Computational Physics

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Lecture - 12
Numerical Integration Part 07

There are other ways of also our more sophisticated ways of improving the random numbers. So, let us look into that.

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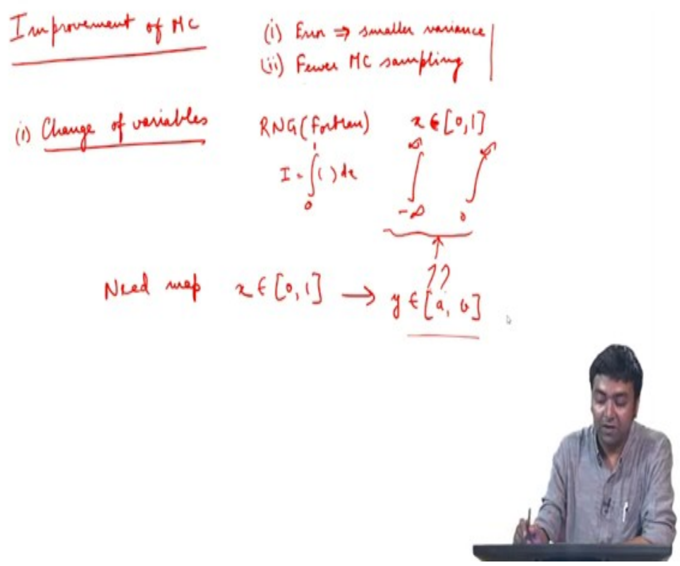

So, what we are going to discuss now is improvement of Monte Carlo integration. So, what does one mean by improvement of Monte Carlo integration? So, we want improvement in terms of two things; one is the error which is of my estimate which implies that the variance should be small. And the second improvement which we want is that the computational cost should be minimal.

So, what that means, is we need to do Fewer Monte Carlo sampling. So, typically the methods which we are going to discuss in these methods for the particularly for the second case we will improve in the time by means of reducing the Monte Carlo sampling. But, the time to do one Monte Carlo step in this modified methods will be more than that of the what we need for the brute force method. So, let us see how this two can be achieved. So, one way to achieve this; so is first of all one can. So, this two are achieved in two ways, one is by doing something called the change of variables.

So, we have all done integration in our calculus where to simplify the integrand we go to some one from one variable to another variable and accordingly we change the limits of the integrals and so on and so forth. So, it is basically the same idea which is applied here. So, my random number generator which comes with Fortran gives me random numbers x that lies between 0 and 1, but it might happen my and in many cases in physics which have seen that the limits of integration. So, with this I can just have integrals whose limits are 0 and 1.

But in many cases I have integrands whose limit extend from minus infinity to plus infinity or 0 to infinity. So, what do I do for these cases? So, precisely for this type of thing what we need to do is we need to map x that belongs to 0 and 1 to another set of random numbers y that belongs to different limits. So, basically you change the variable and in the process also sometimes you need to might need to change the distribution and the second method related to. So, this is change of variables is one thing and the second method is sampling.

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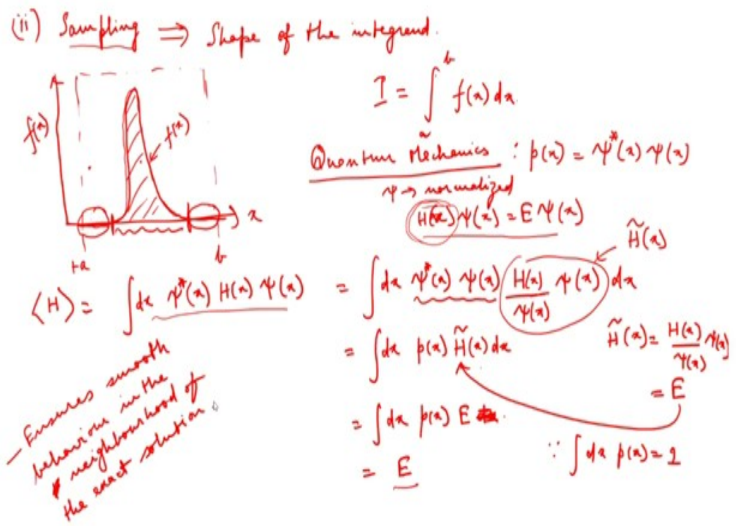

So, what do one mean by fewer sampling? So, what one means by fewer sampling is basically you intend or one intends to use as few as random numbers as possible to compute the integrand efficiently and this sampling is related to the shape of the integrand. So, what do I mean by the shape of the integrand? Let us look at an example 1 dimensional example again. So, suppose I have a function which looks something like this in 1 dimension and I want to do integral say from minus a to sorry from a to b.

