The random walk problem

The random walk problem is one of the most studied problems in statistical mechanics. This problems enables people to simulate diffusion phenomena on a computer. The differential equation and solution to it is the same for random walk and diffusion. Let's try to tackle the problem with whatever we have introduced so far.

The problem is as follows: consider a particle in 1D, or a walker, who works along a 1D lattice. Before each step, he flips a coin. If it is head, he takes a step forward (right). If its tail, he takes a step backward (left). The coin is a fair coin. So, the chances of getting a head or tail is the same — $\frac{1}{2}$. The question

is, what is the probability that the walker will be at a point m after N number of steps, that is, $P(m,N)$.
First of all, each step is independent of all the other steps, since it only depends on head or tail, not on what happened before. Second, for now, we are only considering step length to be 1. Later, we will generalize this.

Now, after N steps, the particle/walker will be in any of the following lattice positions —

$$-N, -N+1, \ldots, -1, 0, 1, \ldots, N-1, N$$

Since all the steps are statistically independent, the probability of the occurance of any sequence is $= \left(\frac{1}{2}\right)^N$.
Try to understand this why is it must be true. Think, what is the probability that a sequence of four consecutive coin toss will be THHT. The first outcome T comes with a probability $\frac{1}{2}$. Given its T, the second outcome H has a probability of $\frac{1}{2}$. So, the probability of getting TH in first two coin toss is $\frac{1}{2}\times\frac{1}{2}$ and so on

Let us now analyze the probabilities for a few steps and try to find a pattern.

For a walk with no steps, $P(0,0) = 1$
" " " one step, $P(-1,1) = \frac{1}{2}$ and $P(1,1) = \frac{1}{2}$
" " " two steps, $P(-2,2) = \frac{1}{4}$, $P(2,2) = \frac{1}{4}$, $P(-1,2) =$
$P(1,2) = 0$, $P(0,0) = \frac{1}{2}$.

For three steps, $P(-3,3) = \frac{1}{8}$, $P(3,3) = \frac{1}{8}$, $P(-1,1) =$

$P(1,1) = \frac{3}{8}$, and others are zero

One thing might be clear from here, that, you can't land on an even site of the lattice after odd number of steps and vice versa. Now, the required probability $P(m,N)$ will be, the probability of a particular sequence $\left(\frac{1}{2}\right)^N$, times the number of all distinct possible sequences of steps that will lead to m in N steps. The number of sequences with N_1 steps towards right and $N_2 = N - N_1$ steps towards left is simply given by the sequence of binomial distribution

$$ {}^N C_{N_1} = \frac{N!}{N_1!\,(N-N_1)!} = \frac{N!}{N_1!\,N_2!} $$

So, the probability of getting N_1 forward steps ~~being at site m after $m = N_1 - N_2$~~ after N steps is,

$$ P(N_1, N) = \frac{N!}{N_1!\,(N-N_1)!} \left(\frac{1}{2}\right)^N \quad \text{—(1)} $$

We could as well generalize the problem with unbiased coin. Say, the head happens with a probability p and tail with $1-p$. The the probability of N_1 number of p is.

$$ = {}^N C_{N_1} \{ p^{N_1} (1-p)^{N-N_1} $$

For $p = \frac{1}{2}$, this reduces to equation (1).

From (1), we can write,

Probability that the walker is at m after N steps,

$$P(m,N) = \frac{N!}{\left(\frac{N+m}{2}\right)!\left(\frac{N-m}{2}\right)!}\left(\frac{1}{2}\right)^N \quad \text{— (1)}$$

Here, we have replaced N_1 by m given by, $m = N_1 - N_2$

$$N_1 - N_2 = m$$

$$\therefore N_1 - (N - N_1) = m$$

$$\Rightarrow 2N_1 - N = m$$

$$\therefore N_1 = \frac{N+m}{2}$$

Similarly, $N_2 = \frac{N-m}{2}$

Now, using Stirlings formula,

$$n! = \sqrt{2\pi n}\left(\frac{n}{e}\right)^n$$

$$\Rightarrow \ln n! = \ln\sqrt{2\pi n} + n\ln\left(\frac{n}{e}\right)$$

$$\Rightarrow \ln n! = \ln(2\pi)^{\frac{1}{2}} + \ln n^{1/2} + n\ln n - n\ln e$$

$$\Rightarrow \ln n! = \frac{1}{2}\ln 2\pi + \frac{1}{2}\ln n + n\ln n - n$$

$$\therefore \ln n! = \left(n+\frac{1}{2}\right)\ln n - n + \frac{1}{2}\ln 2\pi \quad \text{— (11)}$$

