

Advanced Mathematical Methods for Chemistry
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Module - 11
Lecture - 02
Probability Distribution Functions, Binomial, Poisson, Gaussian

In this lecture I will look into more detail into some of the distribution functions. I will talk about the binomial distribution function and then the Poisson distribution and then the Gaussian distribution. These are these are distributions that you encounter frequently in various problems.

So, we will start with the binomial distribution. Now in order to start this let us let us take an experiment where there are only 2 possible outcomes. So, there is one outcome which you can think of as a coin toss. So, you have heads or tails now, but let us say this coin is not a very faithful coin. So, it is slightly biased. So, so there is a probability of one of the outcomes. So, the probability of one outcome is p , and the probability of the other outcome should be $1 - p$, because some of the outcomes should add up to 1.

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The image shows a digital whiteboard with handwritten notes. The title is "Lecture 2: Probability Distribution functions, Binomial, Poisson, Gaussian". The main topic is "Binomial Distribution: Tossing a 'BIASED' coin". It states that each toss has a probability of heads $H = p$ and tails $T = 1 - p$, with a note that there are "ONLY 2 OUTCOMES". A question is posed: "If the coin is tossed N times, what is probability of exactly m heads ($m \leq N$)". The formula for the probability of exactly m heads is given as $p(m) = \frac{N!}{m!(N-m)!} p^m (1-p)^{N-m}$. A red arrow points to p with the label "parameter of the distribution". Below this, the probability of exactly m heads is written as "Binomial Distribution of m ". Specific cases are listed: $p(1) = \frac{N!}{(N-1)!} p (1-p)^{N-1} = N p (1-p)^{N-1}$, $p(0) = (1-p)^N$, and $p(N) = p^N$.

So, I am going to start with the binomial distribution. Now imagine tossing a biased coin such that in each toss probability of heads equal to p probability of tails

equal to $1 - p$. And if p equal to half then it is the it is an unbiased coin. But in general we will say p may or may not be equal to half. Now the question is if the coin is tossed N times what is probability of exactly m heads? So, we call this p of m any m it need not to be the first m need be the need not be the last m ; obviously, we assume that m is less than n , less than equal to n .

So, p of m . So now so, you have to get m heads. So, if you can you can write this following way you can write this as p raise to m and then you have to get you have to get $N - m$ of tails. So, the probability of tails of one tail is $1 - p$ raise to $N - m$. And so this is the probability of getting m heads this is the probability of getting $N - m$ of tails. But this is again for very this is for m to be heads and specific $N - m$ to be tails. So, you have to multiplied this by the number of ways you can choose, you can choose m outcomes out of n . Which we want to be a heads. So, so this is multiplied by factor of N factorial divided by m factorial $N - m$ factorial, which is a number of ways to choose m outcomes out of total N experiments, those m outcomes you are going to have heads.

Now this is referred to as the binominal distribution of m . So, the m is the variable that you are saying. So, the probability that you get exactly m heads or as I said you know you need not be heads or tails you could just be m of outcome 1 and $1 - p$ of outcome 2, so you so the important thing is only 2 outcomes. So, this is where the binominal distribution is used. And this is a very useful distribution. So, the quantity p is a parameter. So, so this is a parameter of the binominal distribution the distribution. Now these 2 p are different the p I referred here is a probability of m .

This is the probability of exactly m heads. So, these 2 are slightly different. I am still using p for both of them, but this is the function of m . So, what is the probability that you get exactly one heads? So, the probability that you get that m . So, then you just substitute m equal to 1 and what you will get is you will get p times $1 - p$. So, p times $1 - p$, $1 - p$ raise to $N - 1$ times N factorial divided by m , m factorial times $N - 1$ factorial, p $1 - p$ raise to $N - 1$ is equal to N times p $1 - p$ raise to $N - 1$.

Now, you can also have a probability of 0 heads. So, probability of 0 heads is just 1 minus p raise to n. So, it means all the others have to be tails. So, you have 1 minus p raise to n. And this is incidentally this is equal to probability of all n. So, probability of N heads is equal to so again you will have one here you will have p raise to n. So, there is a probability of N heads ok.