So, basically; so if I call this function as f x. So, what I am interested to ever know is how much is integration of a to b f x d x. So, in the brute force Monte Carlo what we will do is the following or even in my acceptance rejectance method which is supposed to be improved one what we will do is we will generate lots of numbers that lie within between a and b. So, we will generate lots of numbers that lie between a and b and, but if we look at the shape of the function. So, we see that the function has significant contribution only from this region.

So, only from this part, the rest of the part the function is has a 0 value. So, the area under the curve defined by this as schematic function is 0 for these two circle region, it is only nonzero for this shaded region. So, if I use a uniform if I directly use the random numbers which is generated by my Fortran code which gives the uniform distribution. So, I have a equal probability of getting a random number from here and an equal probability of getting a random number which lies somewhere here in the point of interest.

So, what it means is that it will give me, I need a enormously large number of random numbers to have a reasonable estimate of this integral because most of my points both in the hit and miss method and in the brute force method because most of these points will lie in the region where the contribution to the of the value of the function to its average value is close to 0. So, you are losing l lot of points. So, you do not want to have this. So, rather what we want to do is you want to have a random set of random numbers or you want to generate a set of random numbers whose distribution matches exactly this distribution which should have the same shape as the shape of the function.

One classic example of this is seen in quantum mechanics. So, in quantum mechanics we have a so, we know that my probability distribution function is given by psi star x psi, where I assume that psi is normalized. And, these are eigenvectors of my time independent Schrodinger equation, the psi is are the eigenvectors of my time independent Schrodinger equation. So, if I want to compute the expectation value for example, of H. So, that would be like given by this expression integration dx psi star x H x psi x.

So, this is my expectation value. So, what I can do is I can do some manipulations. So, let us do the following. So, I keep psi star x and then I introduce psi x and then I divide H x by psi x again and I have psi x dx. So, this I can rewrite in the following form. So, if you look at this one psi star x psi x is nothing, but my probability distribution function p x and then this part I call it as H tilde x. So, my integrand become is now a modified function which is given by p x H tilde x.

But from this equation so, I am just writing the H tilde x clearly. So, I have H x psi x psi x ok, but from this equation what I can see is that my H x psi x by psi x that is nothing, but equal to E the eigenvalue. So, what I can do is I can plug in this in place of H psi x. So, my integral is reduced to p x E dx which is nothing, but a constant since integration sorry this d x will not be there since integration d x p x is equal to 1 because my wave functions are normalized.

So, what it has done? It has converted highly non homogeneous type of a function into a constant the in the integrand is quite non homogeneous here as you can see in this case into a constant one. So, basically what it does? So, the idea is you choose in this type of sampling, you choose set of random numbers whose distribution I was probability distribution function p x matches with that of the shape of the function. So, what it does is it ensures smooth behavior in the neighborhood of the exact solution.

So, this is the idea of how one can improve the sampling ok. So, with this brief idea about the change of variables and the improvement of sampling; so, let us come back to the change of variables.

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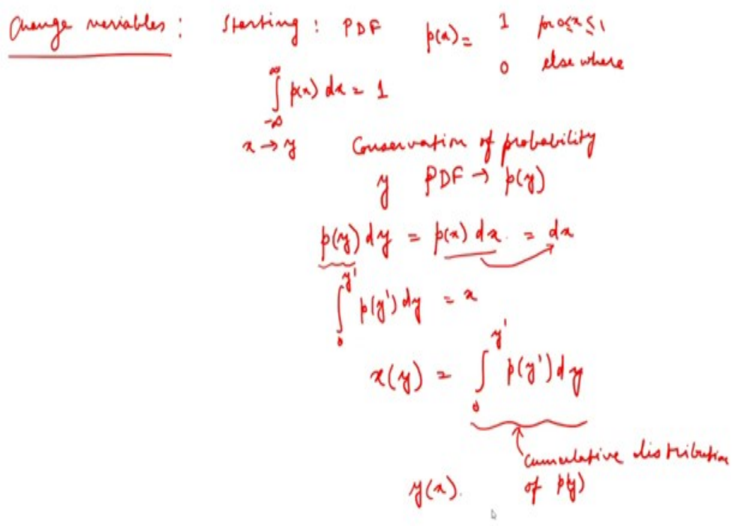

So, we will now talk a bit more about how one can do change of variables ok. So, we keep in mind. So, we will see some examples how you can change your variable and go from one type of distribution to another distribution. So, your starting point; so my starting point one should remember is a set of random numbers with a probability distribution function given as p x is equal to 1 for x less than equal to 0.