Now, if n is very large, in the limit $n \to \infty$, we can write,

$$\boxed{\ln n! = n\ln n - n}$$

Using Stirling's formula given by (III) in equation (II) we get,

$$\ln\left(P(m,N)\right) = \ln N! - \ln\left(\frac{N+m}{2}\right)! - \ln\left(\frac{N-m}{2}\right)! + N\ln\frac{1}{2}$$

$$= \left[\left(N+\frac{1}{2}\right)\ln N - N + \frac{1}{2}\ln 2\pi\right] - \left[\left(\frac{N+m}{2}+\frac{1}{2}\right)\ln\left(\frac{N+m}{2}\right) - \left(\frac{N+m}{2}\right) + \frac{1}{2}\ln 2\pi\right]$$

$$- \left[\left(\frac{N-m}{2}+\frac{1}{2}\right)\ln\left(\frac{N-m}{2}\right) - \left(\frac{N-m}{2}\right) + \frac{1}{2}\ln 2\pi\right] + N\ln\frac{1}{2}$$

$$= \left(N+\frac{1}{2}\right)\ln N - N + \left(\frac{N+m}{2} - \frac{N-m}{2}\right) + N\ln\frac{1}{2} - \frac{1}{2}\ln 2\pi - \left[\frac{N+m+1}{2}\ln\left(\frac{N+m}{2}\right) + \frac{N-m+1}{2}\ln\left(\frac{N-m}{2}\right)\right]$$

$$= N\ln N + \frac{1}{2}\ln N - N + N - \frac{1}{2}\ln 2\pi - C$$

Now, $$C = \frac{N+m+1}{2}\ln\left[\frac{N}{2}\left(1+\frac{m}{N}\right)\right] + \frac{N-m+1}{2}\ln\left[\frac{N}{2}\left(1-\frac{m}{N}\right)\right]$$

$$= \frac{N+m+1}{2}\left[\ln\frac{N}{2} + \ln\left(1+\frac{m}{N}\right)\right] + \frac{N-m+1}{2}\left[\ln\frac{N}{2} + \ln\left(1-\frac{m}{N}\right)\right]$$

$$= \left(\frac{N+m+1}{2} + \frac{N-m+1}{2}\right)\ln\frac{N}{2} + \frac{N+m+1}{2}\ln\left(1+\frac{m}{N}\right) + \frac{N-m+1}{2}\ln\left(1-\frac{m}{N}\right)$$

$$= (N+1)\ln\frac{N}{2} + \frac{N+m+1}{2}\left(\frac{m}{N} - \frac{m^2}{2N^2}\right) + \frac{N-m+1}{2}\left(-\frac{m}{N} - \frac{m^2}{2N^2}\right)$$

where we used the Taylor expansion of $\ln(1\pm x)$ given by,

$$\ln(1+x) = x - \frac{x^2}{2} + \cdots \qquad \Big| \ \frac{m}{N} \ll 1 \text{ for } N\to\infty$$

$$\ln(1-x) = -x - \frac{x^2}{2} - \cdots$$

If $x \ll 1$, $\ln\left(1+\frac{m}{N}\right) \approx \frac{m}{N} - \frac{m^2}{2N^2}$ and $\ln\left(1-\frac{m}{N}\right) \approx -\frac{m}{N} - \frac{m^2}{2N^2}$

$$\therefore \quad C = (N+1)\ln\frac{N}{2} + \frac{m}{N}\left(\frac{N+m+1}{2} - \frac{N-m+1}{2}\right) - \frac{m^2}{2N^2}\left(\frac{N+m+1}{2} + \frac{N-m+1}{2}\right)$$

$$= (N+1)\ln\frac{N}{2} + \frac{m}{N}\cdot m - \frac{m^2}{2N^2}(N+1)$$

$$= (N+1)\ln\frac{N}{2} + \frac{m^2}{N} - \frac{m^2}{2N} - \frac{m^2}{2N^2}$$

$$= N\ln\frac{N}{2} + \ln\frac{N}{2} + \frac{m^2}{2N} \qquad \left(\text{ignoring } \frac{m^2}{2N^2} \text{ since } \frac{m^2}{2N^2} \approx 0 \text{ for } N\to\infty\right)$$

