by the rectangle rule, we should make a trapeze rule. What will happen to our trapezoidal rule? So, on its basis, we defined the trapeze rule. And then if we have to do the composite in the entire interval, then how can we use it? How can we define it? We did that and we defined its error. So, the error is that the second derivative of the second function is happening in this. The error for a linear function is zero. So we have done it till here. Now let's go a little further and see what will happen because till now all the approximants that we have seen, suppose we have three points instead of two points. And the values on this are x0,x1,x2, what? We have been given three points. So what does this mean? How many intervals will all the intervals be? It will be two in this case. So if we have this, what will we do now? Suppose we have our points. Now I am taking this. So, I took xyz somewhere. I took x0,x1 and took x0,x1,x2. Suppose one value is this. The second value, suppose we have this. Okay, the third value is this. Now I am going till here. Now what will we do? So what have I done to this? If the approximation is x minus x1 x minus x2 divided by x0 minus x1 x0minus x2 was plus x minus x0 x minus x2 x1 minus x0 x1 minus x2. Plus x minus x0 and x minus x1 x2 minus x1 we have this interpolator which passes through three points which means it is a quadratic polynomial, right? It is a parabola, this function. So now what we have to do is integrate. So now what I have to do is find out from where to where we have made an interpolating polynomial with P(x), so we will integrate it, okay, x0 from x2. Now if we see this value, we have l0x, this is l1x and this l2x can be written in small letters or capital letters as



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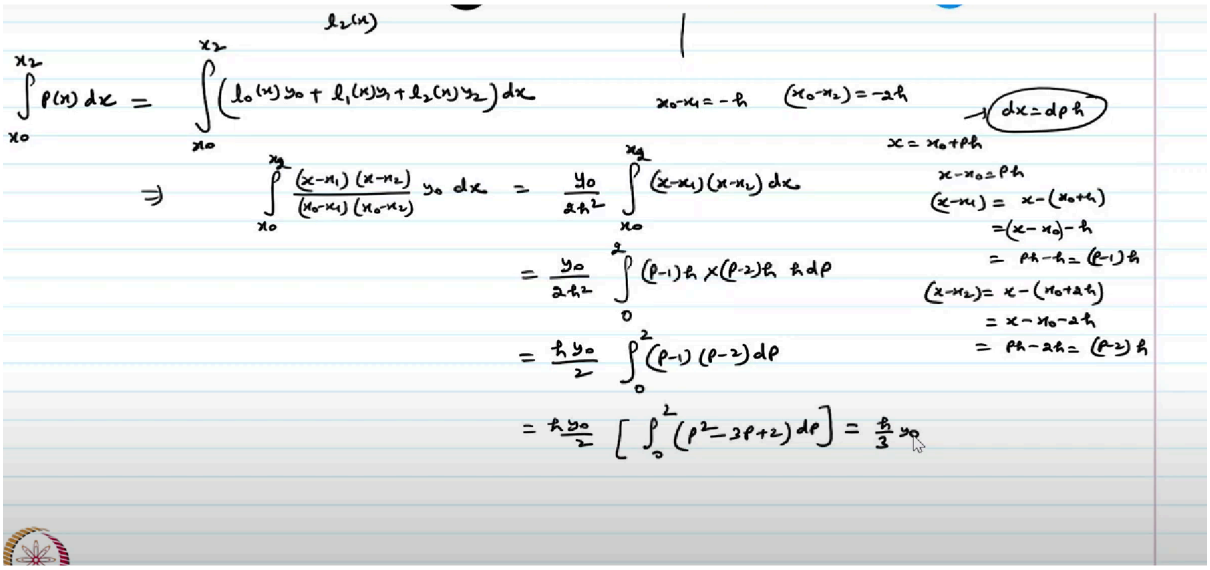
well, so I am calculating this, l0(x) y0, this will go into all, okay, so what comes out is l1(x)y1+l2(x) y2 dx, so we will have to find out each integral part separately, so now let's see what this is, x0 from x1 and I have taken x minus x1 divided by, let me see this, then we will do the second one. We will calculate it. Now let's see, it is a constant. Now see, what is x0 minus x1 x0minus and what is x0 minus x2 and minus and from here if I write, I have minus minus both. So 2h square will come out common. Here I will take it. So inside we are left with x0 to x1 and x minus x2 dx. Now if we have to integrate this, we will see, if we have to integrate it, we will have to make it a little easy. So we know that x is always x0 plus ph. We know, right? So we have defined this value like this. So I am applying this transformation to it. So x minus x0 will become ph. What will be x minus x1? You see, x minus x1 will become x0 plus h. Then x minus x0 minus h. It will come out okay. So if I write x minus x1 as ph and write minus h. It will become p minus 1. It will become like this. I see x minus x2. oh what is that x minus x0 what is x2 okay this becomes our x minus x0 minus 2h and what is this x minus x0 ph minus 2h a so we can write ph minus 2h with these and from here if you see then the dx will become equal to dph in a so what did I do I tried to make this integration a little easy now if we put x0 then what will happen x0 will be zero so see this becomes zero x0 sorry x2 will be okay so if we put more x then what will happen x minus x0 and what will happen equal to 2 so it will come to x minus x1 so this will become p minus 1 * h , x minus x2 ,p minus 2 in h , dx what has become hdp so we have divided it a little bit which will come out pa mive pa minus 2 a so see what will it become hy0 by 2 and this integration zero to 2 p minus 1 p minus 2 d p this is found so this is easy It's easy, okay, so we can calculate this, very easily this will come out and if we see, let's see, this will come out p square minus 3 p + 2 dp, so we will calculate these values, so these values will become h by 3 y0 this, okay, so this will be a hy0/3 this will not come, I can just substitute or cancel all these values, if I change it a little bit, it will become 8/3 – (3/2)* 4+4 will be left, okay and it is already coming here, so we will have this, so