I mean x between 0 and 1 and equals to 0 elsewhere and also the following normalization condition is satisfied by this probability function that if you take the if you integrate it over the whole range you will get 1. So, this we need now need to transform. So, basically we need to transform x to some variable y, what is the general method? So, we will use the idea of conservation of probability ok. So, what were you trying to do? I have set of random numbers which has a uniform distribution and lies between 0 to 1, I want to generate a set of random numbers y whose probability distribution is given by the probability distribution function is given by d y.

So, what I have. So, according to the conservation of probability equation what I have is p y d y should be equal to p x dx. So, here my p y d y is the new probability distribution function which I want to go to, but we already know that my p x is equal to dx. So, this is nothing, but equal to dx the right hand side this part is nothing, but dx because p x equals to 1. So and then we do an integral. So, we do an integral from 0 to y prime p y prime d y this gives me x.

So, basically what I have now is x as a function of y which is given by 0 to y prime p y prime d y. So, this is nothing, but if you look at this is nothing, but the cumulative distribution of p y. So, if we can somehow compute the cumulative distribution of the desired new distribution then we can easily get the mapping. So, once we know x as a function of y if this expression is invertible then we can map also we can get y as a function of caps. So, this is how the transformation is done.

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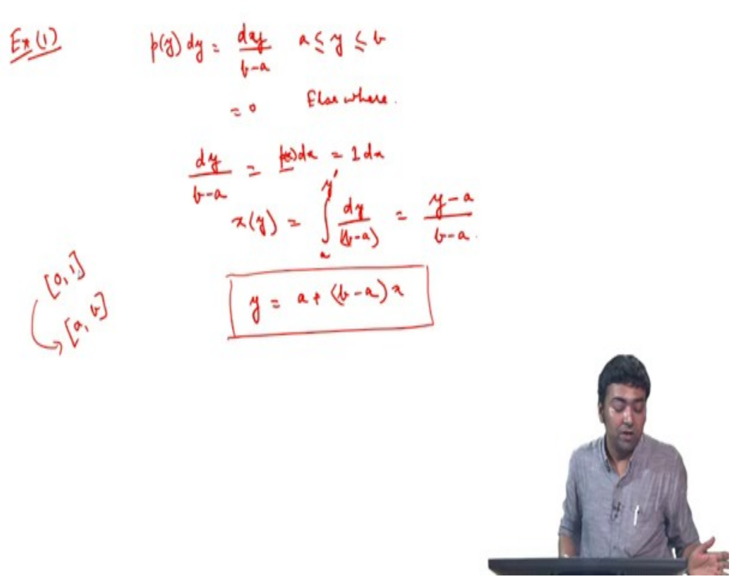

So, we take some example. So, the first example is which is a simple one is that suppose I want set of random numbers which has the following distribution p y d y equals to dx is equal to d y by b minus a. Such that between when a y lies between a and b and is equal to 0 elsewhere.

So, what we do? So, again we use the conservation of probability. So, d y by b minus a equals to p x dx now my p x is my uniform distribution. So, this is dx and then if I do the integral. So, my x and y will lie between a two y prime d y b minus a. So, the value of this integral if we work out is nothing, but y minus a by b minus a right.

So, if I redo the, I mean if I do the algebra I will get y equals to a plus b minus a into x. So, basically what this transformation or this change of variable do is that if I have a set of random numbers with uniform distribution lying between 0 to 1, it converts it to another set of random numbers again with uniform distribution, but now between a to b.

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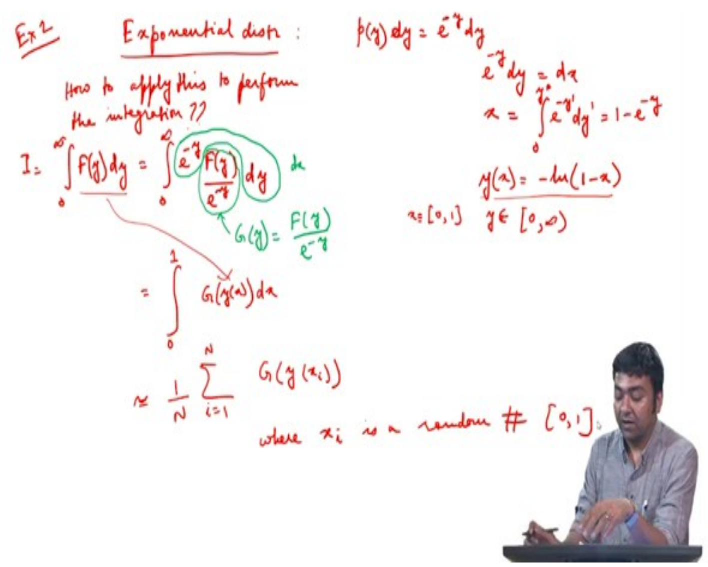

