Lecture 1: Random Walks and 1-D Diffusion

- A localiced high concentration of a substance will spread out to make the concentration spatially homogeneous (2nd Law of thermo)
- Molecules "move" from high to low density
- Individual particles are randomly battered by solvent molecules => causes a random walk
- Many random walks made by many molecules is diffusion
- Diffusion is dominant at les ~1 μm length scales

Show Applet Movie of Random Walk (cannot see little jerks, but can see the large displacements)

Seems remarkable that H_2O collisions perturb μm sphere

Beach ball at concert example

Einstein 1905: while distracted from his thesis

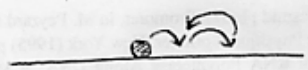
1st observation: pollen particles Robert Brown 1828

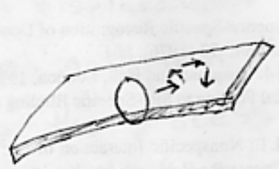
the concept of molecules was contraversial

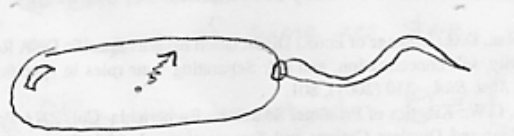
'Brownian motion' was mistaken for a life process

Single molecule measurements: Random walk

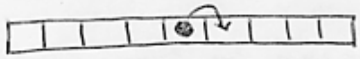
Bulk measurements: Diffusion

1D  transcription factor sliding on DNA
growth of actin filaments

2D  protein traveling in lipid membrane

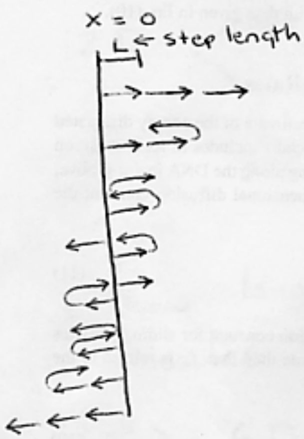
3D  protein traveling in cytoplasm
cell motility

One-Dimensional Random Walk



- flip a coin to determine whether you go left or right
- how far are you likely to go in a random walk
- cannot solve for one walk, but we can determine the <u>average</u> displacement

Enumeration of the possibilities for $N = 3$ steps:



Distance (x_3)	x_3^2
$+3L$	$+9L^2$
$+1$	$+1$
$+1$	$+1$
-1	$+1$
$+1$	$+1$
-1	$+1$
-1	$+1$
-3	$+9$
$\langle x_3 \rangle = 0$	$\langle x_3^2 \rangle = 3L^2$

(mean-square displacement)

for N steps:

$$\langle x_N \rangle = 0 \qquad \langle x_3^2 \rangle = NL^2$$

- the mean displacement of a random walk is zero
- that does not mean that you don't go anywhere!

• Add time to the process

$$N = \frac{t}{\Delta t} \quad \begin{matrix} \leftarrow \text{total time} \\ \leftarrow \text{amount of time per step} \end{matrix}$$

- Define diffusion constant $\mathcal{D} \equiv \left[\frac{\text{length}^2}{\text{time}}\right]$ eg, $\frac{\mu m^2}{s}$

$$\mathcal{D} = \frac{\langle x_N^2 \rangle}{2t} = \frac{NL^2}{2t} = \frac{L^2}{2\Delta t}$$

$$\langle x_N^2 \rangle = 2\mathcal{D}t$$ (mean-square displacement increases linearly with time)

↑ completely arbitrary / convenient later

Any individual random walk will not conform to the diffusion law, even approximately!

- we will observe excursions of any size X as long as we are willing to wait a time $\sim O\left(\frac{X^2}{2\mathcal{D}}\right)$
- can easily experimentally measure $\mathcal{D}$: wait time t, measure displacement, and repeat

Higher-dimensions

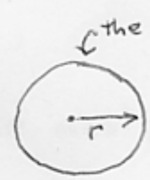
1D $\quad \langle r_N^2 \rangle = \langle x_N^2 \rangle = 2\mathcal{D}t$

2D $\quad \langle r_N^2 \rangle = \langle x_N^2 \rangle + \langle y_N^2 \rangle = 4\mathcal{D}t$

3D $\quad \langle r_N^2 \rangle = \langle x_N^2 \rangle + \langle y_N^2 \rangle + \langle z_N^2 \rangle = 6\mathcal{D}t$

Example

About how long does it take for a sudden supply of sugar molecules to spread uniformly?