ultimately we have this value, next similarly, we want to calculate this as well, x from x2 x minus x0 x minus x2 x1 minus x0 and x minus x2 dx we would like to calculate this as well, so this will come out so I will take out this now Now see how to calculate this, the value is h and this is minus h. So the value that comes here will be y1 by h square minus sign and from here the value of x2 from x-x0 will be left with only this dx . Now if I try to simplify it like this, then it will become zero set x minus x0 which is ph and this p minus 2 h is h d p so this h h a cube will come out. So if we solve this, then the calculation we have will be this, minus y1 * h 0 se 2 p^2 - 2p dp this value will come so - y1 * h and this will come 4 minus if I integrate it, then it will come p ^3 by 3 minus p square zero to 2 will come. So minus y0 and this will come 8 by 3 minus 4. That's it, this is how we will have minus y1 h in minus 4/3 minus When the minus is cut, the value that we got is 4 by 3 so h by 3 into this value y1 ok so this was coming above now this value ah will come next i.e. x0 to x2 x minus x0 x minus x1 x2 minus x0 x2 minus x1 dx will come so we will calculate it like this this is 2h this is h so it will come y2 over 2h square will come in this in this case okay and we have zero to two and this x is zero so this p h p minus 1 hdp in so it will come to us y2 h by two zero to two p square minus p dp will come so if we calculate it then it will come to us h by 3 calculating this we have taken it out so we will substitute the above values y in it ok so I substituted it so let's see what comes out which is p(x) dx one what becomes p one is our lagrange interpolating polynomial It is mial so you will see that its values are h by 3 y0 it was coming h plus 4h by 3 y1 plus h by 3 y2 now what do I do is take a bath as common so it becomes y0 plus 4 y1 plus y2 this is what we have, okay so if we calculate this value, this rule is a bath to bath is coming



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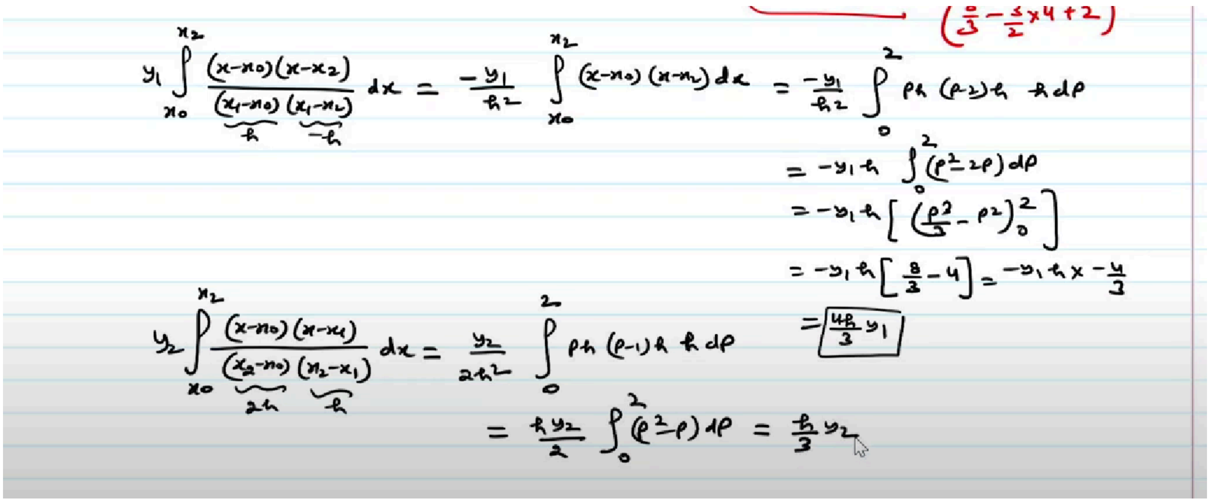
out, so we call this formula as simpson 1/3 th rule or 1/3 by th rule, so the name of its formula is simpson 1/3rule, okay so now we have found out this simpson 1/3th rule, now what will we do, we will see the error in this case, what should be the error, so I want to find out the error between x0 and x2, so I name it R x now we know that this polynomial was a polynomial, so the error that would be there in this case, I will integrate it, a little below x0 and x2 so which The error will be there, I will integrate it between x0 and x2 and what is that error x minus x0 x minus x1 x minus x2 divided by 3 factorial and third derivative one and xi is between x0 and x2 and we know that we have taken out the interpolated polynomial, so we know, okay, so now it has become this and the theoretical one, I have taken it out, now I will make this formula a little easy like we already did, so zero to two ph p minus 1 h (p – 2)h and h dp this will come out, so we will calculate this, so we have calculated it, h h h ah4 a, so h to the power four will come out, taking the third derivative and this is our zero to two p p minus 1 p minus 2 if we solve this, then what will it become? I am doing only this part, what will this part become, so this part will become if we do that, then this p p square. minus 3p plus 2 okay so here if we calculate it then it becomes p3 this becomes p2 and this 2p comes and I delete this part and here we are, row set d okay if I integrate it then p4 / 4 - 3p^3 /3 +p^ 2 / 2 and I put a limit on it like this so if we see what will happen this is getting cancelled by this this is also getting cancelled by this so we will get 2 to the power 4 16 by 4 minus 2 8 plus 4 this value will be left and if we see this it comes to 8 minus 8 so it becomes zero so from here we come to know one thing that Rx in this case will become zero what does it mean that the interpolator that we used in the approach was of second order right so the truncation error that was there was third derivative of the function coming in it right right Third derivative But in this case we have seen that the error that has come is