$$\therefore \quad \ln(P(m,N)) = N\ln N + \frac{1}{2}\ln N - \frac{1}{2}\ln 2\pi - N\ln\frac{N}{2} - \ln\frac{N}{2} - \frac{m^2}{2N} + N\ln\frac{1}{2}$$

$$\Rightarrow \ln(P(m,N)) = N\cancel{\ln N} + \frac{1}{2}\ln N - \frac{1}{2}\ln 2\pi - N\cancel{\ln N} + N\ln 2 - \ln N + \ln 2 - \frac{m^2}{2N} + N\ln\frac{1}{2}$$

$$\Rightarrow \ln(P(m,N)) = -\frac{1}{2}\ln N - \frac{1}{2}\ln 2\pi + N\ln\frac{1}{2} + N\ln 2 - \frac{m^2}{2N} + \ln 2$$

where $\frac{1}{2}\ln N - \ln N = -\frac{1}{2}\ln N$

$$\Rightarrow \ln(P(m,N)) = -\ln N^{1/2} - \ln 2\pi^{1/2} + \ln 2 + \ln\left(e^{-\frac{m^2}{2N}}\right)$$

where $N\ln\frac{1}{2} + N\ln 2 = -N\ln 2 + N\ln 2 = 0$

$$\Rightarrow \ln(P(m,N)) = \ln\left(\frac{2}{N^{1/2}\,2\pi^{1/2}}\right) e^{-\frac{m^2}{2N}}$$

$$\boxed{\therefore \quad P(m,N) = \frac{2}{\sqrt{2\pi N}}\, e^{-\frac{m^2}{2N}}}$$

Let's now take the continuous limit. We had step length of $l = 1$. The position from the origin is obviously given by, $x = ml$. Now let's take $l \to 0$. Also, say, each step is taken after a time interval of τ where $\tau \to 0$. So, after N steps, the total time is $t = N\tau$.

Now, we can calculate the probability $P(x, N)\Delta x$, that the particle is likely to be found between x and $x + \Delta x$, from the probability $P(m, N)\Delta m$, that gives the probability that the particle is found between m and $m + \Delta m$.

$$\therefore \; P(x, N)\Delta x = P(m, N)\Delta m = P(m, N)\left(\frac{\Delta x}{2l}\right) \quad \Big| \; \Delta x > l$$

It might at first glance seem that $x = ml$ and so, $\Delta x = \Delta m \times l$, so $\Delta m = \frac{\Delta x}{l}$. But, this is not correct. Think about an example. You want to find probability between $x = 6$ and $x = 14$. Here, $\Delta x = 8$. But, when you want to calculate Δm, you see that, if you take an even number of steps, you can only land on 8, 10, 12 and 14. The same goes for odd number of steps - 7, 9, 11, 13. So, Δm is really 4, and not 8, and this is why, $\Delta m = \frac{\Delta x}{2l}$.

$$\therefore \; P(x, N)\,\Delta x = \frac{2}{\sqrt{2\pi N}} \, \frac{1}{2l} \, e^{-\frac{x^2/l^2}{2N}} \, \Delta x$$

$$\Rightarrow P(x, t)\,\Delta x = \frac{1}{\sqrt{2\pi \cdot t/\tau}} \cdot \frac{1}{l} \, e^{-\frac{x^2}{2 \cdot \frac{t}{\tau} l^2}} \, \Delta x$$

$$\Rightarrow P(x,t)\,\Delta x = \frac{1}{\sqrt{2\frac{t}{\tau}l^2\pi}}\, e^{-\frac{x^2}{2\cdot\frac{t}{\tau}l^2}}\,\Delta x$$

$$\boxed{\therefore P(x,t)\,dx = \frac{1}{\sqrt{4\pi Dt}}\, e^{-\frac{x^2}{4Dt}}\,dx}$$

with $D = \frac{l^2}{2\tau}$, which is called the diffusion co-efficient. The probability density is then given by,

$$\boxed{P(x,t) = \frac{1}{\sqrt{4\pi Dt}}\, e^{-\frac{x^2}{4Dt}}}$$

Connection to diffusion

To make a connection to diffusion, we can write the probability as a stochastic difference equation. Let us consider the probability $P(ml, (N+1)\tau)$ that gives the probability that the particle is at ~~at~~ position $x = ml$ at a time $(N+1)\tau$. For this to happen, the particle has to be either at $x=(m-1)l$ or $x=(m+1)l$, at $t = N\tau$.

