Advanced Mathematical Methods for Chemistry

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Lecture - 03
Poisson Distribution, Gaussian Distribution

So now we just saw about the binomial distribution. Now another there are couple of other famous distributions and I will just explain I will just describe them briefly. So, the first one is called the Poisson distribution.

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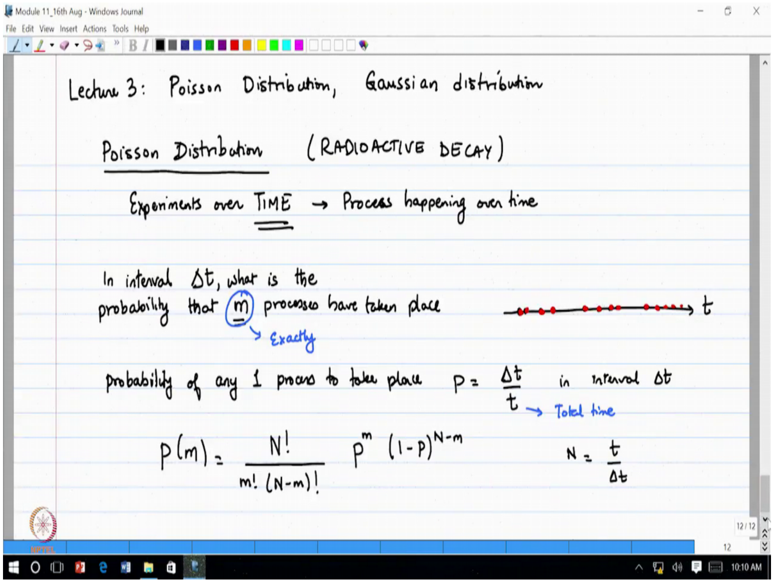

And this is like a limiting value of the binomial distribution. So, like a limiting value of the binomial distribution. Let us to motivate it let us consider let us consider that you do experiments over time. So the idea is idea is that there some process or some process happening over time. The most common example is that of radioactive decay. So, so where what you think of is you have a nucleus of a radioactive element. And over some it might it decays. And each decay is one instant or one single process.

So, in one decay one atom decays then later on some other atom might decay. So now, what you think of is you look at these processes over time. And you might have one happening here another one happening here next one happening here next one happening here and so on. You might have actually let me show this in red. So, the decay process takes place at various each of these corresponds to one of these processes happening. So, if you have if you have something like this happening, then you can ask what is the So, we can we can ask a question that in interval delta t what is the probability that m processes have happened have taken place.

So, if this process is radioactive decay then what is the probability that exactly m atoms have decayed in interval delta t exactly m. So, it is very important when you say m you mean exactly m. And what will assume is that the probability of any one process to take place p is equal to delta t by t. So, take place in interval delta t, t as total time. So, that means, during each interval there is a probability that even take place which is delta t by delta t. So that means, over this whole time t basically this process all the I mean this the probability that will decay over this entire time t goes to one.

So, in this case now you are you are you can you can write you can write the probability that exactly m processes have taken place as n factorial divided by m factorial n minus m factorial just like the binomial distribution. And you have p raise to m 1 minus p raise to n minus m. So, so where n is equal to t divided by delta t. N is the total number of intervals, which is t divided by delta t. So, so what you are imagining is that you are breaking that this interval of times from 0 to t into unit is of delta t. This is your t and you are breaking to unit is to delta t. Now we just go ahead and we say that n factorial.

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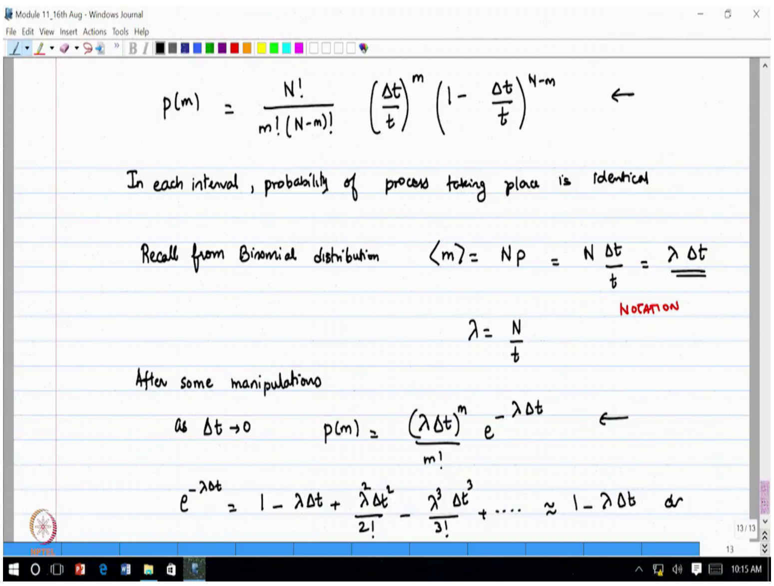