zero. This means that we can say from here that it implies that this Simpson rule by the 1/3 rule gives exact results for cubic R. It is not only that it will give the exact answer for the second order polynomial. It will also give the exact value for the third polynomial because if I take the second degree polynomial, then what will happen if I take its third derivative and it will come out to be zero. This means that it will give the exact solution till the second polynomial. But if we have seen in this case that we take the cubic polynomial, even then the result that we are getting is not showing any error. This means that Simpson's th rule is giving good result even for the third degree polynomial. So after the third degree, if we go to the fourth degree, then what will happen? Now we will have to calculate the error. So now the error will become, suppose I write in Rx. Now what we have to do is the third degree derivative. We do not have to go till there till the fourth derivative. If we have to go till the fourth derivative, then we have only three points, x0, x1, x2. So if we have to calculate the error, then we will have to increase the polynomial by one degree of error, then we will have to take the derivative of the degree and I divide it by 4 factorial and the amount that we have to get should be brought between x0 and x2, but now it is cubic, so for cubic we have just seen that it is giving the right result, so what do we do, we will square the mid point. We can also square x minus x0, okay we could have squared x minus x2 as well, but generally we square x minus x1, so that this mid point, both sides will be equal, it will get divided. Now if we calculate this, then if you see in this, the fourth derivative has been folded and inside we have x2 from x0, so this is the square of x minus x0 x minus x1, so this is the remainder, so we have our fourth derivative. We will calculate this in the same way, this is the part, so if we find it in the same way, then the error that we will get in this case is, I am directly writing it as minus h to the power 5 by 90 f. And we know what is xi going on between x0 to x2. This is our truncation error, the error in this case is y. So it means that the sinth rule gives us a very good result, up to cubic polynomial, we do not know beyond that. So in this we will say that up to cubic gave a good result, but in the fourth polynomial, if we do its approximations, we get some errors and that error is this . So in this case we have calculated this. Now, if we see the work that we have done, we did it only in the first three points. This one, now the next point can also be after x. So there is x4 somewhere and then x. So now we have three points, one point this has come. One value was this and one value was suppose this was like this, so what did we do, I had three points in it, so I calculated it like this, this is our quadratic, in the middle of it we took out the area, so what should we have, x after x4 and one in the middle, so it means there should be four sub intervals, there should be two sub intervals, it will go on like this, so if you see, if we want to use the composite formula for the whole data, then the first task before us is that the number of sub intervals should be even, if they are even then only we can apply the sines nth rule, okay, so even sub interval means the nodal value, so we should have odd nodal values and how many should be 3 5 7 no 11 13 15, only then we will get even number of sub intervals, so the first condition is that the first condition of the application of simpson is that the sub intervals should be even number of off, so okay So we took out all the ones like this. After that, the next thing I am writing is the composite formula. So what is in the composite formula? Now we have to go from x0 to xn. Okay, always. And in this case, n will be even. Okay, so if n is there, we can take 2n as well because we need one. So now we know that it should be even. So what will it be? This is divided between x0 and x2. Okay, plus x4 from x2 plus x4 from x6. And in the end, what we have is xn. This is xn minus 2. And the function is like this. So let us simplify it a little.



