Computational Physics

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Lecture - 14
Numerical Integration Part 09

Now, the question is I could have stopped here only, but why did we do this part this extension into this Box Muller transformation.

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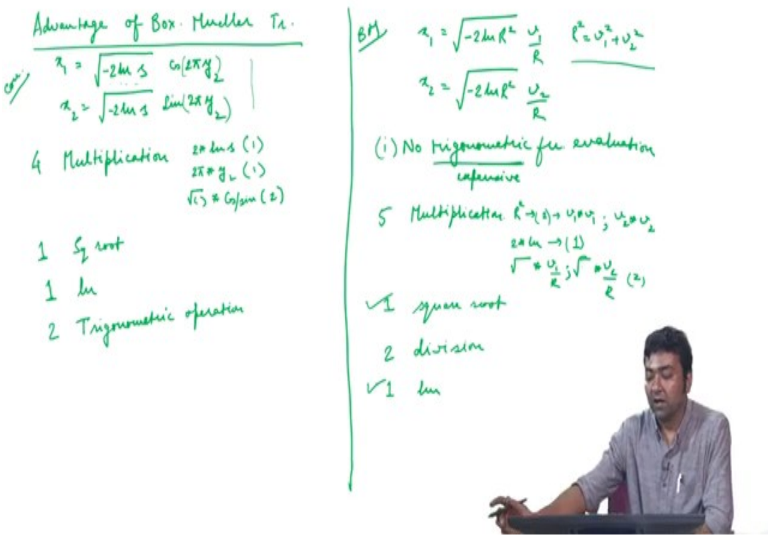

So, we will see that now. So, what we were looking at now is the advantage of Box Muller transformation ok. So, look into that let me just write down the two expressions which I have. So, the conventional one is x 1 is equal to root over minus 2 log s cos twice pi y 2 and x 2 equals to minus 2 log s sin twice pi y 2.

And so this is the conventional one and this is my Box Muller. So, where I have x 1 is equals to minus 2 log R square v 1 by R and x 2 equals to root over minus 2 log R square v 2 by R. So, now, let us see how many mathematical operations we need to perform to for each of these two cases to get a pair of random numbers. So, let us start with the conventional one. So, the first mathematical step is one is to do is multiplication. So, how many multiplications do we need to do?

So, in order to get these two values of x 1 and x 2. So, what we need to do is we need to do one multiplication that is a 2 into log s. So, this is one step which we need to do once and then what we also need to do is we need to do multiply twice pi and with y 2. So, this is one; so this step this multiplication we do 1 time and then this multiplication we do 1 time and the other multiplication is we multiply all the term under the square root with the cos or the sin term. So, these are two multiplications. So, in total to generate one pair of x 1 and x 2 we need to do 4 multiplications ok.

Then the next function operation is we need to do also a square root. So, how many square root we can we need to do? So, if I evaluate this square root term ones I can use it both for x 1 and x 2. So, basically what it means is I need to evaluate do perform 1 square root operation and in a similar way we need to perform 1 logarithm operation and then we also need to evaluate the cos or the sin of 2 pi y 2. So, that implies that we need to perform 2 trigonometric operations.

Now, let us look at this Box Muller transform 1. So, the first difference which we see between Box Muller transform and the conventional one is here there are no trigonometric functions so, no trigonometric operations evaluation. So, remember this is the most expensive part, this is the expensive thing. So, I am getting read of these two trigonometric operations and what is extra which is coming on. So, let us re visit the multiplication operation.

So, now for the multiplication operation, so, we need to evaluate R square which is given by v 1 square plus v 2 square. So, for this R square we need to do two multiplications here. So, basically a product of v 1 here v 1 into v 1 and v 2 into v 2. So, basically two multiplications which involves v 1s star v 1 and then v 2 v 2 star v 2 and then we need to do to one more multiplication which is the product of 2 into log R square and this we can do only once and use for generating both the numbers.

