Computational Physics
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Lecture - 13
Numerical Integration Part 08

So, far we have seen how to change the variable and how to improve the sampling. So, with changing the variable , the idea was to go from one from a uniform distribution to a desired distribution of the random numbers. So, there looked like one for example, we looked into how to get an exponential distribution from a uniform and distribution of random numbers.

But there is another distribution which is quite common and we have not talked about it that is how to generate set of random numbers having the normal distribution or Gaussian distribution.

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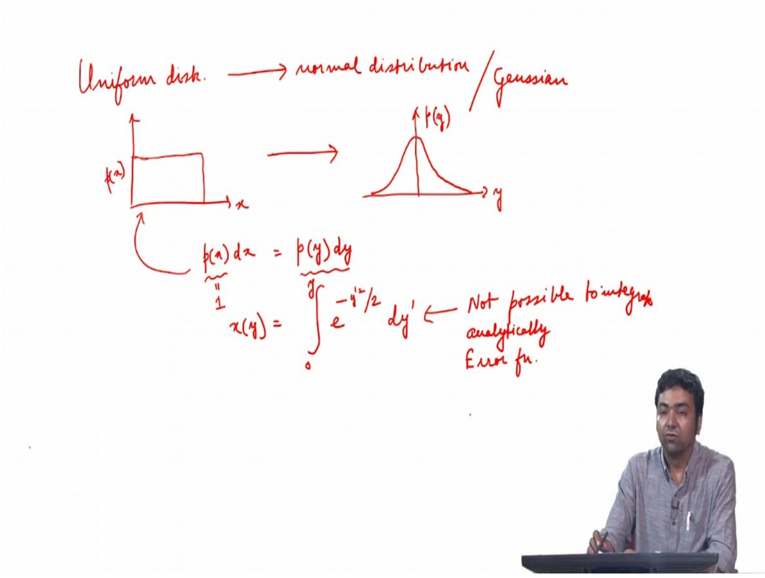

So, basically the idea is I have a set of random numbers which is generated by my machine which has a uniform distribution and I go to or I transform them to another set of random numbers, which has a normal distribution or it is also called the Gaussian distribution normal or Gaussian distribution.

So, if I plot the distribution. So, basically what it means is, I have. So, if this is my probability distribution function p x for a uniform one and so, I want to convert it to something like this for a like a Gaussian function this is x. So, if we remember the recipe. So, what we did it let me let me just call it as y. So, if you guys remember what was the recipe; the recipe was we use the principle of conservation of probability a that is this equation and where we set p x to this is equal to 1 for this particular case.

And then what we did is, we did we computed basically we wrote x as a function of y to be the cumulative distribution of this new or the desired pdf. So, that is 0 to y prime, 0 to y not y prime sorry the integral 0 to y and if I take my Gaussian distribution to be e to the power minus x square by 2. So, this is what is called a normal distribution normal Gaussian distribution y press dy prime. If you remember the conditions which this recipe or this function should have is that one it needs to be integrable.

But if you look at this function, we know that this is not possible to integrate analytically. The popular name of this function is it is also called the error function. So, now, we cannot so, but it is clear from this is that, we cannot using this recipe generator Gaussian dist or a normal distribution of random numbers so, but again as I mentioned there are several places in a physics where these type of the Gaussian distribution is followed system follows or the system can be represented by a Gaussian functions there are many examples in physics.

So, it is an important problem to need to solve. So, the question is what is the way out and so, in order to achieve this or to get this new distribution. So, we have to use some unconventional technique and the most proper and the book the popular technique which is typically used is called the Box-Muller transform.

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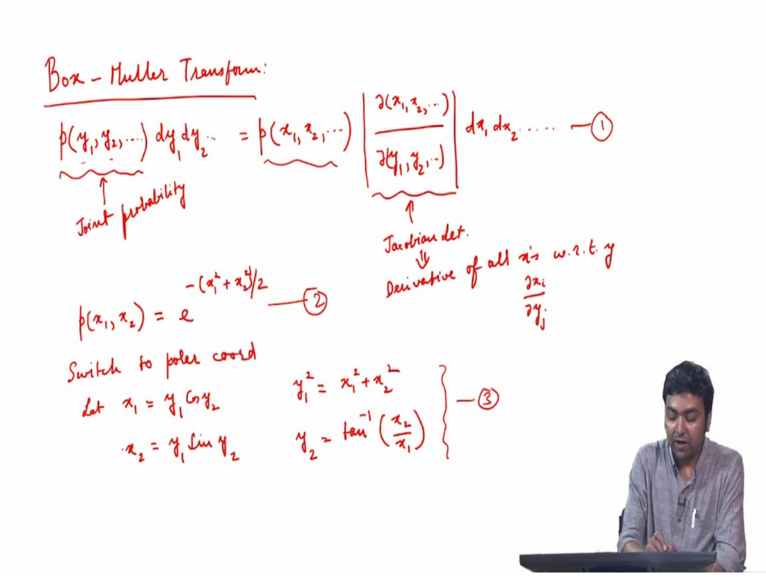