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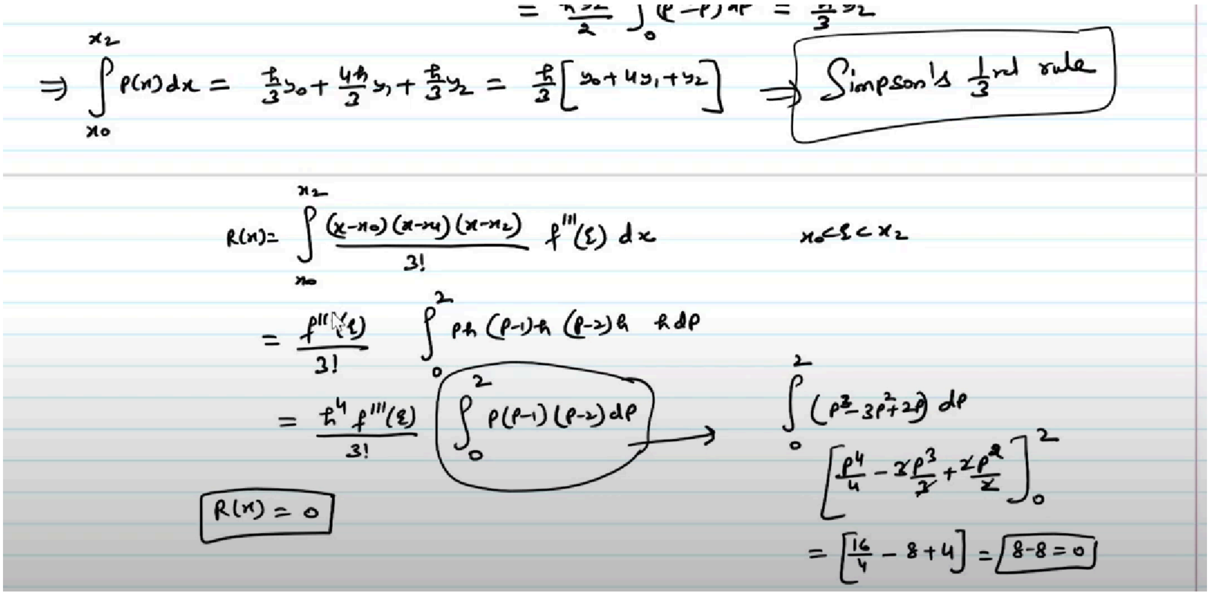
Now see what is coming in the first one. This value is coming. So if I write this, what will come out? h by 3 y0 plus 4 times y1 plus y2 plus h by 3 because h by is equally spaced. So we can write it like this. Now y2 plus 4 times y5 plus we will calculate it like this in the end we will get h by 3 y n minus 2 plus 4 times y_n-1 +yn this will come I will take h by 3 common to all of them so you will see first y0 zero came now 4 y1 is coming plus 4 5 plus this value is coming okay so the total values of this will have to be calculated so this function which will be formed with us if we see then 4 y1 plus y5 how it will come to this sorry y 3 plus 4 y 3 +y4 like this okay so 4 after that y5 then yn-1 and in the end it will go up to yn-1 plus two times two y2 +y4+y6 like this and in the end we will have y n minus 2 plus in the last y so this is left we have this formula this composite formula this value so in this you see the odd value has to be multiplied by four For even values, leaving the boundary, we have to multiply it by two and so on and so this value is y we have calculated and with this we have y now we have to see the error in all so what will be the error it will keep getting divided by all it will keep getting divided by all, so the error that we will have in this case the total error that will be formed will be minus n h to the power 5 of h and if xi is 90 then it will become 180 what will be the error that will be formed by x0 from xn now how did 180 come because we have n by two and interval is xi right so if we have 10 then 5 all interval will be formed in this way so I did it by a by two and multiplied it by 90 so this value is h so we have y and I can also write it as b minus a to the power 4 by 180 so this is the total error that we had y okay so this is the error that we have that is four derivative and this When we got the value, we called it the Simson's rule.