$$\therefore P(ml, (N+1)\tau) = \frac{1}{2}\times P((m-1)l, N\tau) + \frac{1}{2} P((m+1)l, N\tau)$$

$$\Rightarrow 2P(ml, N\tau+\tau) = P(ml-l, N\tau) + P(ml+l, N\tau)$$

$$\Rightarrow 2P(ml, N\tau+\tau) - 2P(ml, N\tau) = P(ml-l, N\tau) - 2P(ml, N\tau) + P(ml+l, N\tau)$$

$$\Rightarrow \alpha\left[P(x,t+\tau) - P(x,t)\right] = \left[P(x-l,t) - P(x,t)\right] - \left[P(x,t) - P(x+l,t)\right]$$

$$\Rightarrow \alpha\tau \frac{P(x,t+\tau) - P(x,t)}{\tau} = l^2 \frac{\frac{P(x-l,t) - P(x,t)}{l} - \frac{P(x,t) - P(x+l,t)}{l}}{l}$$

$$\Rightarrow \frac{\partial P(x,t)}{\partial t} = \frac{l^2}{\alpha\tau} \frac{\partial^2 P(x,t)}{\partial x^2}$$

$$\therefore \boxed{\frac{\partial P(x,t)}{\partial t} = D \frac{\partial^2 P(x,t)}{\partial x^2}}$$

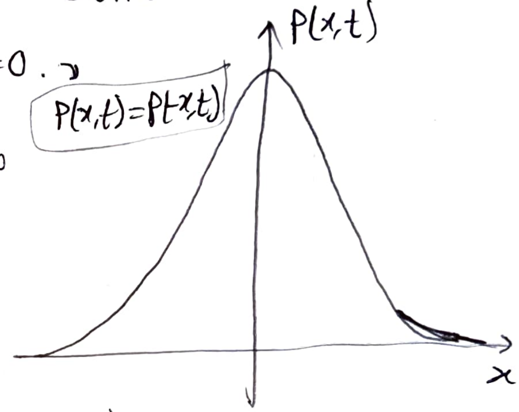
This is the famous diffusion equation. We will later show in diffusion chapter that the solution to this diffusion equation is exactly our $P(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}$.

Comments on probability distribution of random walk

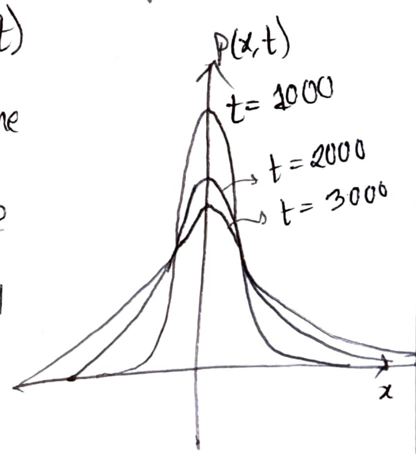
$$P(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

This is a Gaussian probability distribution function, which we found after taking $N \to \infty$ limit in the binomial distribution of random walk. The distribution function is obviously symmetric w.r.t. $x=0$. $\to$ $\boxed{P(x,t)=P(-x,t)}$

It looks like as shown in the graph for a particular time t as a function of x.



As a function of x, the $P(x,t)$ at different times are shown in the graph. You see, as t increases, the peak of the distribution decreases and it flattens out, so the area under the curve remains 1.



The peak of the function occurs at $x=0$ (you can verify by using the idea of derivatives and stationary points).

$$P(x,t)\Big|_{max} = P(x,t)\Big|_{x=0} = \frac{1}{\sqrt{4\pi Dt}}$$

So, if we divide $P(x,t)$ by $P(x,t)|_{max}$ for different t, then their peaks will coincide to 1. However, we can also divide $P(x,t)$ by just $\frac{1}{\sqrt{t}}$, and they will still coincide (since $\frac{1}{\sqrt{4\pi D}}$ is just a constant).

We can then compare the widths of the distribution with time properly, since the half maximas are now at the same height.