So, another type of distribution which we often find in particularly in the area of physics is my exponential distribution which is example 2. So, what I mean is basically, what do I do is I want to generate. So, this is my desired distribution of random numbers is equal to e to the power minus y d y. So, again I apply the conservation of probability, so what I get is the following.

So, e to the power minus y d y is equal to d x and if I integrate it on both sides. So, 0 to y prime e to the 0 to y sorry e to the power minus y prime d y prime and this is nothing, but gives me 1 minus e to the power minus y if I do the integral and then I can express y as a function of x will then be given by minus log 1 minus x. So, now, you see, so what will be the new limits?

So, my y; so x belongs to 0 and 1; so, for x equals to 0 here we get y is 0, but for x equals to one we have the open limit that is y becomes infinity. So, now, the question is how we apply this; so how to apply this to perform the integrand? So, suppose I want to use this distribution to form the following integration I equals to 0 to infinity F y d y. So, how will it I do it? So, what I will do is from this F y I will pull out e to the power minus y. So, I have e to the power minus y if y divided by e to the power minus y d y.

So, now if I look carefully in this equation; so, this term here this is nothing, but my dx and this other term f to the power y minus a divided by e to the power minus y this I am calling as G y. So, G y is equal to F y by e to the power minus y. So, once I have that then what I can do is I can rewrite this into the for this integrand in the following way. So, I have now G y which I know is the function of x from this expression here. So, G y which is the function of x in terms or in terms of x dx; so, this is what my original integral F y is converted to.

Now, what will be the limits? So, my y was. So, now, we will need to go the other way around. So, when my y is equal to 0 here, so y x will also become 0, but when my y is infinity. So, this one will go to infinity and x becomes 1. So, this is how the after the variable transformation how the integrand will look like and then this I can use the Monte Carlo to approximate it in the following way.

So, instead of evaluating this function F y now I will evolve find out the average of this function G y x i where my x i is random number in the interval between 0 and 1. So, in this similar fashion if you want to if you know the form of the mathematical form of the desired distribution of random numbers you can just do the change of the variables.

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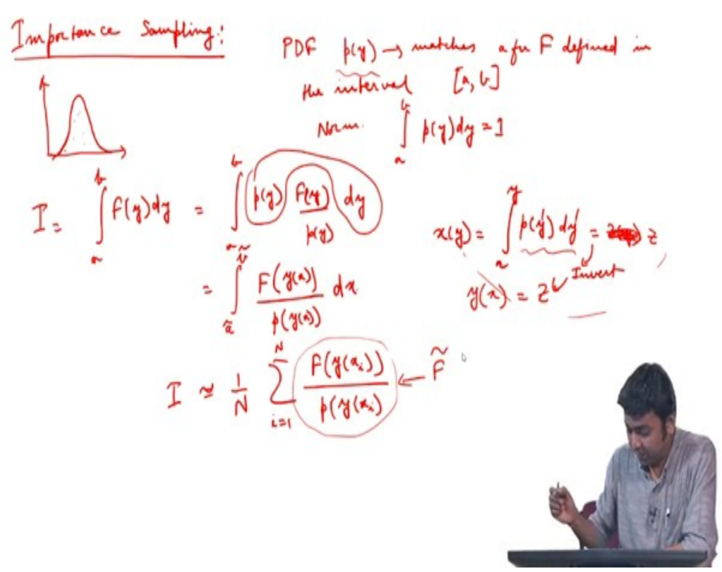

So, in the last part we go to the second part of this improvement method which we call as important sampling. So, the idea is already explained briefly a couple of slides back I am just reiterating. So, basically what I need to do is I need to generate a random number in this case whose distribution maps or whose distribution or the shape of the distribution matches with the shape of the function.

