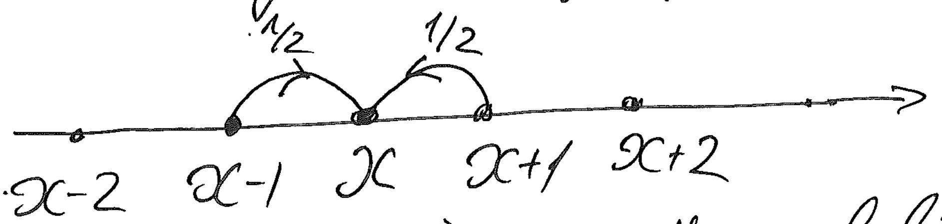
Lecture 4

1D Random walks and ~~[illegible]~~ diffusion

We are studying random walks on 1D chain with symmetric jumps



We introduce $P(x,t)$ as the probability that at time t our particle is in the point x. Let us find a relationship between $P(x,t+1)$ and $P(x,t)$:

jump on the right ($x-1 \to x$)   jump on the left ($x+1 \to x$)

$$P(x,t+1) = \frac{1}{2}P(x-1,t) + \frac{1}{2}P(x+1,t)$$

Initial condition:

$$P(x,t=0) = \delta_{x,0}$$

(the particle in in the point $x=0$)

~~[illegible]~~ Behavior at large time $t \gg 1$ and large $|x|$:

We use the Teylor expansion

$$P(x,t+\Delta t) = P(x,t) + \frac{\partial P}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 P}{\partial t^2}\Delta t^2 + \dots$$

$$P(x+\Delta x,t) = P(x,t) + \frac{\partial P}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 P}{\partial x^2}\Delta x^2 + \dots$$

Then the equations

$$P(x,t+1) = \frac{1}{2}P(x-1,t) + \frac{1}{2}P(x+1,t)$$

takes a form $(\Delta x = \pm 1, \Delta t = 1)$

$$\cancel{P(x,t)} + \frac{\partial P}{\partial t}\Delta t + \frac{\partial^2 P}{\partial t^2}\Delta t^2 =$$

$$= \cancel{\frac{1}{2}P(x,t)} - \cancel{\frac{1}{2}\frac{\partial P}{\partial x}} + \frac{1}{4}\frac{\partial^2 P}{\partial x^2} + \dots$$

$$+ \cancel{\frac{1}{2}P(x,t)} + \cancel{\frac{1}{2}\frac{\partial P}{\partial x}} + \frac{1}{4}\frac{\partial^2 P}{\partial x^2}$$

We get an equation

$$\frac{\partial P(x,t)}{\partial t} = \frac{1}{2}\frac{\partial^2 P(x,t)}{\partial^2 x^2}$$

It is the well-known diffusion equation in 1D.

Solution of the diffusion equation

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

In a general case

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

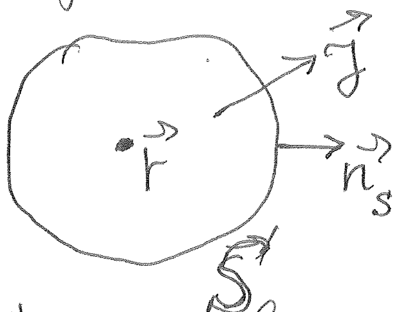
$$P(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}$$

$P(x,t)$ is the density of particles at point x at time t.

The diffusion equation is the consequence of the particle conservation law.

The particles do not disappear and do not appear. They only move ~~s~~ from one region ~~the~~ to another region.

Let us consider a region of a small volume ΔV around point $\vec{r}$. The volume is surrounded by a surface S. $\vec{n}_s$ is the unit vector normal to the surface.



The number of particles in the region is

$$\rho(\vec{r}, t)\, \Delta V$$

During time interval Δt, the number is changed

$$\delta \rho\, \Delta V = \Big(\rho(\vec{r}, t+\Delta t) - \rho(\vec{r}, t)\Big)\Delta V = \frac{\partial \rho}{\partial t} \Delta t\, \Delta V$$

This change is due to the fact that ~~...~~ there is a flow $\vec{J}$ of particles through the surface. The number of particles that left the ~~...~~ volume during the time Δt is

$$\Delta t \oint_{S} \vec{n}\vec{j}\, dS$$

So we have

$$\frac{\partial \rho}{\partial t} \Delta t \Delta V = - \Delta t \oint_{S} \vec{n}\vec{j}\, dS$$

The sign (-1) shows that particles left the volume $(\vec{n}\vec{j} > 0)$.

