Computational Physics
Dr. Apratim Chatterji
Dr. Prasenjit Ghosh
Department of Physics
Indian Institute of Science Education and Research, Pune

Lecture - 06
Numerical Integration Part 01

Welcome to the second module of this course. So, in this module what we are going to learn about is how to perform integrations numerically, but compared to the conventional numerical integration methods, our focus will be more on stochastic methods which are typically used to do multi dimensional integrals. So, what are stochastic methods and those things, I will explain to you in a short time, but before that let me just list what the topics we are going to cover.

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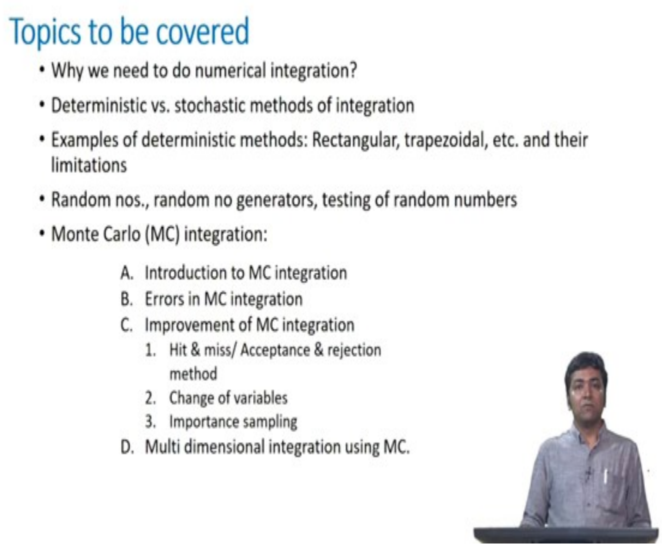

So, I will start this module by briefly motivating, why we need to do numerical integrations, when numerical integrations are required under what circumstances. I will then tell briefly about deterministic versus stochastic methods of integration and then as a example of the deterministic method, we will talk very quickly on the following methods which some of you may have already seen before. For example, the rectangular method, the trapezoidal rule and what their limitations are, how the errors are of what how does one make estimates of the error, how the errors scale with the system size so on and so forth.

And then we will move on to the stochastic methods, which is primarily what we are going to talk about is the Monte Carlo integration method, but before we go move into the Monte Carlo integration. So, what one needs is to have some basic idea of random numbers. So, I will very briefly introduce you to random numbers are and very shortly tell you in a very precise way, how random numbers are generated and then most important part, we will tell you how random numbers are tested.

Here we are not interested in how random numbers are generated; we assume that we have some way to generate the random numbers. So, most of the focus will be on testing the random numbers. By testing, what I mean by testing the random numbers is whether the random numbers are in reality random or not, how does one know that. Then this is a very important thing because if the random numbers are correlated then these methods fail. So, we have to be absolutely sure about the quality of the random numbers we are using.

So, we will talk more about that when we come to this topic and then within the Monte Carlo integration, I will talk give start by giving brief introduction to Monte carlo integration, we will see how the errors scale in Monte Carlo integration and then we will talk about three ways to improve the conventional Monte Carlo integration scheme.

So, the first one is the hit and miss or acceptance and rejection method, the second one is how one can change the probability distribution by changing the variables and the third one is how one can change the sampling by using a method called importance sampling. And finally, so throughout this discussions I mean I will give you examples and the most of the examples will be like in the form of you writing a code to get a feel of the method. And then finally, we will look into an example of how multi dimensional Monte Carlo integration can be done from using the things which we have learnt from A to C.

So, with this brief summary of the topics that we are going to cover in this module , let us start. So, when do we need to do a numerical integration. So, numerical integrations are typically necessary when we do not have or we do not know the functional form of my integrand. I suppose we are all familiar with doing integration.

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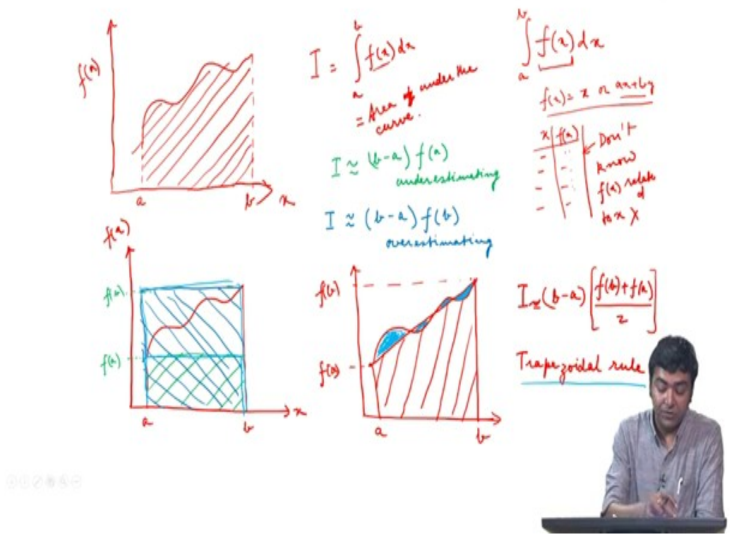