So, suppose if I have a exponential Gaussian this function here which I want to integrate I would rather prefer set of random numbers which has a normal distribution or a Gaussian distribution than a set of random numbers which has a uniform distribution. So, how one change the shape of the sampling is done in a following way. So, let us assume; suppose let us have say that we have a PDF probability distribution function p y which matches a function F which is defined in the region a and b. So, and the normalization condition is integration a to b p y d y is equal to 1.

So, what we are going to do is we are going to evaluate the integral of this function F y dy; so, as before as in the previous case. So, we will use the same trick. So, I multiplied the integrand with p y and also divide the integrand with p y. So, I have now p y d y d y and then we can see that this is nothing by dx and this is my modified function. So, what I do is. So, I change the variables accordingly a my b and then I have my modified functioned p y x and again p as a function of x dx, where my x as a function of y is given by the cumulative distribution of my original of this probability distribution function p y of the desired probability distribution function p y ok.

So, once we have this then it is the simple standard procedure where we instead of keeping it as a continuous we discretize the thing, so y in my function my integrand. So, that is F y as a function of x y by p y as a function of x i. So, this gives me then estimate of the integrand ok. So, so this is how the. So, now, this shape of this function. So, you are basically modify what you are doing is you are modifying this function to in such a way that you can have maximum number of sampling points lying in that.

So, but this is nontrivial to do having said that it is a important and its a very efficient method, its non trivial. So, there are certain conditions that needs to be satisfied, that my desired probability distribution function should satisfy.

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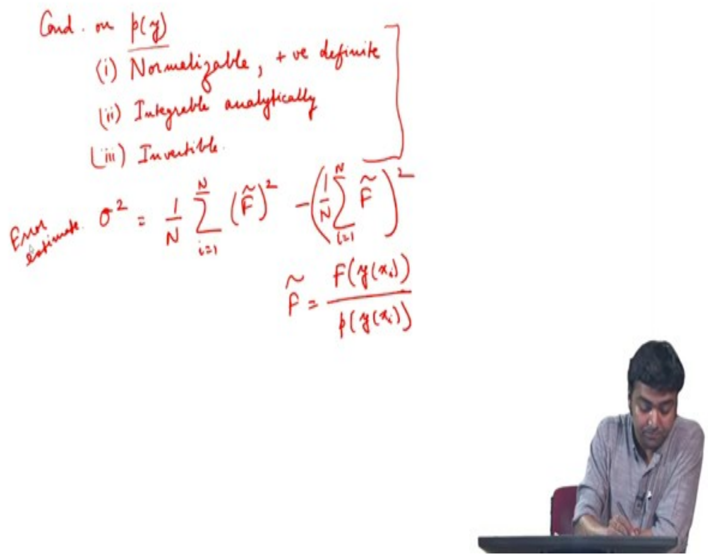

So, first of all since this is a probability of distribution function; so, the first thing is p y has to be normalizable. So, you should be able to normalize p y what it means is if you take the integral over of p y it should give you about the complete interval, it should give you one and not only that since probability is always positive and it has a unique at a given value of y it has it should have a unique value.

So, it should be positive definite throughout the desired range this function p y should be positive definite and as you saw that what we need to do is we need to compute the cumulative integral ok, we need to compute the cumulative integral of p a cumulative distribution of p y. So, in other word what it means is that p y should be integrable analytically So, given assuming that you can integrate solve this integral analytically. So, say you will get some value let us say z y; so I say some value z.

So, to get y I need to invert this equation. So, I need to put this back here and I need to write y as a function of z some z prime. So, this is obtained by; so I invert this and I get this. So, what it means is that in addition to these two conditions it should be invertible ok. So, these are the very three strict conditions and in many case most cases it is very difficult to satisfy all the three conditions particularly the integrable analytically and the invertible one. So, having said this, if we can come up with a probability distribution function whose shape matches with the shape of the integrand that we are interested to compute the integral of; so, this is one of the very efficient way and the error or the variance can be computed then in the following way.

So, where sum over I equals to 1 by N F tilde square minus sum over 1 by N sum over I equals to 1 to N F tilde and then whole square where my F tilde is this modified function this is my F tilde. So, I will just write it here where my F tilde is equal to F of y x i by p y x i. So, this is my error estimate . So, so let me just summarize these two things. So, basically what we have learnt is how to improve the efficiency or how to improve of my Monte Carlo integration. Improve the efficiency not compared to the grid based method, but compared to the brute force Monte Carlo.

So, we do it in two ways we change the variable and we change the distribution of the random numbers. So, we choose a new distribution of the random numbers which typically a matches the shape of the function which we want to integrate and this way we can do it very efficiently the integration with fewer sampling points.