Now the basic idea of Poisson distribution is that is that in each interval probability of process taking place is identical. In other words if you think in terms of radioactive decay then within each interval the probability that one atom one particular atom will decay is the same which is p.

Now, the idea is we want to we want to consider the case. So, so we will make a few changes in this. We recall from binomial distribution, that average value of m is equal to n times p is equal to n times delta t by t. And we will call this as lambda times delta t where lambda is n by t. So, this is the notification. So, what you can do is that is that your mu or average value of m this is mu is lambda times delta t. What we will do is we will we will try to eliminate t and write wherever we have t we will write it as n by lambda. So, we will write t as n by lambda. So, lambda is equal to n by t or t equal to n by lambda and what you can do is that after some manipulations, we can show that as delta t tends to 0 as a intervals it become very small p of m can be written in the following form can be written as lambda delta t raise to m divided by m factorial times e to the minus lambda delta t.

Now I have skipped quite of few steps in this in this derivation, but the basic idea that will use is that e to the minus lambda delta t is equal to 1 minus lambda delta t plus lambda square delta t square by 2 factorial minus lambda cube delta t cube by 3 factorial plus and so on. So, use this infinite series now what will see is that as delta t become goes to 0 then you can truncate this to only some part. You can approximate this by only part of the expression and that is what we have going to use in order to in order to show that show that this is the same as this. So, so we can say approximately equal to 1 minus lambda delta t as delta t tends to 0 ok.

So, once you use that then you can show that this result and what you have here are essentially the same. So, with this we can so now, now that we have we have this result in place. So, we will just use this result p of m is equal to lambda delta t raise to m divided by m factorial e to the minus lambda delta t.

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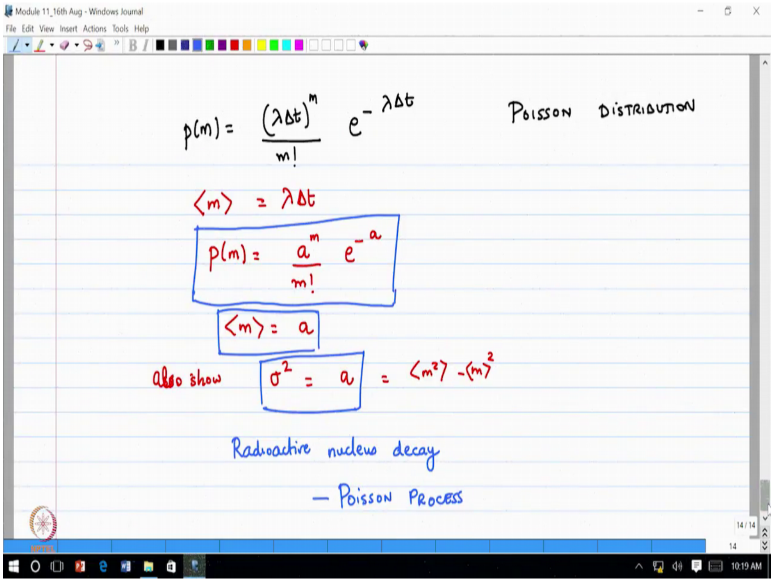

This is called a Poisson distribution. And what are the properties? Average value of m is equal to lambda times delta t. So, so sometimes you can write p of m as a raise to m and divided by m factorial e raise to minus a. Where a is the average value of and average of m is equal to a and again this is something that you can show fairly easily. Now what about the standard deviation? So, so you can also show sigma square is equal to a is equal to average of m square. So, so these are the 2 characteristics of this or 2 properties of this Poisson distribution. And this is something that is you know fairly widely used let me just highlight these points. So, so this is another widely trend you can used in used for example, in radioactive nucleus decay. General this Poisson distribution can be shown to work for general. So, this is called a Poisson process, where the important thing is that in any interval delta t. So, if you take any of these intervals delta t the probability that the process happens is equal.