So, what is done in Box-Muller transform? So, what we need to do to avoid this particular . So, far we were restricting ourselves to only one dimension by one dimension I mean we are using just a single variable. So, there is only dx and on the right hand side also there is only one variable dy; but rather than that what we will do is now we will move to do multiple dimensions and there we can write down again the probability conservation in this form.

Suppose we have a probability distribution function which is given by p y 1, y 2 and dot dot dot. So, it has n number of values then the conservation equation now becomes the following. So, we have the probability distribution as a function of x then we have this Jacobian matrix. So, x 1 x 2 dot dot in terms of delta y 1 y 2 like this it goes and then I have d x 1 d x 2 and so on and so forth.

So, these type of probability distribution functions these are also called joint probability distribution functions because they depend on more than one variables and this determinant here is the Jacobian determinant it is called the Jacobian determinant and the information it contains is the derivative of all x's with respect to y. So, basically it is a determinant containing elements of this form, del x i del y j. So, now, for our purpose what that is to generate this Gaussian distribution?

So, what we will do is we will use two variables. So, let me consider a joint probability function which is given by which is a function of two variables p x 1 x 2 which is equal to e to the power minus x 1 square plus x 2 square by 2. So, this is basically a two dimensional Gaussian function or you can in terms of since we are talking about probability distribution function. So, we can total it as a two dimensional Gaussian distribution, whose sigma is equal to 1. So, this is the distribution which I want and what I have in my hand is the set of random number or my random number generator which gives me the uniform distribution random numbers having uniform distribution. So, what I do is to simplify this. So, I will switch to polar coordinates. So, what do I mean by that? So, by that what I mean is, I rewrite x 1 and x 2 in the following form.

Let x 1 is equal to y 1 cos sorry cos y 2 and x 2 is equal to y 1 sin y 2. So, what is the relationship between x 1 x 2 and y 1 y 2? So, if you if I take the square of these two equations and add them up. So, what I will get is y 1 square is equal to x 1 square plus x 2 square and if I divide one equation by the another one. So, and what I will get is y 2 is equal to tan inverse x 2 minus x 2 by x 1.

So, now I have got this thing and what I will do is, if I call this as my equation 1 this is 2 and this set of equations we call it as 3. So, what I will do is, I will take this 1 and 2 and I will plug it in this one in this particular equation. So, what I will get is in this case.

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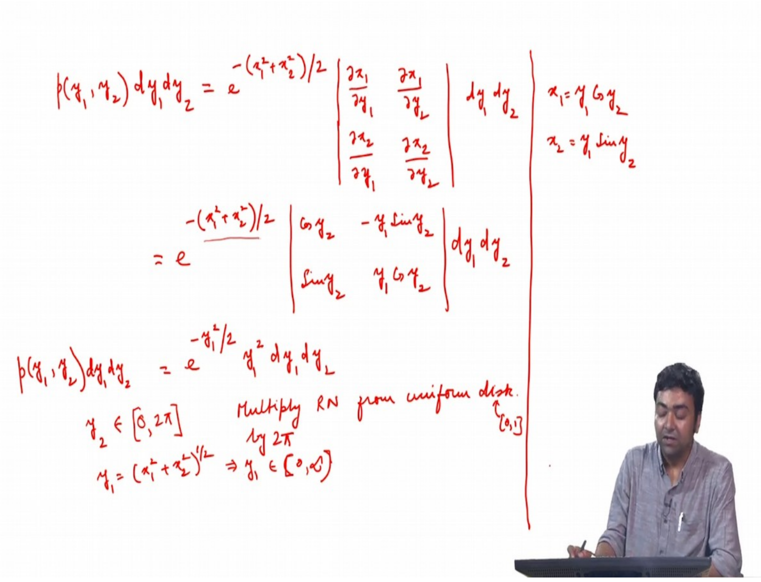

If I do that so, I will get p y 1 y 2 as a function of d y 1, d y 2 this will be equal to. So, my p x 1 x 2 from equation 2 is my this Gaussian distribution here,which is e to the power minus x 1 square plus x 2 square by 2. So, that is e to the power minus x 1 square plus x 2 square by 2 and then what I need to come have is this Jacobian.