We use the Gauss-Ostrogradsky theorem

$$\int_{V} \underbrace{(\vec{\nabla}\vec{F})}_{\mathrm{div}\,\vec{F}} dV = \oint_{S} \vec{n}\vec{F}\, dS$$

Therefore

$$\frac{\partial \rho}{\partial t} \Delta t \Delta V = - \Delta t \int_{V} \vec{\nabla}\vec{j}\, dV$$

$$\approx - \Delta t \Delta V\, \vec{\nabla}\vec{j}$$

we get

$$\frac{\partial \rho}{\partial t} = - \vec{\nabla}\vec{j}$$

The flow of particles

$$\vec{j} = - D \vec{\nabla} \rho$$

The particles move from a region with low concentration to region with a high concentration

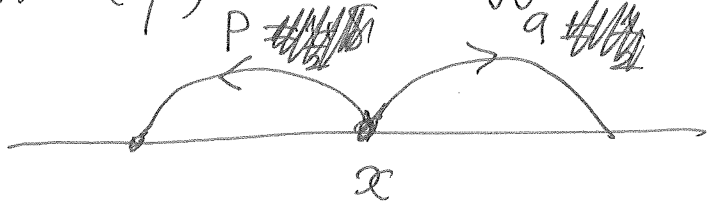
$$\Rightarrow \quad \frac{\partial \rho}{\partial t} = D \Delta \rho$$

$$\Delta = \vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Lecture 5

Assymetric random 1D walk with drift.

We consider the case when the probabilities to jump on the left (p) and on the right (q) are different.



$p \neq q$

$p + q = 1$. Assymetric jumps:

$$\begin{cases} p = \frac{1}{2} - \delta \\ q = \frac{1}{2} + \delta \end{cases}$$

The probability to find the particle at point x at time t (i.e., after t jumps) is

$$P(t,x) = C_{n_+}^{t}\, p^{n_-}\, q^{n_+}$$

n_- ~~is~~ the number of jumps on the left
n_+ is the number of jumps on the right

$$\begin{cases} n_+ + n_- = t \\ n_+ - n_- = x \end{cases} \Rightarrow \begin{cases} n_+ = \frac{t+x}{2} \\ n_- = \frac{t-x}{2} \end{cases}$$

$$P(t,x) = C_{n_+}^{t} \left(\frac{1}{2} - \delta\right)^{n_-} \left(\frac{1}{2} + \delta\right)^{n_+}$$

we get

$$P(t,x) = \frac{C_{n_+}^{t}}{2^t}(1-2\delta)^{\frac{t-x}{2}}(1+2\delta)^{\frac{t+x}{2}}$$

~~thus~~ it is the probability for symmetric jump.

Let us find

$$(1+2\delta)^{\frac{t+x}{2}} = \exp\left[\frac{t+x}{2}\ln(1+2\delta)\right] \simeq$$

$$\simeq \exp\left[\frac{t+x}{2}\left(\cancel{1}2\delta - \frac{1}{2}(2\delta)^2\right)\right]$$

$$(1-2\delta)^{\frac{t-x}{2}} \simeq \exp\left[\frac{t-x}{2}\left(-2\delta - \frac{1}{2}(2\delta)^2\right)\right]$$

we get

$$(1+2\delta)^{\frac{t+x}{2}}(1-2\delta)^{\frac{t-x}{2}} =$$

$$= \exp\left\{\begin{matrix}\cancel{t\delta} + x\delta - t\delta^2 - \cancel{x\delta^2} \\ -\cancel{t\delta} + x\delta - t\delta^2 + \cancel{x\delta^2}\end{matrix}\right\}$$

$$\simeq \exp(2x\delta - 2t\delta^2)$$

We obtain for assymetric jumps

$$P(t,x) = \frac{1}{\sqrt{2\pi t}}\exp\left\{-\frac{x^2}{2t} + 2x\delta - 2t\delta^2\right\}$$