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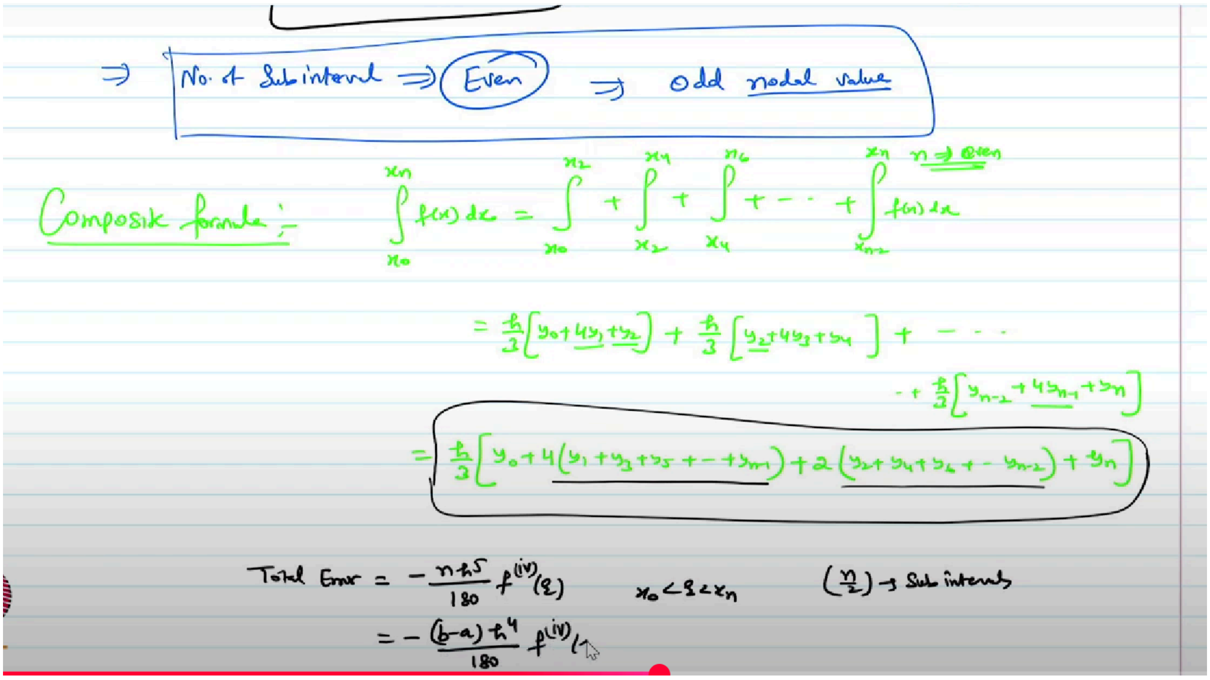
Now, the best advantage of Simpson's rule is that it is giving the result for cubic as well. Now, our next point came, so we said, if we keep doing it like this, then suppose we get the points x0, x1, x2, x3. Let's take four points. Now, as soon as we take four points, we know that the polynomial, the lagrange polynomial, will come to us. l0 y0, l1 y1, l2 y2 and l3 will come. Now we will integrate it. So, I integrate it. x0 to x3, l0 x dx, I took x. I will try to calculate it. So, we have this integration which is coming to us.



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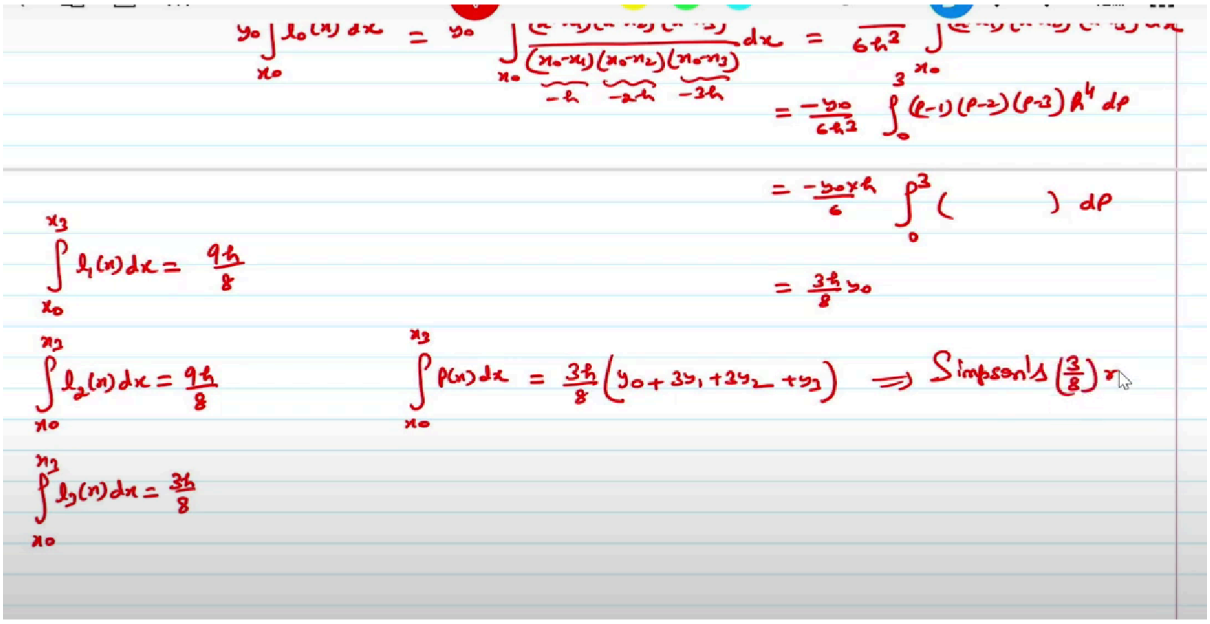
And this will come to x minus x1, x minus x2 x minus x3, x0 - xv minus x2, and x0 minus x3 will come to us. Okay, so now what we have to do is calculate this. So we will calculate it, look here it comes minus it comes -2h and this comes -3h, if we see it, it will come to us minus y0 by 6h ^3, okay and from above it comes to us x0 to x3 and this is like this, so we have come to know that we can easily calculate it by changing the transformation, so it will come from zero through 3 it will come p minus 1 p minus 2 p minus 3 into p in h to the power four because then y will come from h it will become d, so we have calculated this, h came y0 by 6 in a and this is its calculation, it will become a little big and complicated, so if we solve it, then the value of this will come to 3 h by 8 y0 this value will come, okay so 3 h by 8 y0 will come next, we will calculate it, so I am writing directly, so from here I am going to calculate x0 to x3 If we calculate l1(x)dx, then the value that will come out is h x0 from x3 l2(x) dx, if we calculate it, then it will come to us 9 h /8 and this x0 from x3 Easily we can calculate it by sitting and it will come out to us 3 h by 8. So if we have calculated all of this, now we have x0 from x3 and px is dx p(x) which was our polynomial, which seems to be a polynomial, which is cubic, so if we calculate it, then see, now I can take 3 h/8 common, so it will become y0 plus 3 y1plus 3 y2 plus, this will become okay, so now 3 /8 is common in it, so we will name it simpson 3/8 and simpson 3/8 , okay, so this is the formula of simpson 3/8 and if there will be an error in it, then if we have to calculate the error, then we know that it is cubic So the error that will come from the integration of x0 to x3 x minus x0 x minus x1 x minus x2 x minus x3 for derivative by 4 factorial x or ok so we will calculate it, if we calculate it then we will get minus 3 h to the power f by 180 by h f derivative and what is xi going on x0from x3 is not of much use because in this also the error is coming in the power of 4 degree and the same was there in Simpson too, so there is not much change in the error, so what does it mean that the Simpson 3/8 rule will not be very useful in this case, so what we generally do is we use Simpson and we use Simpson 1/3 hardly because we have seen that the cubic