Here since I have two variables by Jacobian will be our two cross two determinants and that will be given by del x 1, del y 1, del x 1, del y 2 and in the second row we will be having del x 2 del y 1 and del x 2 del y 2 and then we have d y 1 and d y 2. So, just for recap let me just write down here the expression of x 1, x 1 is equal to y 1 cos y 2 and x 2 equals to y 1 sin y 2.

So, if I evaluate these two these four derivatives and plug it in here. So, what I will get is the following. This equation the right hand side of this equation we can rewrite in the following form minus x 1 square plus x 2 square by 2, then the derivative of x 1 with respect to y 1 will give me cos y 2; the derivative of x 1 with respect to y 2 will give me minus y 1 sin y 2, the derivative of x 2 with respect to y 1 will give me sin y 2 and the derivative of x 2 with respect to y 2 will give me y 1 cos y 2 and then I have d y 1, d y 2.

So, what I can do now is again if you look at these two equations. So, y x 1 square plus x 2 square that is nothing, but y 1 square. So, I plug in y 1 square here. So, I get e to the power minus y 1 square by 2 and then if I evaluate this determinant. So, what I will be getting is, y 1 y 1 cos y 2 square plus y 1 sin y 2 square and together that gives me y 2 square sorry y 1 square and then I have dy 1 dy 2.

So, this is what my probability distribution function will look like based on the new transformations that we have made. Now these y 1 and y 2 these we need to generate from my random numbers which has the uniform distribution. So, in that case so, let us see what values y 2 can take. So, y 2 if you remember. So, y 2 is tan inverse x 2 by x 1. So, basically what it means that my y 2 will vary or y 2 can vary from 0 to 2 pi.

So, how will I get these value different values of y 2 from the uniform distribution? So, what I need to do is, multiply the random numbers from my the random numbers from uniform distribution by 2 pi. So, this will then generate a set of numbers whose range is from 0 to 2 pi uniform distribution. So, where this range is 0 to 1 and what will be the range of y 1? y 1 can take any value because y 1 is x 1 square plus x 2 square to the power half.

So, in principle y 1 belongs can take any values ranging from 0 to infinity. So, now, the question is how to relate y 1 to a set of random numbers which lie between 0 to 1. So, to prove that we make another assumption. So, what we say is ok.

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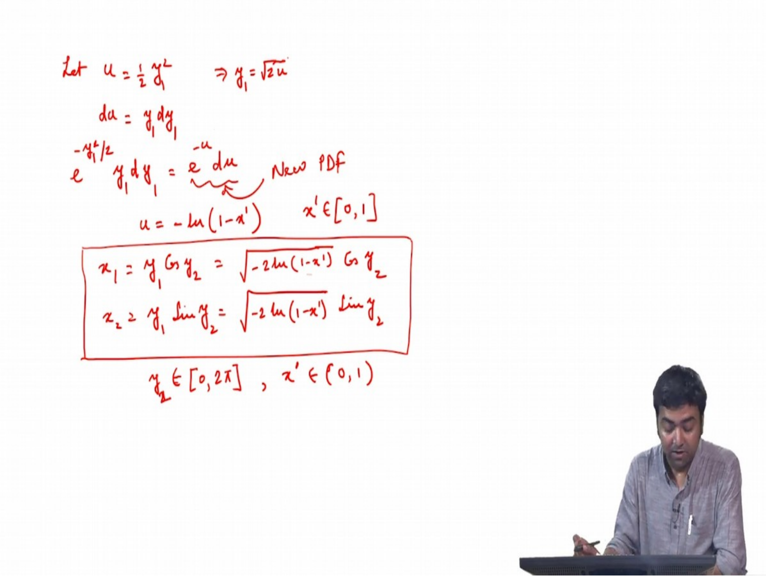

Let me define a new function which is u is equal to half y 1 square. So, that implies y 1 is equal to root 2 u. So, from here if I take the d u, d du will be given by y 1 d y 1.

So, what I will do now is, I will plug this in into this expression. So, what will happen is the following. So, in this expression if we focus on this particular term e y 1 square sorry there is a mistake here will be just y 1 not y 1 square sorry for that. So, what we will do is, we will replace this part with my this function. So, what I have is e 1 square e 1 to the power minus y 1 square by 2 y 1 dy 1 this I can write into e to the power minus u du. So, this is my new probability distribution function and we have already seen that. That this is the probability distribution function is exponential and for that we know x in terms of y or in other words a in this case we can write down u as a function of x.