So, we need to have 2 star log; so this multiplication term v 2 ones and then we need to do two more multiplications. So, that is the product of this term under the square root into this fraction so, that we need to do for two different numbers. So, basically the term under the square root into v 1 by R and the term under square root into v 2 by R. So, this is another two multiplications ok.

So, total we need to do 5 multiplication operations then the square root is same as this one. So, we need to do just 1 square root operation because once we evaluate the square root of minus 2 log R square that we can use in both x 1 and x 2 and then finally, one more thing is we need to do 2 divisions. So, we need to find v 1 by R and we need to find v 2 by R.

So, my and sorry I forgot also we need to do 1 logarithm evaluation also. So, where we kept compute the log of R square. So, this and this step these are also same in the conventional method, but; so what we did is we got read of this expensive trigonometric operation by a doing 3 extra mathematical operations that is I do 1 extra multiplication and 2 extra divisions.

But this is but the overall cost of this will still be less than this one because trigonometric operations are very expensive and remember you have to use some millions and millions of random numbers to in your calculation when you do a Monte Carlo integration. So, repeating and doing this trigonometric operation millions of time. So, even though if the difference may be of a fraction of second on computing random number generating appear of random number using this versus this, but if you multiplied by million times then it becomes a large number .

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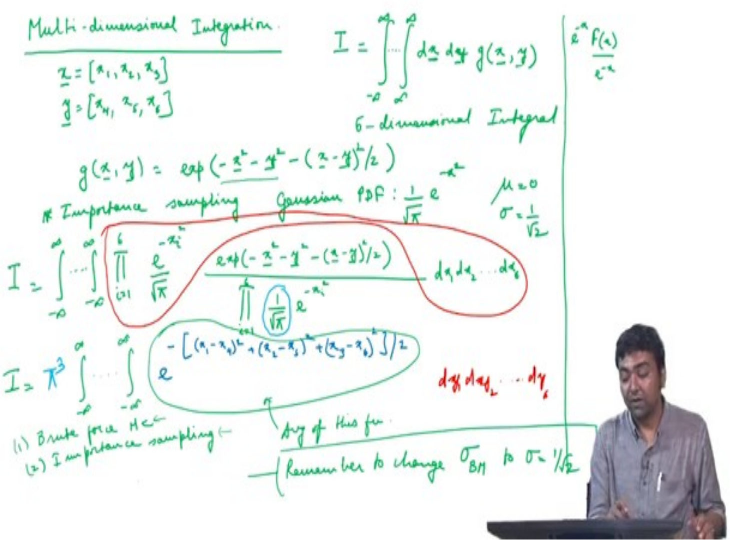

So, with this we will come to the last part. So, what we will do is we will look into how multi dimensional integrations are done . So, what we want to do is. So, the way we will do it is rather than using abstract equations. So, we will take a example and see how one can tackle it. So, what I am interested to do is I want to integrate perform these integrations using numerical tool and to more specific using Monte Carlo simulations. So, this is a multiple multi dimensional integral. So, where I have this vectors quantities d x d y these remember this are vectors. So, each of them have 3 components so, and then I have of a function which is a function of x and y.

So, basically what it means is my x vector that x is a contains x 1 x 2 and x 3 and my y contains x I write it y in this form x 4, x 5 and x 6. So, this is a 6 dimensional integral . And the form of my g x y is in this is the following, so I write by function to be exponential function. So, which is exp minus x square minus y square remember each x y these are all vectors minus x minus y whole square by 2. So, this is my functional form.

So, if we; so how do we do this integration? So, if we look into the function carefully, so what you can see is that this is like a I mean it has a resemblance to a multi dimensional Gaussian function, if I forget about this term then this part here. So, basically what. So, this first 2 terms if suppose this term is not there this minus a x minus y whole square. So, if I just have this terms it looks like a Gaussian function. So, I can evaluate this function in two ways one is by the at this integral two ways one is by the brute force method where I do not care about using a different distribution I use just the simple uniform distribution of random numbers to compute the integral.