So probability that happens process is equal, and just using that you can derive this Poisson distribution. Next distribution that is extremely popular is what is called a Gaussian distribution.

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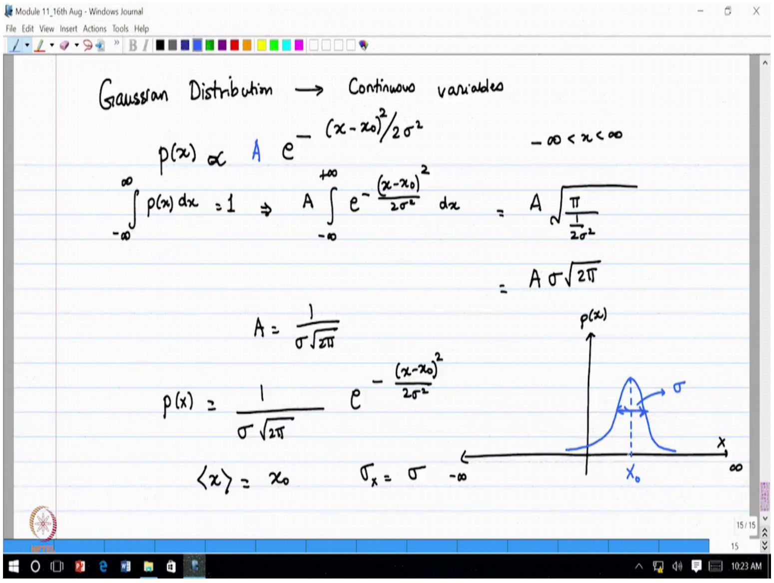

And this is typically for continuous variables. So, here p of x is written as is proportional to e to the minus x minus x 0 whole square divided by 2 sigma square. And what is this consent of proportionality? So, so the first thing is you can say that to determine this consent of proportionality. So, you impose integral p of x d x and the range of x is minus infinity less than x less than infinity. So, integral p of x the p of x from minus infinity is equal to 1, this is equal implies a which is this factor that is there here a. And now you have integral from minus infinity to plus infinity, e to the minus x minus x 0 whole square divided by 2 sigma square d x. This is a Gaussian integral ok.

So, this works on to be a times square root of pi divided by 1 by 2 sigma square. So, what this implies is that and this is equal to a times sigma root 2 pi. So, therefore so this equal to 1 implies a is equal to 1 by sigma root 2 pi. So, p of x can be written as 1 by sigma root 2 pi e to the minus x minus x 0 whole square divided by 2 sigma square. This is a So, average value of x is equal to x 0. And standard deviation of x equal to sigma. And what just look like? This Gaussian function is it is look like a Gaussian distribution function. So, if this is minus infinity this is your x access p of x show on this access. So, what is done is that you take some point it is x 0 and this looks like, this function looks like this spread is equal to sigma is of order sigma. This is the mean this is in the standard deviation is the measure of this spread, let us let us calculate the calculate the quantity call the full Width at half maximum of p of x.

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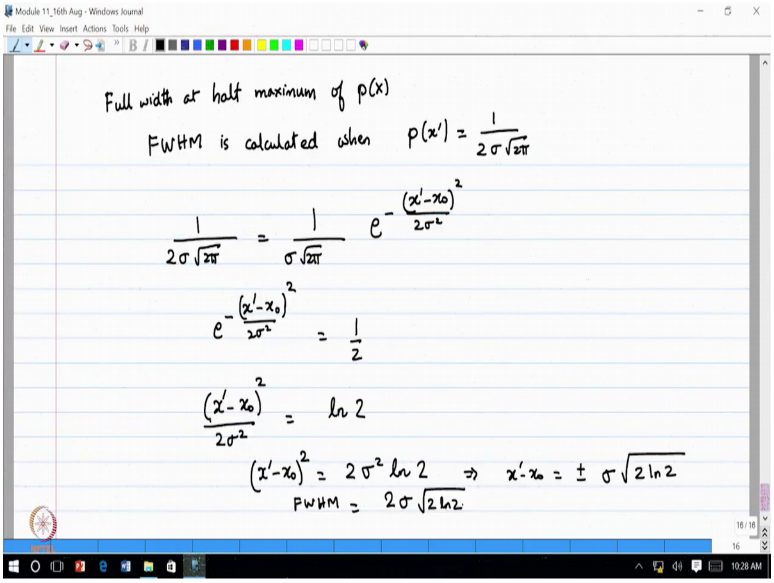

