Lecture 2 - Random walks

Random walks are usefull in simulating physical processes as they are related to solutions of the diffusion equation

Diffusion equation in 1D:

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

where D is the diffusion coefficient

- for a quantum particle $D = \frac{\hbar^2}{2m}$
- $P(x,t)$ is a PDF which quantifies the probability of a particle being in the interval $(x, x+\Delta x)$ at time t.
- in 3D $\quad \Delta f(x,t) = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) f(x,t)$

Mean-square displacement $\langle x^2 \rangle$ and the average position $\langle x \rangle$?

- $\langle x(t) \rangle = \int_{-\infty}^{\infty} x \, P(x,t)\, dx$

Multiply by x diffusion eq. and integrate

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

$$\text{l.h.s} = \frac{\partial}{\partial t} \int_{-\infty}^{\infty} x \, P(x,t)\, dx = \frac{d}{dt} \langle x(t) \rangle$$

$$\text{r.h.s} \underset{\substack{\text{integration}\\ \text{by parts}}}{=} \underbrace{D x \frac{\partial P(x,t)}{\partial x}\Big|_{x=-\infty}^{\infty}}_{\emptyset} - D \underbrace{\int_{-\infty}^{\infty} \frac{\partial P(x,t)}{\partial x} dx}_{\underbrace{P(x=\infty,t) - P(x=-\infty,t)}_{\emptyset}}$$

due to boundary condition

$$\begin{cases} \frac{d\langle x \rangle}{dt} = \emptyset & \text{- i.e. } \langle x \rangle \text{ - const} \\ x = \emptyset & \text{at } t = \emptyset \end{cases}$$

$\Rightarrow \quad \langle x \rangle = \emptyset$ at any moment of time

- for calculation of $\langle x^2 \rangle$ multiply by x^2

$$\int_{-\infty}^{\infty} x^2 \frac{\partial p(x,t)}{\partial t} dx = D \int_{-\infty}^{\infty} x^2 \frac{\partial^2 p(x,t)}{\partial x^2} dx$$

$$\text{l.h.s} = \frac{\partial}{\partial t} \int_{-\infty}^{\infty} x^2 p(x,t)\, dx = \frac{\partial}{\partial t} \langle x^2 \rangle$$

$$\text{r.h.s} = \underbrace{D(2x) \frac{\partial p(x,t)}{\partial t} \Big|_{-\infty}^{\infty}}_{\emptyset} - D \int_{-\infty}^{\infty} 2x \frac{\partial p(x,t)}{\partial x} dx$$

$$= \underbrace{-D\, 2 \frac{\partial p(x,t)}{\partial t} \Big|_{-\infty}^{\infty}}_{\emptyset} + D \cdot 2 \cdot \underbrace{\int_{-\infty}^{\infty} p(x,t)\, dx}_{1}$$

$$= 2D$$

The resulting diff. equation is

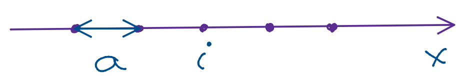
$$\frac{d}{dt} \langle x^2(t) \rangle = 2D \qquad \langle x^2 \rangle = 2Dt + \cancel{\text{Const}} \to \emptyset$$

$$\langle x^2(t) \rangle = 2Dt \qquad \text{if } \langle x^2(t=0) \rangle = \emptyset$$

- In d - dimensional space $2 \to 2d$: $\langle x^2 \rangle = 2Ddt$
- The random walk and the diffusion equation have the same time dependence, let us show it

Random walk equation

Consider a discrete process in which a particle can move by taking steps to right or left with 1/2 probability on a lattice with spacing a



The master equation: discrete space, discrete time

$$p(i, N) = \frac{1}{2} \left[p(i+1, N-1) + p(i-1, N-1) \right]$$

where PDF $p(i, N)$ describes the probability of being at site i after N steps

In order to take continuous limit we identify

$$t = N \Delta t$$
$$x = i \cdot a = i \cdot \Delta x$$
$$p(x,t) = \frac{1}{a} p(i, N)$$

where $\frac{1}{a}$ factor takes into account the proper normalization and proper units

$$\sum p(i,N) = 1 \to \int p(x,t)\, dx = 1$$

normalization and proper units

$$\sum_i \underbrace{P(i,N)}_{\text{dimensionless}} = 1 \rightarrow \int P(x,t)\, \underbrace{dx}_{\text{units of length}} = 1$$

$P(x,t)$: units of inverse length

$$p(x,t) = \frac{1}{2}\left[p(x+\Delta x, t-\Delta t) + p(x-\Delta x, t-\Delta t)\right]$$

subtract $p(x, t-\Delta t)$ and divide by Δt

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

Continuous limit $\Delta x \rightarrow 0$

$\Delta t \rightarrow 0$

$D \equiv \frac{\Delta x^2}{2\Delta t}$ - Const

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

i.e. PDF satisfies the diffusion equation

NB 1 Traditional way to solve diffusion equation or similar differential equations is Crank-Nicholson or other deterministic methods.