And I can do a better way I can use this concept of importance sampling and change of variables. So, now, since as I mentioned that this function looks like a Gaussian function, so, what I will try to do is I will try to map this or I will try to use a setup random numbers which has the Gaussian distribution and to generate those setup random numbers we can use the method which you just learnt. So, this Box Muller transform method.

So, and also what we need to do is we need to modify the variable. So, the why we do it is following. So, we use importance sampling and for that we use Gaussian PDF which is of the form following form 1 by root pi e to the power minus x square. So, this has a mean of 0 and a variance sigma is 1 by root 2. Remember when you try to implement this in a code, so the Box Muller method gives you a Gaussian function which is in which the mean is still 0, but the sigma is 1 where as when we are using a Gaussian distribution for this particular course with a sigma 1 by root 2.

So, one needs to be careful and keep that in mind when one is generating the Gaussian distribution. So, you need to change your distributions variance from sigma equals to 1 sigma equals to 1 by root 2 and one way (Refer Time: 12:29) I mean one way to do that is just multiply your you generate your random number as with a Gaussian distribution with sigma equals to 1 using the previous method the Box Muller method and you just multiplies by the random number by 1 by root 2. So, that changes your distribution.

So, how do we simplify this? So, let us; so what we do is we rewrite the integral in this form. So, now, you see we have 6 variables here, so I need to multiply it with 6 such distributions. So, if you remember what we did in the earlier class. So, if I have a function say F x which is which has like an exponential which is like an exponential function or similar to exponential function. So, what I do is I multiplied by e to the power minus x and divided by e to the power of minus x.

So, that is precisely the same thing which we are going to do here. So, we are going to multiply it by e to the power minus x square by root pi. Now, since we have 6 variables, so for each case we need to multiplied by e to the power x square. So, basically we need to multiplied by e to the power minus x 1 square by root pi into e to the power minus x 2 square by root pi still its e to the power x 6 square by root pi. So, instead of writing it explicitly I write it in a compact form. So, pi means here basically a continuous product where this I goes full. So, this is still i; i goes from 1 to 6.

And then I have my function which is following form exponential minus x square minus y square minus x minus y whole square by 2 and this I divide once again with this term. So, in the product 6 times product of 1 by root pi e to the power minus x i square. So, if I and then I have d x 1, d x 2 to all the way to d x 6. So, if I do the simplification, so what I see is if I take this term here this I can rewrite as basically d x 1 d x sorry d y 1, d y 2 and d y 6.

I have my integral as the limits are same and then what I can also see is that this term. So, I have in the denominator I have 1 by root pi whole to the power 6. So, that basically becomes pi cube and then if I divide this the numerator with e to the power minus x 1 square x 2 square and so on so forth. So, basically what I will get is, so I will be having e to the power minus.

So, this terms will cancel out x 1 square, x 2 square, x 3 square and x 4 square, x 5 square and x 6 square and I will be left with this term here which is nothing, but I can write it as x 1 minus x 4 whole square plus x 2 minus x 5 whole square plus x 3 sorry x 3 minus x 6 whole square by 2. So, this is my simplified or modified integral this become my modified integral. So, now, what we need to do is basically generate the random numbers with a Gaussian distribution and find out the basically find out the average of this one.

So, that will give me the integral. So, to write it in a piece of code, so remember to change sigma Box Muller to sigma equals to 1 by root 2. So, otherwise your integral will be wrong. So, what I expect is that you write a code of your own and find out the value of integral.

So, you can do two things you can write the code with the brute force Monte Carlo and then you can write another code with the important sampling that is the way we have discussed here. And compare how quickly you will reach the same level of accuracy by how quickly I mean with how many random numbers you need for the case 1 versus how many random numbers need for case 2 to have the same level of accuracy in the value of the integral.