So, so this is called as FWHM ok.

So, to calculate this, p of x is maximum. So, we can do this we can see this p of x is maximum. And when it is it is it is maximum at x equal to x 0 when x is equal to x 0, then this quantity e to the minus x minus x 0 square by 2 sigma square as e to the 0 which is one. So, this value is just one over sigma root 2 pi. So, what you have to do to calculate the full width at half maximum is, So is calculated when p of x prime is equal to now it will be one over 2 sigma root 2 pi. So, so when you have t equal to 1 about sigma toot 2 pi. Then what you will say is that one over 2 sigma root 2 pi is equal to 1 over sigma root 2 pi times e to the minus x prime minus x 0 whole square divided by 2 sigma square ok.

So, basically e to the minus x prime minus x 0 whole square divided by 2 sigma square equal to half and if you take logarithm on both sided logarithm or half is minus logarithm of 2. And so, what you will get is x minus x 0 x prime minus x 0 whole square divided by 2 sigma square equal to natural log of 2. Or you can write that x prime minus x 0 whole square equal to 2 sigma square natural log of 2. And this implies that x prime minus x 0 is equal to 2. So, so you can just look at the width. So, there are 2 possible values, x prime minus x 0 equal to plus minus plus minus sigma root 2 ln 2. So, so that implies that full width that half maximum is equal to so, it will be twice this separations. So, I can just write this as 2 sigma square root of 2 ln t wook.

Now, natural log of 2 is about 0.69. So, 0.69 into 2 is about 1.38. So, square root of 1.38 it will be about 1.11 and so and so and so, what you get is about h m is approximately equal to sigma into 2.37. So, essentially this spread at full with half maximum. So, of order to sigma is approximately sigma into 2.37. So, so in other words is proportional to sigma and it is some small multiple of sigma. So, sigma measures the spread of this distribution.

Gaussian distributions Are ubiquitous as you seen them everywhere in sciences.

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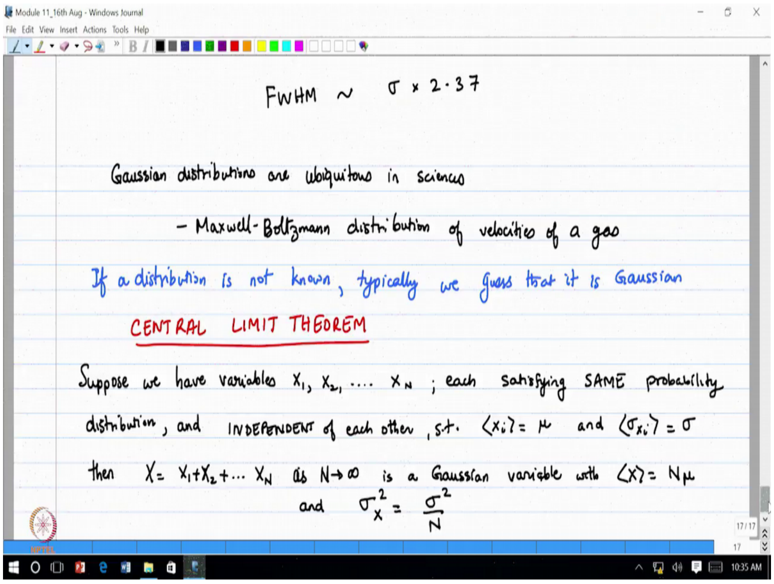

Example is Maxwell Boltzmann distribution of velocities this is one example of a gas. But there are several other examples and in fact, what is important about situation is that is that is that if a distribution is not known then typically we guess that it is Gaussian. This is a very important idea that is underline lot of the things that we do s we also I mean for example, you know when you when you do your experiment you calculate you do a measurement many times. What you do by default is to calculate the average and standard deviation. So, you are implicitly under need that you will be it turns out that you are assuming that your variables are distributed like a Gaussian with this mean and standard deviation. And in fact, in fact we use that to analyze the 2 estimate the error we will see that in the next lecture ok.