Transformation

$$-\frac{x^2}{2t}+2x\delta-2t\delta^2=$$

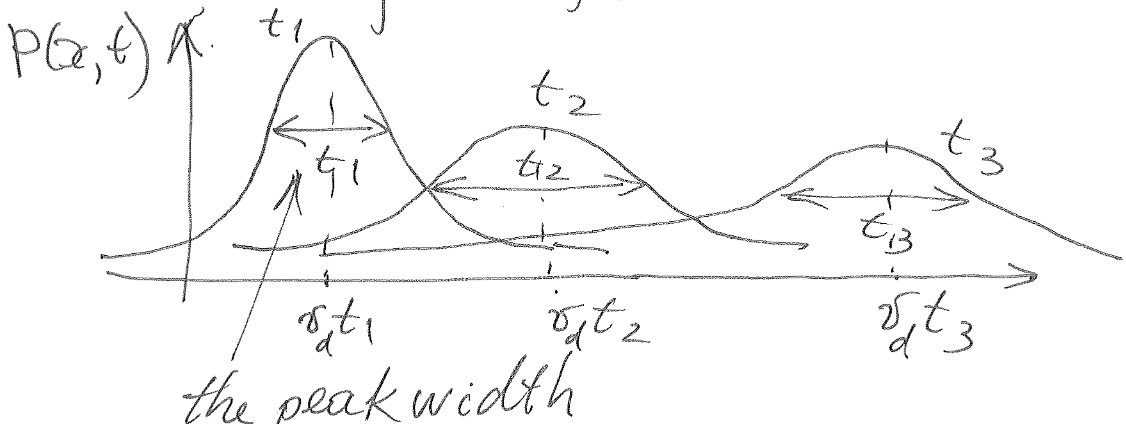
$$=-\frac{1}{2t}\left(x^2-4xt\delta+4t^2\delta^2\right)=$$

$$=-\frac{1}{2t}(x-2\delta t)^2$$

So we get

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

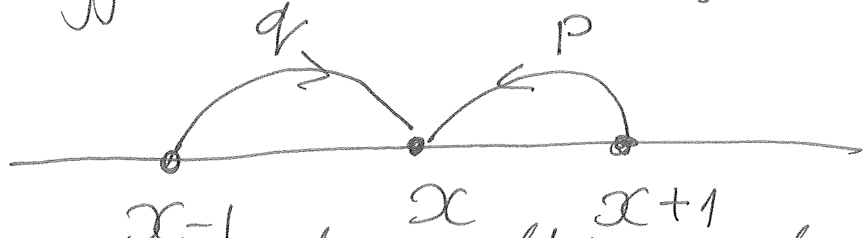
Here $v_d=2\delta$ is the drift velocity of the maximum of $P(x,t)$



$$\max P(x,t)\Big|_{x=2\delta t}=\frac{1}{\sqrt{2\pi t}}$$

$$x_{max}=v_d t$$

Diffusion with a drift



Assymetric random walks are described by

$$P(x,t+1) = q\, P(x-1,t) + p\, P(x+1,t)$$

$$P(x,t=0) = \delta_{x,0}$$

$$P(x,t+1) = \left(\frac{1}{2}+\delta\right) P(x-1,t) + \left(\frac{1}{2}-\delta\right) P(x+1,t)$$

$$= \frac{1}{2} P(x-1,t) + \frac{1}{2} P(x+1,t) + \delta\, P(x-1,t) -$$

$$- \delta\, P(x+1,t)$$

using the Teylor expansion

$$P(x+\Delta x,t) = P(x,t) + \frac{\partial P}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 P}{\partial x^2}\Delta x^2 + \dots$$

$$P(x, t+\Delta t) = P(x,t) + \frac{\partial P}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 P}{\partial t^2}\Delta t^2 + \dots$$

$$P(x-1,t) - P(x+1,t) = \cancel{P(x,t)} - \frac{\partial P}{\partial x} + \cancel{\frac{1}{2}\frac{\partial^2 P}{\partial x^2}}$$

$$- \cancel{P(x,t)} - \frac{\partial P}{\partial x} - \cancel{\frac{1}{2}\frac{\partial^2 P}{\partial x^2}} = -2\frac{\partial P}{\partial x}$$

We obtain

$$\frac{\partial P}{\partial t} = \frac{1}{2}\frac{\partial^2 P}{\partial x^2} - 2\delta\frac{\partial P}{\partial x}$$

Here $v_d = 2\delta$ is the drift velocity

We obtain the diffusion with a drift.

$$\frac{\partial P}{\partial t} = \frac{1}{2}\frac{\partial^2 P}{\partial x^2} - v_d \frac{\partial P}{\partial x}$$

The solution of the equation

$$P(x,t) = \frac{1}{\sqrt{2\pi t}} \exp\left[-\frac{(x - v_d t)^2}{2t}\right]$$