The same equation can be solved stochastically by using Random Walks

NB Implementation of complicated boundary conditions can be rather tricky in deterministic methods and are staightforward in Random Walk formulation

Solution of the diffusion equation in free space

Fourier transform can be used to solve the diffusion equation

- use of conjugate variable (momentum)

$$FT[P(x,t)] = P(k,t)$$

- Fourier Transform of m^{th} derivative

$$FT\left[\frac{\partial^m}{\partial x^m} P(x,t)\right] \sim k^m P(k,t)$$

Diffusion equation

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

- multiply by e^{ikx} and integrate over x

$$\partial t \qquad - \qquad \partial x^2$$

- multiply by e^{ikx} and integrate over x

$$\int_{-\infty}^{\infty} \frac{\partial p(x,t)}{\partial t} \cdot e^{ikx} dx = \int_{-\infty}^{\infty} D \, \frac{\partial^2 p(x,t)}{\partial x^2} \cdot e^{ikx} dx$$

$$\text{l.h.s} = \frac{\partial}{\partial t} \underbrace{\int_{-\infty}^{\infty} p(x,t) e^{ikx} dx}_{p(k,t) \text{ - definition of Fourier Transform}} = \frac{\partial}{\partial t} p(k,t)$$

r.h.s = (integration by parts)

$$D \frac{\partial p}{\partial x} e^{ikx} \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} D \frac{\partial p}{\partial x} \cdot ik \, e^{ikx} dx$$

$\frac{\partial p}{\partial x} \to 0$ at $\pm \infty$

second integration by parts

$$= -D \, p(x,t) \, ik e^{ikx} \Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} D \, p(x,t) (ik)^2 e^{ikx} dx$$

$p(x,t) \to 0$ at $\pm\infty$

$$= -D k^2 \int_{-\infty}^{\infty} p(x,t) \, e^{ikx} dx = -D k^2 p(k,t)$$

In momentum space

$$\frac{\partial p(k,t)}{\partial t} = -D k^2 p(k,t)$$

Solution is a Gaussian in momentum space

$$p(k,t) = \exp\left(-Dk^2 t\right)$$

In coordinate space: FT of a Gaussian is anothe Gaussian

$$p(x,t) = FT^{-1}\left[p(k,t)\right]$$

$$= \int_{-\infty}^{\infty} p(k,t) \, e^{-ikx} \frac{dk}{2\pi}$$

$$= \int_{-\infty}^{\infty} \exp\left\{-Dk^2 t - ikx\right\} \frac{dk}{2\pi}$$

Quadratic form in k

$$-Dk^2 t - ikx = -Dt \cdot k^2 - 2 \cdot \sqrt{Dt}\, k \cdot \frac{ix}{2\sqrt{Dt}} \pm \left(\frac{ix}{2\sqrt{Dt}}\right)^2$$

$$= -\left(\sqrt{Dt}\, k + \frac{ix}{\quad}\right)^2 + \left(\frac{ix}{\quad}\right)^2$$

$$-(2\sqrt{Dt})$$

$$= -\underbrace{\left(\sqrt{Dt}\,k + \frac{ix}{2\sqrt{Dt}}\right)}^2 + \left(\frac{ix}{2\sqrt{Dt}}\right)^2$$

$$k' = \sqrt{Dt}\,k + \frac{ix}{2\sqrt{Dt}}$$ change of variables

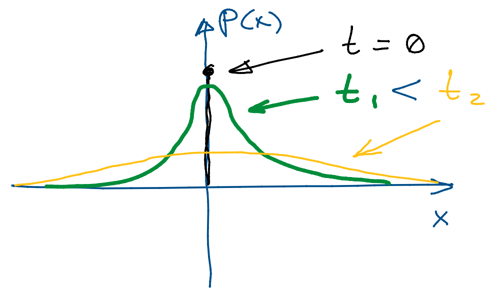
$$dk = \frac{dk'}{\sqrt{Dt}}$$

$$p(x,t) = \int_{-\infty}^{\infty} e^{-k'^2}\, e^{-\frac{x^2}{4Dt}}\, \frac{dk'}{\sqrt{Dt}} \cdot \frac{1}{2\pi}$$