So, and here remember we are primarily talking of a finite integral. So, this is something of this form. So, if I know what my integrand is that is f x what is the functional form of it that is whether f x is equal to a x or f x is equal to a x plus b y, I can do these integrals, but suppose if I have a set of data. So, I have a set of data where I have x and the value of f x. So, these are just numbers and I do not know the functional form how f x is related to x.

These I do not know, under these circumstances one typically use the numerical integration. So, as we have learnt in our introductory courses to integration method so, the geometrical way to reproduce an integration problem is the following way. Suppose, so, for simplicity I am talking about a 1 dimensional integral, but this can also be extended to a multi dimensional integral. Suppose, this is my x-axis and here I have my f x right.

Suppose, I have a function which looks something like this and I want to integrate this function from this limit a to the limit b. Now, what will be the integral? So, geometrically the integral will be the area under this curve so, this will be our integral. So, if somehow we can compute the area under the curve then we can have an estimate of the integral. So, what I want to do is, to summarize is, that I want to evaluate this where I do not know the functional form of f x and that this will be the one way to do to estimate the value of this quantity is I measure the area under the curve.

So, if I can do that I am done with my integrals so, how does one do that. So, in order to do that the simplest way, the simplest approximation of this which I can make is the following. So, again suppose this is my a this is my b, I am trying to draw the same curve here this is my x and this is my f x. So, what I do is, I say as a first approximation. So, let me suppose that at this is the value of the function at a which I am calling as f a.

And this is the value of the function at b which I am calling as f b. So, one very brute approximation is I can say that let me draw a line parallel to my x-axis from the point a and up to the point b and let me calculate this area so, this will be an approximate value of my integral right. So, this area will be equal to this length into this height. So, basically b minus a into the value of the function at a, i.e f(a) ok.

So, but the problem with this is that if you see here so, we are missing out this part of the function this part of the function is not taken into so, basically this whole unshaded region, we are missing out. So, what we are doing here is in this case we are just underestimating severely the integral the value of the integral. So, then another option might be one can think of is in this case we are underestimating so, how about let me start from the point b and then draw a line parallel to the x-axis up till the point a.

So, basically what I am doing here is now, I am trying to find out the area, sorry... the area under this rectangle. So, now, this is my blue shaded rectangle this is what I am calling as my new estimate of the area under the curve. So, this is approximately equal to b minus a f b now, what happens for this case. So, for this case if you look carefully so, what you will find is that this part of the rectangle, this in reality does not belong to the area of the curve under the curve determined by this red line.

So, what we are basically doing here is we are severely overestimating. So, both this ways give me a very crude idea or very crude estimate of the area under the curve. Now, let us suppose how about instead of taking one point or instead of taking this other point here so, what happens if I do it in the following way so, again this is my curve here.

So, this is my a ,b sorry... this is my a. So, so far what I have been doing was, I was either taking this area or I was taking this larger area. So, instead of that what I say is let me join this point at a with this point at b and then I estimate the area under this trapezoid, under this circumstance what will be the value of the integral.

So, this integral will be given by the area of this trapezoid found by a, f (a), f(b) and b these four points and this will be b minus a by height of the trapezoid and the half the sum of the parallel sides that is f(b) plus f(a) by 2. So, this is my approximate estimate of the integral and this way of estimating the integral is known as the trapezoidal rule.

So, if you see here now I mean there are still numerical errors in this calculation, but this numerical errors are primarily restricted to these regions so, basically these shaded regions. So, here we are overestimating in this region, we are missing out this part here, we are again overestimating this part and we are overestimating and here we are sort of getting this, we are underestimating here and overestimating in this point, sorry for that error so..., but overall if you look at this is a much better estimate than defining the area only either using this part under the curve or using this part under the curve.

So, this trapezoidal rule gives us a better estimate of the area than if we use these rectangular ones. Now, the next question is, is there some way we can sort of increase the efficiency or if we can, can we improve the estimate.