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Binomial distribution \rightarrow Application in Random walk
 Model for Diffusion

$$\langle m \rangle = \sum_{m=0}^N m p(m)$$

$$= \sum_{m=0}^N m \frac{N!}{m!(N-m)!} p^m (1-p)^{N-m}$$

$$= mp$$

Evaluation is not straight forward but can be shown

$$p(m) = \frac{N!}{m!(N-m)!} p^m (1-p)^{N-m}$$

One of the terms in B.E. of $(p + (1-p))^N$

$$\Rightarrow \sum_{m=0}^N p(m) = (p + (1-p))^N = 1 \quad \text{NORMALIZED}$$

The last 2 are very initiative ideas. So, the binomial distribution is actually I mean though it is seems like a very simple distribution. So, so binomial distribution has applications in what is called as a random walk or this is model for diffusion. So, random walk is a model for diffusion of particles.

This is again very important non equilibrium transport. So, so the binomial distribution has a very important application, in it is generally you will see it in lot of places I mean you will see it sometimes you are doing when you are doing in statistical mechanism we use the binomial distribution. Now what is the average value of m? So, this will be given by some over I equal to 0 now m can take value of 0 to it can go all the way to n. $M p m$ and this we can write as m times. So now, now if you want to evaluate this it take bit of work, but if you finally, evaluate it you will get an answer you will get this answer that this is equal to m times p. So, just say evaluation not straight forward. I will just I will just say that it is not straight forward, but what I want to emphasize is that can be done, but it can be done.

So, what I mean is if you just look at this series as a by itself, it does not look like it does not look like something that that you can that you can get that result, but; however, the idea is idea is if you take if you realize that this is part of a binomial this is a coefficient of a binomial term. So, so the idea is p of m is equal to N factorial divided by m factorial N minus m factorial p raise to m 1 minus p raise to N minus m . This is this is coefficient of p plus 1 minus p raise to n or other one of the terms, one of the terms in binomial expansion of this. And what we immediately see is that is that this implies that sum over m equal to 0 to N p of m is equal to p plus 1 minus p raise to N which is equal to 1 .

So this is normalized. So the way the way the probability is structured you can you can immediately see that this is part of this binomial expansion and so and so, it is going to be normalized. And now what is done to show. So, so what you can due to show this next result.

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The image shows a handwritten derivation in a digital journal. The steps are as follows:

$$\langle m \rangle = \sum_{m=0}^N P(m) m = \sum_{m=0}^N m \frac{N!}{m!(N-m)!} p^m (1-p)^{N-m}$$

Set $1-p = q$

$$(p+q)^N = \sum_{m=0}^N \frac{N!}{m!(N-m)!} p^m q^{N-m}$$

$$\frac{\partial}{\partial p} (p+q)^N = \sum_{m=0}^N \frac{N!}{m!(N-m)!} [m p^{m-1} q^{N-m} - (N-m) p^m q^{N-m-1}]$$

$$p \frac{\partial}{\partial p} (p+q)^N = \sum_{m=0}^N \frac{N!}{m!(N-m)!} [m p^m q^{N-m} - (N-m) p^{m+1} q^{N-m-1}]$$

$$\langle m \rangle = \sum_{m=0}^N \frac{N!}{m!(N-m)!} (N-m) p \cdot p^m q^{N-m-1}$$

Is to show that what the idea idea is show that average value of m equal to sum over m equal to 0 to N p of m times m and this is equal to m N factorial divided by m factorial N minus m factorial into average value is not m p it will be N p sorry, I made a mistake there. It should be equal to m N times p . So, this times p raise to m 1 minus p raise to N minus m . So, what you can show is that this is actually related to the derivative of derivative of the binomial expansion coefficients ok.