So, basically what we need here is what it means is that, we need to have a set of numbers random numbers which follows the exponential distribution. And that we can generate again from big from a set of random numbers which has a uniform distribution and lying between 0 to 0 prime 0 and 1 and if we call that as x prime so, that we can write down as minus log 1 minus x prime. So, where my x prime belongs to between 0 and 1. So, if I plug in all these things now. So, what do I get is x 1 is equal to the numbers which I started off with is equal to y 1 y 1 cos y 2 and y 1 we know is given by a root 2 u.

So, what I need to do is basically take the log of. So, it is minus 2 log 1 minus x prime and then we have cos y 2 and similarly x 2 is equal to y 1 sin y 2 which is given by again minus 2 log 1 minus x prime sin y 2. So, this is how I generate my uniform this a normal distribution random numbers and what are the limits on y 1 and x prime?

So, y 1 will go from sorry y 2 will go belongs to your 0 and 2 pi 0 to 2 pi and similarly your x prime that will belong to 0 to 1. So, now, if you look one thing. So, if my x prime a is 1 then this term is always this term becomes log 0. So, and log 0 is undefined. So, that is why I have a open bracket here. So, x prime will be actually less than 0 less than 1.

So, now that next question is can we do some more simplification to this? Because you see these involves lot of operations when you try to calculate it. So, it involves estimation of expensive cos trigonometric functions, the sin and the cosine and the log then square root. So, all this takes time to compute in the computer. So, the idea is can we simplify it further to something which is much more cheaper to compute?

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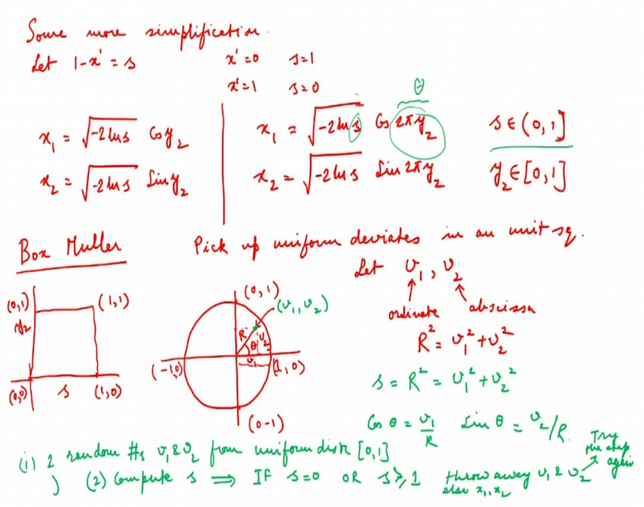

So, let us see how we do it. So, some more simplifications. So, to do that what we assume is, let us do some more change of variables. So, we assume 1 minus x prime is equal to s. So, when x prime is equal to 0, I have s equals to 1 and when x prime equals to 1 I have s equals to 0. So now, if I rewrite. So, my x 1 will be equal to minus square or within the square root minus 2 log s cos y 2 and then x 2 will be equal to minus 2 log s sin y 2.

So, this I can rewrite in a slightly different way which is the following. So, instead of. So, if I take y 2. So, is if you remember as we talked earlier. So, y 2 we have to generate from a distribution of random numbers which lie between 0 and 1. So, we need to multiply 2 pi by to this to those random numbers to get y 2. So, rather than doing that what we can do is, we can rewrite this in this fashion. So, x 1 the first part is same as on the left hand side we have and then instead of cos y 2, we just write 2 pi y 2. In the similar fashion, x 2 is equal to root over minus 2 log s then we have sin 2 pi y 2.

And the restrictions on s and y 2 will be again s should be 0 between 0 and 1 it, but it should not be equal to 0 and neither it should be equal to 1 because if it is equal to 0 then where these x 1 x 2 becomes undefined and if it is equal to 1 then we will always get 0 as my 2 sets of random numbers which we do not want. So, this is a sort of an open interval we are putting in here and then y 2 now since we have written it as 2 pi into y 2. So, we can directly use the random numbers given by my uniform distribution or the my pseudo random number generator available in the code. So, thus goes between 0 and 1. So, there is some further way to simplify it and this is what Box Muller proposed. So, we will first see why what we are doing, what simplification we are doing and then I will explain to you how this simplification makes the computational cost lower.

So, if I look at this these two variables. So, this I can put in two axes. So, if along the x axis I say this is my s and along the y axis I have my y 2. So, if we look at this. So, basically I have start from the origin, then I have 1 0 that is the range of x and what I can do is, I can draw a rectangle with these coordinates 0 0 1 0 1 1 and 0 1.