But there is a deeper reason why Gaussian distributions are assumed. And this has to do which something called the central limit theorem. So, the central limit theorem. So, what it say is that suppose we have, we have variables x 1 x 2 up to x n x n. So, these are different variables. Each satisfying same probability distribution and independent of each other each other, and independent of each other. So, they are independent of each other and satisfying the same probability distribution, such that average of any x I is equal to mu and sigma of x I is equal to sigma. So, each of them have the same average and standard deviation ok.

Then the x is equal to x 1 plus x 2 up to x n, the sum of these variables as n tends to infinity. So, if you have a very large number of variables as n tends to infinity the sum of these variables x is a Gaussian variable with average x equal to n times mu. And average or sigma of n sigma of x is equal to sigma divided by square root of n. So, so in other words I can write sigma x square equal to sigma square divided by n. So, this theorem basically says that if you have a large number of variables and these variables might satisfy any distribution, but they should satisfy the same probability distribution and they should be independent of each other. Then their sum looks like a Gaussian variable and the important thing is that the sum of these random variable is a Gaussian.

Now, you can this seem are very obscure statement, but you know when you make any physical measurement it is like making a number of small measurements and you are taking I said the sum is Gaussian distributed with this distribution, you can also take the average and if you take the average then.

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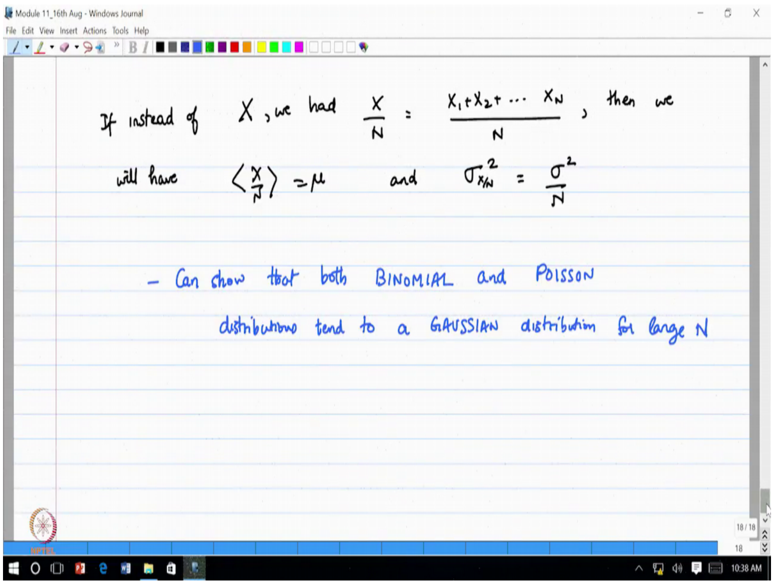

So, if instead of Instead of x we had x by n equal to equal to x 1 plus x 2 plus x n by n we will have average value of x by n equal to mu. And sigma of x by n is equal to it remains the same that is sigma of x by n square equal to sigma square divided by n. So, basically if you think of any macroscopic measurement as average of lot of small microscopic measurements then the Gaussian distribution is very natural. If you think of very large number of measurements then things do look Gaussian. And in fact, you can you can show this we can show that can show that both binomial and Poisson distributions tend to a Gaussian distribution for large n ok.

So, the Gaussian distribution appears very naturally and that is the distribution that we see and that is the distribution that we used most of most often I will conclude this lecture here. So, in the next lecture what I will describe is the idea of error estimation. So, we will look at what are the standard estimates of error. And what I want to emphasize is that underlying the whole error analysis is the idea that your variables are have somehow distributed like a Gaussian. So, I will I will stop here for now.

Thank you.