So, the idea is suppose you suppose you set, let us say set $1 - p$ equal to q . Now you now you say that suppose you have $p + q$ raised to N , this is sum over m equal to 0 to N , N factorial divided by m factorial $N - m$ factorial, p raised to m q raised to $N - m$. Now if I take if I take d by $d p$ of $p + q$ raised to N , this is equal to sum over m equal to 0 to infinity. Now you have N factorial divided by m factorial $N - m$ factorial and you have $m p$ raised to $m - 1$, q raised to $N - m$. And now if I if I multiply this by p So then, what is done is to So suppose you multiply this by p , then what you will get is that So, p this is equal to So, let me let me just work this out again. So, so there should be a second term which comes from derivative of this with the respect to with respect to p .

So I will just write that second term also. So now, we will get minus. So, I have all this as it is minus $N - m p$ raised to $m q$ raised to $N - m - 1$. So, that will be the other term. The minus term is there is because p is $1 - q$. And so now, if I multiply this by p , then what I will get is minus $N - m p$ raised to $m + 1 q$ raised to $N - m - 1$. So, so what you can see is that left hand side should be 0 , then you get exactly what we are interested in which is the first term. So, that should be equal to the second term. And so what you end up with is that is that you will you will end up with the average value of m is equal to some over m equal to 0 to infinity, N factorial divided by m factorial $N - m$ factorial times $N - m p$ into p raised to $m p$ raised to $m q$ raised to $N - m - 1$ ok.

And now again you can because you have just factor of $N - m$ here, what you what you have to do is actually do a few more manipulations ok.

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The image shows a handwritten derivation on a digital notepad. The first line is the definition of the mean $\langle m \rangle$ for a binomial distribution:
$$\langle m \rangle = \frac{Np}{q} \sum_{m=0}^{\infty} \frac{N!}{m!(N-m)!} p^m q^{N-m} - \frac{p}{q} \sum_{m=0}^{\infty} \frac{N!}{m!(N-m)!} m p^m q^{N-m}$$
 The second line shows the result of the derivative:
$$\langle m \rangle \left(1 + \frac{p}{q}\right) = \frac{Np}{q}$$
 The third line gives the final result:
$$\Rightarrow \langle m \rangle = Np$$
 Below this, it states: "Binomial Distribution has $\mu = \langle m \rangle = Np$ " and "Standard Deviation $\sigma = \sqrt{Np(1-p)}$ ".

So, the so, the first term first term is you can take the Np outside, and then you will have 1. So, if you just take the N times p . So you so, you multiply and divided by q . So, I can write this as, and now again this so what I have done is I have exactly got average value of m here. So now, if I just take this to the left hand side. So, this is exactly average value of m is a p is a additional p factor.

So, what I can show is that average value of m if I take this to the left hand side times $1 + p/q$ is equal to Np/q . And this is exactly equal to 1. This quantity is exactly equal to 1 because of the normalized distribution. So now, now what is this $p + q$ divided by q that is $1 + p/q$. So, therefore, this implies average value of m equal to N times p . So, it is a bit of work show this average value of m , but you can you can work it all. So, the so, the binomial distribution has μ equal to average value of m equal to N times p . This is a very intuitive quantity because each time you can think of it as each measurement you make your you are you are sought of you sought of p is a fraction of each measurement that you get m . So, if you make N measurements then the average number of times that you get it should be N times that fraction.

Ok. So now, this trick that I used where I took the derivative that can be used to calculate higher order moments also. So, suppose you want to calculate the value of average value of m square, I will do the same thing, but I have to take 2 derivatives when you take 2 derivatives you will get you will get m times $N - 1$. And you go through the same

arguments you go through the same manipulations and finally, you will also end up with the average value of average value of sigma square.

So, I will just mention that the standard deviation of the of the binomial distribution. So, the standard deviation sigma is equal to equal to $N \times p(1-p)$. So, so square root of this. So, it is a little bit, but you can show this. So, that is a so, much about the binomial distribution now binomial distribution is a I said one kind of distribution that is fairly widely used. There are other distributions which are called the Poisson distribution and the Gaussian distribution, which can actually be derived from the binomial distribution. But I will do this as part of the next lecture.

So, I will conclude this lecture here. And in the next lecture we will talk about the poisson and Gaussian distributions.

Thank you.