So, the idea is the following. What we do is we pick up uniform deviates in. So, the side of each of this square is one in an unit square. So, uniform deviates by uniform deviates what I mean is that, the random number which has a uniform distribution and then we defined 2 variables let v 1 and v 2. So, where v 1 is my ordinate and v 2 is my abscissa.

So, what we do is using these two we draw a circle. So, what we have is basically the idea is the following say we have a circle whose radius is unity. So, this is a bad drawing.

So, basically I mean what I mean is this is this side it will be 1 and this side it will be minus 1 1, 0, 1, 0 and this coordinate this will again be 0 1 and this will again be 0 minus 1. So, this is my circle whose radius is 1 and we took 2 points v 1 and v 2.

So, such that we have radius which is given by r square equals to v 1 square plus v 2 square. So, what it means is. So, basically this is my v 1 the this part here and then this is my v 2 or this normal is my v 2 and then I can get the angle theta as the angle sustained by v 1 and v 2 and this distance from. So, basically this the coordinate of this particular point let me use a different colour to show the point. So, let us choose green.

So, I have this green coloured point here. So, the coordinate of this point is given by v 1 and v 2 and the distance of this point from the origin is sort of you can think of as the radius. So, if you look into these equations. So, we need one variable which gives me one number which gives me this one, and the other number is and then we need something analogous to an angle. So, we need a s and we need an angle. So, what we do is. So, what the suggested is, let us take is s the as the square of the distance from the origin of my circle to the point v 1 and v 2 described by v 1 and v 2. So, that is v 1 square and v 2 square.

And so, if I think of this as some variable theta. So, for these cases the coordinates what I get is I get cos theta will be v 1 by R and sin theta will be v 2 by R. So, what I now do is basically the following. So, I pick two numbers from my uniform distribution of random numbers random out rather in other words random numbers have a uniform distribution and lying between 0 and 1 I pick 2 numbers I compute s.

So, I need to check about s because s is crucial because the value of s can make this two newly generated random numbers to 0 or it can make them to be undefined. So, as part before. So, this was the restriction on s. So, what we do is we. So, you choose two random numbers. So, the step is following you two random numbers v 1 and v 2 from uniform distribution and lying between 0 and 1. So, the second step is compute s. So, from here what you do is you check s if my s is equal to 0 or s is equal to is greater than or equal to 1. So, what I do is, I throw away v 1 and v 2 if these conditions are not satisfied then else I mean the random numbers which are generated x 1 and x 2 generated using this formula that we will be using as an new set of random numbers.

And if this condition is satisfied then what you need to do is you need to try the step again. So, this is the whole idea of generating the things.

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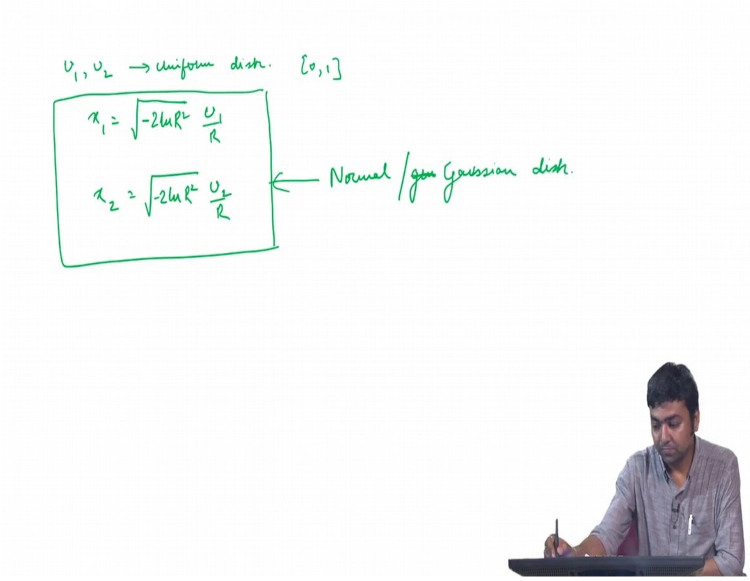

So, at the end of the day what you have is you take two random numbers v 1 and v 2 which has a uniform distribution form a uniform distribution and lying between 0 and 1 and then you do this following transformation. So, you write you generate two new set of random numbers which is given by minus 2 log r square v 1 by R and then you have x 2 equals to root over minus 2 log R square v 2 by R. So, these are my new set of random numbers which forms the normal or Gaussian distribution.