$r \approx 1\ \mu m$ for bacterium
$r = 10\ \mu m$ for neutrophil
$r \sim 1000\ \mu m$ for nerve cell

$\langle r_N^2 \rangle = 6\mathcal{D}t \qquad$ sugar $\mathcal{D} \sim 500\ \frac{\mu m^2}{s}$

$$t \sim \frac{\langle r_N^2 \rangle}{6\mathcal{D}}$$

$$t_{coli} \sim \frac{(1\ \mu m)^2}{6\left(500\ \frac{\mu m^2}{s}\right)} = 0.0003\ s$$

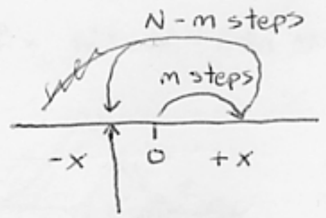
$$t_{neu} \sim \frac{(10)^2}{6(500)} = 0.03\ s$$

$$t_{nerv} \sim \frac{(1000)^2}{6\ (500)} = 300\ s$$

Compare with $\mathcal{D} \sim 5\ \frac{\mu m^2}{s}$ for an average-sized protein in the cytoplasm.

Explicit calculation of the probability distribution

- 1D random walk



final displacement probability $P(m,N)$

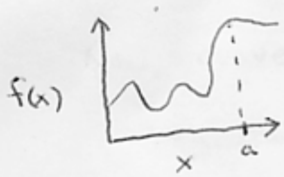
- each step is like flipping a coin $P_+ = P_- = 1/2$
- How many heads in 100 flips?

- Binomial probability distribution: $P(m,N) = \left(\frac{1}{2}\right)^N \frac{N!}{m!(N-m)!}$

- factorals are mathematically intractable
- want to approximate function P

- Calculate a Taylor series around the most probable end point m^*

reminder: purpose of a Taylor Series is to approximate a function with a simpler mathematical expression



$$f(x) \approx f(a) + \left(\frac{df}{dx}\right)_{x=a}(x-a) + \frac{1}{2}\left(\frac{d^2f}{dx^2}\right)_{x=a}(x-a)^2 + \ldots$$

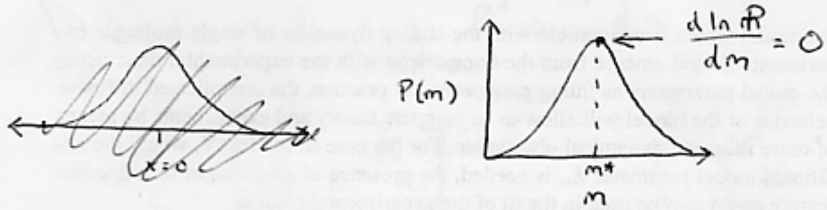
- Approximate $P(m,N)$ - work w/ log is easier

$$\ln P(m) = \ln P(m^*) + \left(\frac{d\ln P}{dm}\right)_{m^*}(m-m^*) + \frac{1}{2}\left(\frac{d^2 \ln P}{dm^2}\right)_{m^*}(m-m^*)^2 + \ldots$$

Need to evaluate the derivatives $\left(\frac{d\ln P}{dm}\right)$ and $\left(\frac{d^2\ln P}{dm^2}\right)$

Take log of 1 and use Stirling's Approximation $(\ln N! \approx N\ln N)$

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



A $$\left(\frac{d\ln P}{dm}\right)_{m^*} = 0 = -1 - \ln m^* + \ln(N-m^*) + 1$$

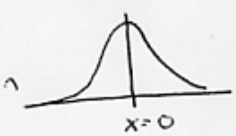
solve for m^*, $m^* = \frac{N}{2}$ (makes sense, right?)

B $$\left(\frac{d^2\ln P}{dm^2}\right)_{m^*=N/2} = \left(-\frac{1}{m} - \frac{1}{N-m}\right)_{m^*=N/2} = -\frac{4}{N}$$

Put A + B into Taylor Series

$$\ln P = \ln \underbrace{P^*\cancel{\left(\tfrac{N}{2}\right)}}_{P \text{ at } m^*} + 0 + \tfrac{1}{2}\left(-\frac{4}{N}\right)(m-m^*)^2$$

$$P = P^* e^{-\frac{2(m-m^*)^2}{N}}$$] form of Gaussian Distribution



Now, convert from m to x

~~forward progress~~ displacement is forward - reverse steps

$$x = m - (N-m) = 2m - N$$

$$m = \frac{x+N}{2}$$

$$P(x) = \underbrace{P^*}_{\text{at } x=0} e^{-\frac{x^2}{2N}}$$

- Now, calculate P^*
  - this is a probability distribution that needs to be normalized

$$\int_{-\infty}^{\infty} P(x)\,dx = 1 = \int_{-\infty}^{\infty} \underset{\substack{\uparrow \\ \text{const}}}{P^*}\, e^{-\frac{x^2}{2N}}\, dx$$

$$P^* = \left[\int_{-\infty}^{\infty} e^{-\frac{x^2}{2N}}\, dx\right]^{-1} \qquad \left(\text{can look up } \int_{-\infty}^{\infty} e^{-ax^2}\,dx = \sqrt{\pi/a}\right)$$

$$= \frac{1}{\sqrt{2\pi N}} = (2\pi N)^{-1/2}$$

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

a Gaussian of this form $\langle x^2 \rangle = N$

from the Diffusion law

$$\langle x^2 \rangle = 2\mathcal{D}t = N$$

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

- can calculate $\mathcal{D}$ if you have a distribution
  $P(x)$ ~~at [illegible]~~ of displacements at time t