Diffusion

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Mathematical Modeling and Simulation

Learning Objectives

1. Describe the process of diffusion.
2. Understand how diffusion can be modeled by random walks (microscopic theory).
3. Understand Fick's Laws of diffusion (macroscopic theory).

Diffusion

Diffusion definitions

- Common: Diffusion is the process by which particles move naturally from regions of high concentration to regions of low concentrations.
  - What is natural? How do they “know” where to move?
- Particles collide forcing them to wander around - execute a random walk.
- Particles initially confined in a small region of space wander around in all directions and spread out.
- Alternative: Diffusion is the migration of molecules or small particles due to random motion.

Characterize Diffusion

- How far do particles spread?
- Where do they end up?

Diffusion models

How do we model diffusion? Two theories:

- Microscopic view
  - Look at random walks of individual particles.
  - Stochastic - we can't predict the motion of a single particle.
  - Investigate probability distributions.

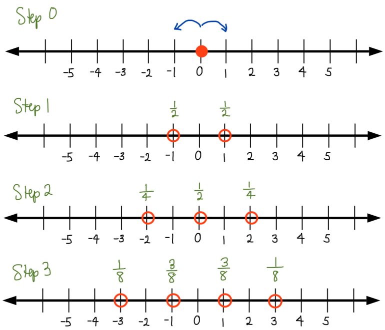
Diffusion models

How do we model diffusion? Two theories:

- Microscopic view
  - Look at random walks of individual particles.
  - Stochastic - we can't predict the motion of a single particle.
  - Investigate probability distributions.
- Macroscopic view
  - Look at average motion of a larger number of particles executing random walks.
  - Deterministic - we can predict average motion of particles.
  - Use continuous models - Fick's Laws of Diffusion.

Random walk - one dimension

Consider motion of particles along x axis.

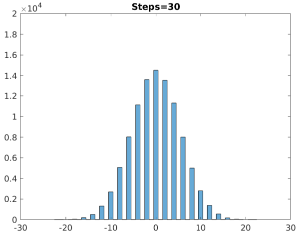


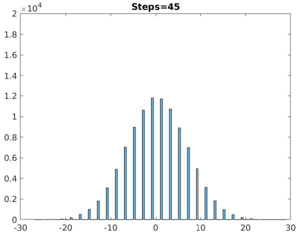
1. Start at time $t = 0$ and position $x = 0$.
2. Each time step Δt: move one unit to the left -1 or to the right $+1$ with 50% probability and steps are independent.
3. Particles don't interact.

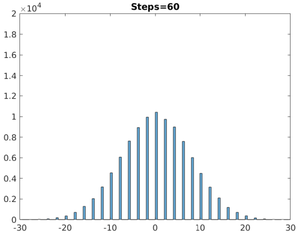
Simulating a 1D random walk

- Consider a single particle.
- Note down the final position of the particle after n steps.
- Repeat N times eg. 10^5 (equivalent to having N particles).
- Plot a histogram of the final positions of particle.

Final particle positions





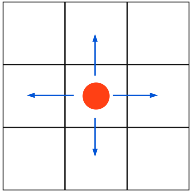


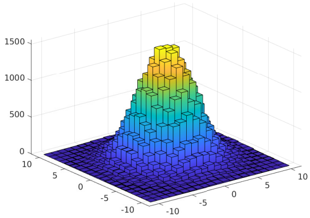
- The particle most likely returns to start position.
- Probability to return to center falls with more time steps.

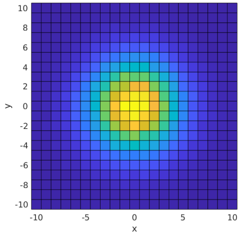
Discussion

- Variance is n - the number of steps.
- Particles execute n steps in $t = n\Delta t$ so the standard deviation is $\sqrt{n}$.
- Standard deviation is proportional to $\sqrt{t}$.

2D random walks



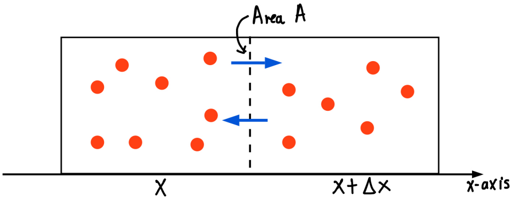




- Follow rules 1) and 3) of a 1D random walk in both directions.
- Assume there is equal probability to move in any of the four directions.

3D random walks are similar.

Diffusion - macroscopic theory



- Consider two cells in 1D with centers shown.
- The concentration of particles C in each cell in known at some time t.
- What is the net flux J through area A in some time t?
- Flux - number of particles passing an area per time.

Fick's 1^{st} Law of Diffusion

$$J = -D\frac{\partial C}{\partial x}$$

- Net flux is proportional to minus the concentration gradient.
- Constant of proportionality D – diffusion coefficient.
- Particles move from high to low concentrations.
- If particles are uniformly distributed, $\partial C/\partial x = 0$ then $J = 0$.
- If $J = 0$, the distribution doesn't change and system is in equilibrium.

1D Diffusion equation

Also known as Fick's Second Law of Diffusion or Heat equation.

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

- Rate of change of concentration in time is proportional to the curvature of concentration.
- D is the diffusion coefficient.

Interpreting $\partial C/\partial t = D\partial^2 C/\partial x^2$

- $\partial^2 C/\partial x^2 > 0 \Rightarrow C(t,x)$ is concave up $\partial C/\partial t > 0 \Rightarrow C(t,x)$ increases.
- $\partial^2 C/\partial x^2 < 0 \Rightarrow C(t,x)$ is concave down $\partial C/\partial t < 0 \Rightarrow C(t,x)$ decreases.
- $\partial C/\partial x$ constant $\Rightarrow \partial^2 C/\partial x^2 = 0 \Rightarrow \partial C/\partial t = 0$ and the concentration is stationary – there is equal exchange of particles.

Simulation macroscopic diffusion

- If we know initial distribution and what happens at the boundaries of region being considered, we can figure out later distributions.
- A nonuniform distribution of particles will redistribute itself in time.

Conclusions

- Diffusion arises from random motions of particles resulting in spreading out.
- We can characterize diffusion on a microscopic with random walks or macroscopic level with Fick's laws.
- Diffusion acts to dilute concentration and reduce gradients of concentration.