$$= \frac{e^{-\frac{x^2}{4Dt}}}{\sqrt{Dt}} \cdot \underbrace{\int_{-\infty}^{\infty} e^{-k'^2} dk'}_{\sqrt{\pi}} \cdot \frac{1}{2\pi}$$

$$\boxed{p(x,t) = \frac{1}{2\sqrt{\pi D t}} \exp\left\{-\frac{x^2}{4Dt}\right\}}$$

- Free solution is a Gaussian $e^{-\frac{x^2}{2\sigma^2}}$ of width $\sigma = \sqrt{2Dt}$
- initial moment corresponds to a Gaussian of zero width, $\lim_{t\to 0} p(x,t) = \delta(x)$
- the width increases with time



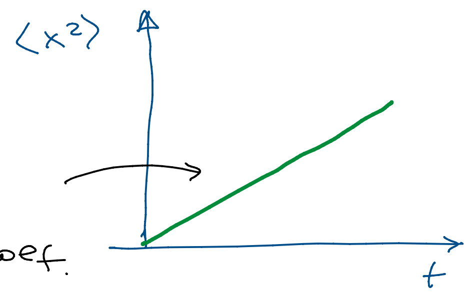
- mean-square displacement

$$\langle x^2 \rangle = \frac{\int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{4Dt}} dx}{\int_{-\infty}^{\infty} e^{-\frac{x^2}{4Dt}} dx} = 2Dt$$

- average position

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x\, e^{-\frac{x^2}{4Dt}} dx}{\int_{-\infty}^{\infty} e^{-\frac{x^2}{4Dt}} dx} = 0$$

NB 1 We obtained Einstein equation for the diffusion



$\langle x^2 \rangle = 2Dt$

slope : diffusion coef.

NB2 Gaussian distribution can be obtained from a Random Walk process

CLT : summing up random variables ends up in a Gaussian probability distribution

NB3 : How to cook a good pasta?

diameter of spaghetti d

Question: time to cook t as a function of d?

Solution : evolution of the temperature distribution $T(x,t)$ is governed by the heat equation

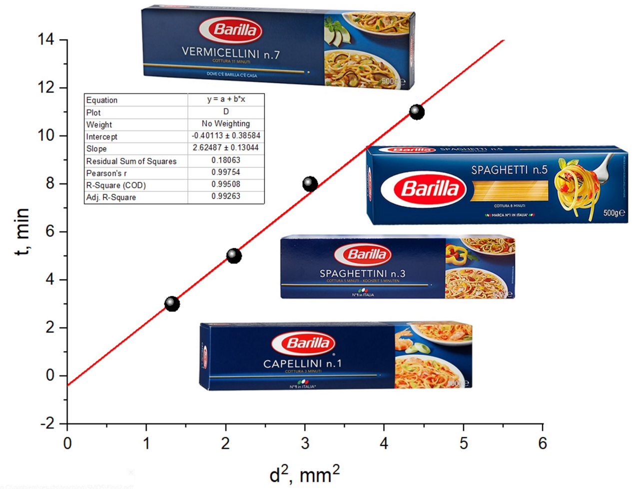
$$\frac{\partial T(x,t)}{\partial t} = D \frac{\partial^2 T(x,t)}{\partial x^2}$$

time needed to diffuse from the border

$\langle x^2 \rangle \sim t$

Considering pasta of different diameters d ;

cooking time $t \sim d^2$



Coef. of proportionality $\quad 2{,}62 \ \frac{min}{mm^2}$

Random Walk solution to Laplace equation

Advantages:

1) arbitrary shape of the boundary can be used

2) differently to deterministic and iterative methods there is no need to solve $p(x,t)$ everywhere

   ⇒ Ex. it's easy to find the value in a single point

3) solution can be found even if the space is infinite, contrarily to the usual methods

Disadvantages

1) the result has some statistical error

But:

- it is controllable
- can be reduced $\sim \frac{1}{\sqrt{M}}$