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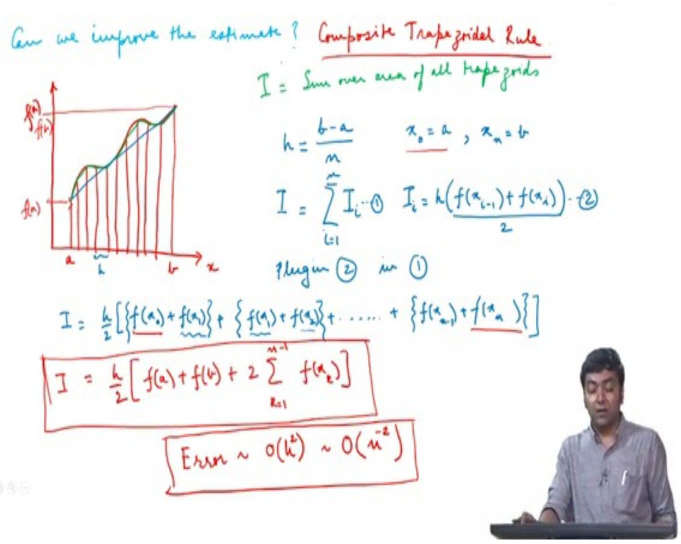

So, the question is, can we improve the estimate? The answer to this is yes, we can do that and let us see how we can do that. So, let me just redraw the graph again here whose integral we are interested in evaluating. So, let us suppose it is something like this. So, now, what I do is I just say that instead of taking the trapezoid by joining from a to b, what I will do is I will divide my segments between a to b into smaller finite segments so, something like this.

So, divide it into n smaller segments which for my purpose I am assuming they are equally spaced. So, in this case what I have is for example, 1 2 3 4 5 6 7 8 9 10. So, if I just connect this with this I have one trapezoid and now instead I have divided this one trapezoid into 10 smaller segments and at each segment I connect the starting point with the beginning point of the trapezoid of this segment.

So, what it will help me to get is, I will get lots of trapezoids here. So, now, I am connecting it like this then I am connecting it like this, like this, this, this, this and so on and so forth and then what I am saying is my area is equal to sum over area of all trapezoids. So, I have divided this segment into smaller finer segments and I have smaller trapezoids, I compute the area of each of this trapezium and then I sum them to get the total area under this curve which is nothing, but my integral.

So, what we have if you now look at this figure here so, you will see that compared to this line the I mean our previous way where I was using this larger trapezoid here, the error here is much smaller. So, the error is significantly reduced ok. So, how do we put this in mathematical terms. So, suppose between the segment b and a, we divide it into n equal segments and we call that as the width h.

So, each of this is my width h here and let us suppose my x0 is 'a' so, what I am doing here, I am basically discretizing this segment into n segments or n minus 1 points. So, my x 0 is 'a' and my x n is equal to 'b' ok. So, what now I have is n as I mentioned before I have now because of this discretization into smaller parts, I have now n trapezoids. So, what my integral will amount to is basically the area of my i th trapezoid and the sum over i where i runs from 1 to n.

So, if I now how to evaluate I this term here, then I can easily do the sum so, what is my subscript i. So, this is nothing, but again the area of the trapezoid. So, that will be the height of the trapezium and the product of f(xi-1) plus f(xi). So, if I call this as equation 1 and this as equation 2 now, if I plug-in equation 2 in 1. So, and try to expand it... sorry there will be by 2 here. So, what I will get will be the following. So, I will get h by 2 then f (x0) plus f (x1) plus f (x1) plus f(x2) plus so on and so forth until we get f(xn-1) plus f(xn-2) ....sorry... f(xn) ok.

So, now what we see here is that there are certain terms like x1, f(x1) which appears twice then similarly f(x2) which will appear twice and so on and so forth. So, basically apart from this first and the last term here which I mark by this red colour so, apart from this term and this term, all the other terms in the middle that will come to be that will come twice in this expression. So, just to simplify this, what I do is, I rewrite this in the following way.

So, I write my 'i' as, 'i' equals to h by 2 then f(a) plus f(b) because f(x0) is nothing, but by definition the value of the function at x equals to 0 at x(0) and x(0) is 'a' so, that will be here f(a) and then this is similarly f(b). So, f(a) plus f(b) plus 2 into sum k equals to 1 to n minus 1 f(x) k. So, this is my formula final expression for computing the integral using this trapezoidal rule, but where I am dividing the big trapezium into several small trapeziums and computing their area of each small trapezium and summing them up. So, this rule method is called the composite trapezoidal rule.

And, one can show that in this case, the error of the calculation or the error in the estimated value of your integral, this goes as order h square or in other words, this also we can write it as n to the power minus 2. So, this is the error which we get in this case ok. So, this was about the 1 dimensional case.