polynomial is at least so we see Simpson 1/3th, okay and the error will come in the derivative and we used the 3/8 rule in that Meaning, the calculation in it increased, our calculation increased but we saw that the error in it was also same, so that is why we will use the simpson. So this Simpson and 1/3 rule can be calculated like this.



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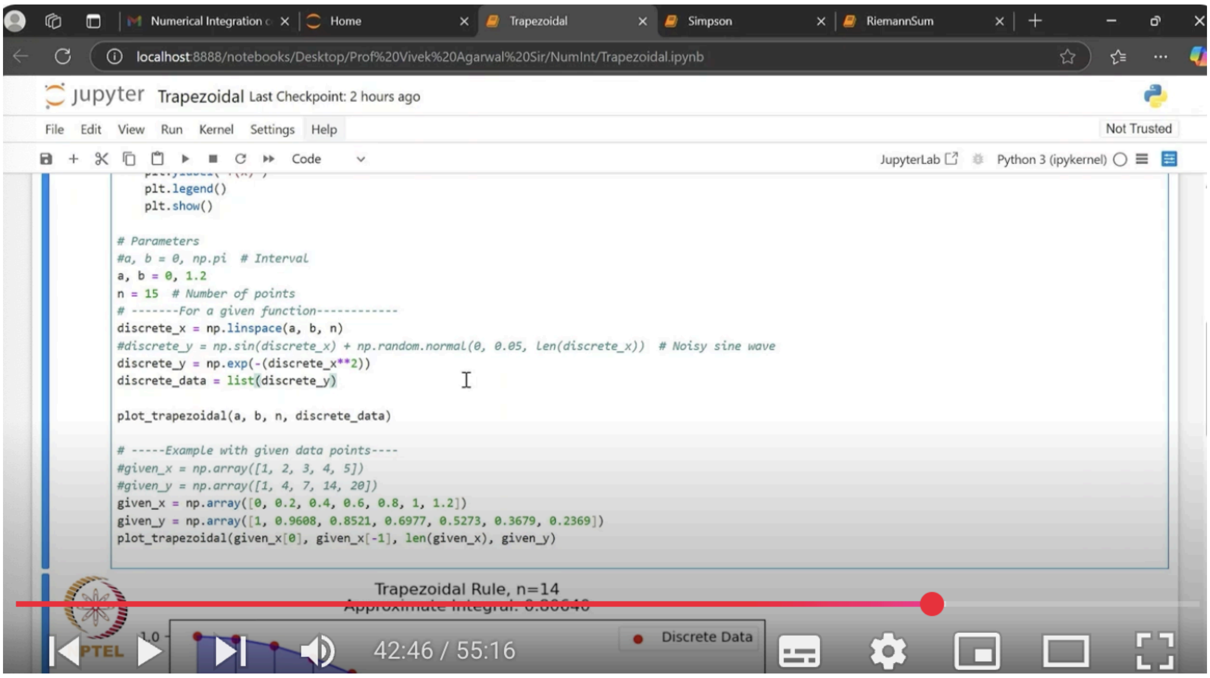
Now the code that we have is Python code, let us see how we can use it. So now let me first check the trapezoidal rule. So the trapezoidal rule is that we know that the rule is the top which we will create for the entire data, we will create a trapezoidal there and we will find out the area of the trapezoidal. So we have defined this function over the trapezoidal rule and in this we are taking only discrete data, so and discrete data is okay and we have our space, we have taken x points, dx, which is h, we have defined the value of h, we have defined the value of y over the discrete data. We will apply the value and we have defined the sum, after that we returned the values and here we have given the plot, so the plot of the trapezoidal rule will appear, okay, so the code that we have given for this, there is not much in it because what we need is just x and x2 and after that we make it even, we have made it even, okay this side into times, what we have, the internal overlapping nodal value becomes two times and the first and last one remains like this, we have already seen and this is our sum, so the trapezoidal rule is that we have plotted a function, what will we do in it, we will define the plot, okay, the scattered values will give discrete values, after that we will define its plot, so what have we done here, we have defined the function till here, after that I will put in the values of a and b in it and the number of sub intervals to be taken, how many to take, we will define or we will define the number of points, after that from the line space we get equally spaced points, between a and b, n number of points, okay and what have we done with it, we will define it like this, if we are taking any other function, then we will define on its basis that what am I taking, I am taking x or I am taking x s or I am taking x why or I am taking exponential and what we will do I have defined discrete data. Now I took this data, just like we did in the previous example, I squared e to the power minus x. So, look, what I am defining here is the same as e to the power minus x. Whatever discrete value we get, I will square it. I squared the exponent minus the discrete x.



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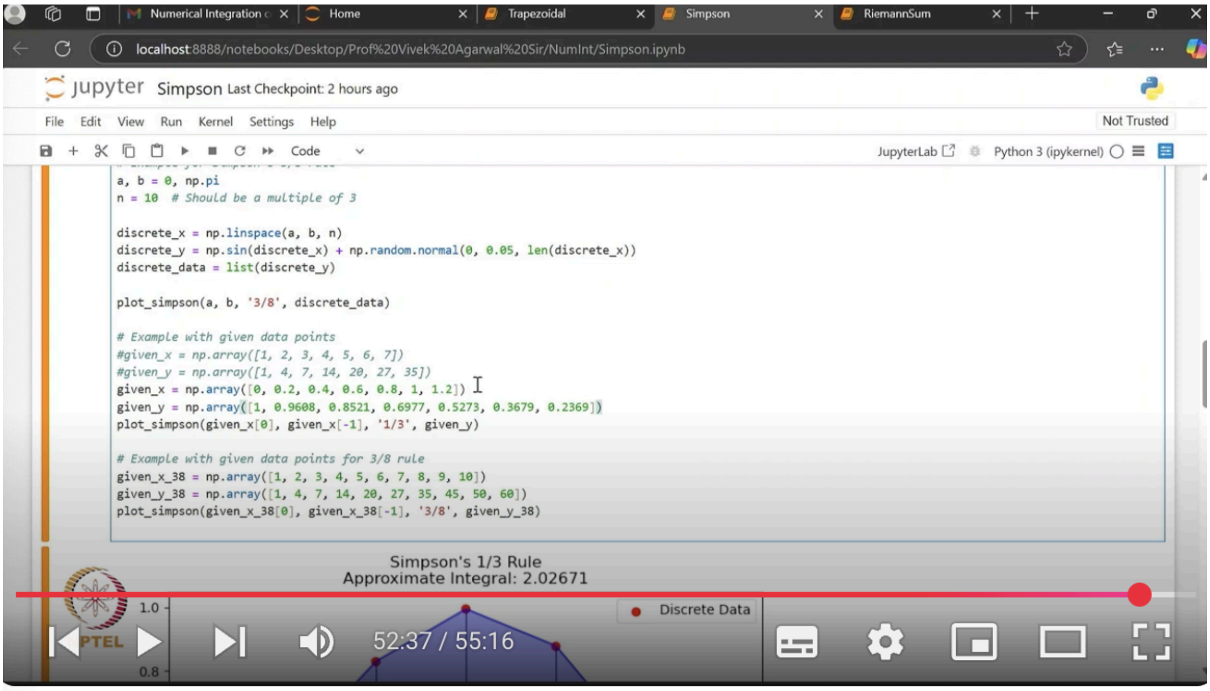
So, this is what we have. Now what have we done, we have defined this data. So this is my data, the same one that we used last time in the Riemann Sum. We used the same data in Riemann Sum. So, I am taking the value 0.24 p 6.81 1.2 and the values on it are y and I plotted it. So, now we ran it. So, after running it, we have the top rule and we have it. So, this is the first trapezoidal, this is the second trapezoidal, this is the third trapezoidal. We have to calculate our trapezoids like this. After that, we used the composite method. So the discrete data that we had was this, so by trapezoidal rule we got .8064, okay, so we calculated it, changed it and took n= 6. Now what did we do first, we calculated on this, that means the data that we have, the function that is given, we divided it, okay, now we have only the data value given, okay, to th fur 5 6 is sane point, so it means there will be six sub intervals, so now we used this function for approximations, see, our tuple is this, which is the first tuple or the second tuple is this, so in this way we have six numbers of it, we calculated the area, so after calculating, we saw the result that came out approximally, so these are the values, basically we calculated it using the function and this value we did for discrete data, so what we have is this, okay, so in the same way we can calculate for different data, if we have the function di If it is not given then we will get only the second graph. If we have a function also given then what are we doing, first we are finding it using the function and after that we are finding it using the trapez rule. So the verification that we are getting from both is that the error, which means integral approximations, is done by the same method, so the first condition in the graph is this. If we have to find the simpson th rule and apply it, then there should be an even number of sub-intervals. So we will apply the first condition here. So see, the model value should be zero. It means that the number of mesh points minus should be exactly divided by two. So we have applied this condition. If it is not so, then we will get this.

The even rule requires an even number of intervals and an odd number of points. This is the remark that we have, it will be written here. The warning will be written here. Then what do we have to do, we will change it and make it, after that all the work is the same, just that the sum value has been changed, so son, this is A, this is G and this was the last one left, after that see, A into the odd values and 2 into the even values, the sum of all of them and it will return us the value like this, in Simpson 3/8 we have to multiply by 3/8 and all the values will keep getting calculated like this, okay, so what did we do after that, we plotted it, so we will plot Simpson 1, we will plot Simpson 3/8, now the value that we have is given in this way, now see, now I am calculating it for sine, if we calculate it for sine function, see this sine function is this one, in this case we have the function given, so what are we doing, the values that we are taking out are being taken out from sine, so the sine values are, we took them out from this and we added some error in it so that there is no exact value, okay. Random numbers are normal distributors, we added it, so that the values that we have are absolutely exact. Now after that we defined a and b from zero to pie and made them number of 10. So if it is an even number, it will work, no problem. After that we will calculate it, we will do it for 3/8 also and we will solve our examples. As soon as I run it, we will get this. So we had taken the sine function, so it was taken between zero to pie. The value of pie is 3.14, so it is going up to here. See, if you see with this simpson th rule, then this value is coming, so our area came out to be 2.02 and this is what we have done, we have done it with 3/8, so what should be in simpson 3/8, it should come in multiplication of three, because what is happening in it, in the first one that we had calculated. X0 x1 x2 x3 There should be this many number of points, then x3 x4 x 5 x 6 So it means the value should be till here, so it means that there should be multiples of three numbers, only then the 3/8 rule can be applied to us, so we changed the rule a little and increased the number of points, see in this, from 1 2 3 four 5 6, the number o how many are coming in this, tooth 5 5 6 7 8 9 10, so 3 in 3 psv became 10, so we did this in approx and got 944, now this was done for discrete data, so the value came from there and simpson 3/8 was done, so this value is ok, so what we have in this case is data points and we have this function sign, so we have done it for both, so in this the number of points should be and n means the number of sub intervals should be even, so we have given these sub intervals, here there should be multiple of i plus 1, so like x 6 is x9, so x9 will be the point of 9 plus zero which will become 10. So similarly we have calculated it according to 10. So from here we have calculated it. So now this code can calculate both the things. If we have data, then we will put the data value here and if we have a function, then we can use the function sin here as well. So whenever we use the function, we will have to input the value of a and b here and we will also have to give the number of sub intervals. If I don't use this and just use the data, then I will use data on y so that we get the data value, then we will calculate it and the values that we have in approx will come. So if I do the same work that we had done for s, let's do it in trapezoidal order. So I had taken these values in trapezoidal order, so let's use it and see one two three 4 Yes, this will work for this, right? So what do I do? I write its values here. So what I did in the previous one, I am doing the same thing here. Only the number of data points is seven in this as well. See, if you look at it, it should be from 5 to 6. So it is odd.



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Okay, let me use this 3 by 8 rule. No problem. So if we see this, all the graphs will come out the same. Just this has been changed. So see, here if we see, in the approximations that came out, ours was coming out to be 0.86. When we did it in trapezoidal, it was coming out to be 0 4. At 0804, it should have been 0.86. But we did the same thing with Simpson. So see how good it came out. It came up to 0.86. So it means the accuracy up to three digits has come in simpson 1/3 th. In trapezoidal, the accuracy was up to two digits. So in Simpson we know that Its accuracy increases. So we have taken Simpson and the functions that we have taken are e to the power of x, so it is a Gosh function and Gosh functions are obviously non-linear, so in that case we know that we can calculate the error, so the error that will be calculated by this calculator will be known to us with the help of the formula that we have defined.

So this is Simpson, the trapezoidal, simpson, simpson 3/8 rule, we have done all the calculations and we have run it according to that. So we have checked our Python code that it is working for the 1/3th, 3/8th and the trapezoidal rule. So similarly, with its help, we can take any function, we can take discrete values and we can find out the area, we can do numerical integration. So I hope that This is the lecture by Simpson 1/3, Simpson 3/8 and you must have understood the error that is evolving in it and thank you for watching this lecture. Hello