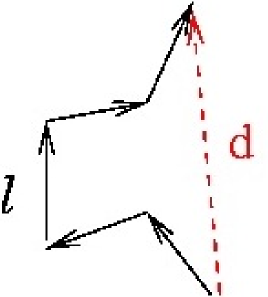
Lecture 6:
Random Walks

Lightning strike See: MIT course on surface growth



Example random walk Credit Michael Richmond

Random systems: Motivation

- In Previous lectures: we examined deterministic systems: these were described by a differential equation
- Random system are described probabilistically rather than deterministically. *Probabilistic* means described by a probability distribution.
- Two generic cases of systems that are described probabilistically:
  - Quantum mechanical system

    wave function describes probability of being in a given state
  - System with large number of degrees of freedom (dof)

    deterministic description impossible: equations cannot be solved and initial conditions cannot be determined anyway. Examples: Brownian motion, stirring of cream in coffee or tea
- ‘Random’ has well defined meaning: probability distribution is known

  result of computation is mean value and dispersion around mean, rather than detailed ‘microscopic’ state

Random systems: Pseudo-random numbers

- Desired: generate a set of numbers that correctly sample a given probability distribution
  Example: random numbers uniform in the interval $x = [0, 1($: $\mathcal{P}(x) = 1$,

  return a random set of choices from a given set, as for example the faces of a die
- Extensive literature for generating 'pseudo' random numbers

  set of numbers that samples a distribution function without **artificial** correlations or periodicity

  Pseudo random numbers because *any* random number generator does have artificial correlations
- Seed: often it is useful to be able to generate *the same* random sequence multiple times for example for debugging. This can be done by starting the random sequence from a given seed

  if seed is not set, generator uses time + date to set the seed
- *numpy* has (pseudo) random number generator

  random.randint(0, 10): random integer between 0 and 10; random.rand(0,10) uniform float in [0,10(

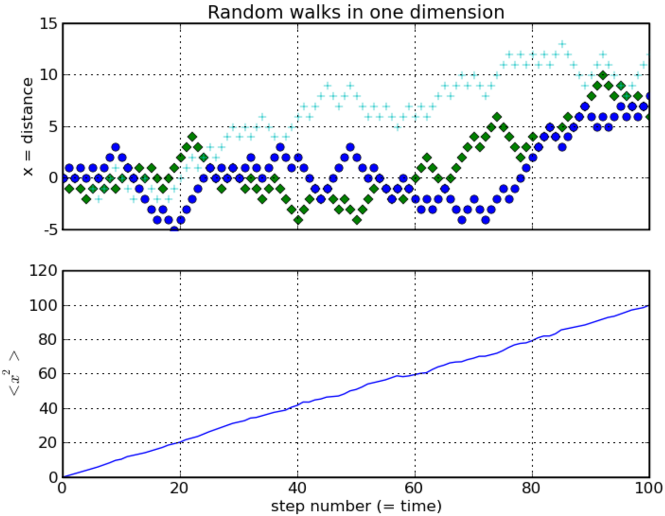
Random systems: Random walk

- 1D one dimension: each step changes the location of the walker by ± 1 chosen with equal probability ('at random'), for example $\Delta x =$ np.random.choice([-1,1])
- nD n dimensions: in addition, randomly choose dimension to step in
- Example of random walk:
  - Einstein's paper on Brownian motion: small particles in a liquid gets pushed around by colliding with molecules
  - Trajectory of milk 'particle' in hot tea

Random Walks: Pseudo-code

Initialise: start m random walkers at $x = 0$, $i = 0, 1, \ldots, m-1$.
Calculation: ▶ For each walker: choose direction to step in ▶ After each (time) step t compute: ▸ the mean displacement $\langle x(t) \rangle$ averaged over walkers ▸ the mean squared displacement $\langle x^2(t) \rangle$
Plot the results.

Random walks: Results.



Random walks: Results.

- 'No' identical random walkers if good random number generator used
- Average (signed) displacement of all random walkers:

$$\langle x(t) \rangle = 0 \,.$$

as expected, since $\Delta x = +1$ equally likely as $\Delta x = -1$

- Average mean *squared* displacement

$$\langle x^2(t) \rangle = t \,; \quad \langle x(t)^2 \rangle^{1/2} \propto t^{1/2} \,.$$

  - Increases linearly in time meaning with the number of steps taken
  - Closely related to the physics of **diffusion**

    relation is worked out in more detail later on

Random walks: Analytical analysis

- Write the position of a walker after n steps as:

$$x_n = \sum_{i=1}^{n} s_i \ , \quad \text{where} \ \ s_i = \pm 1 \ \ \text{with equal probability}$$

$$\langle s_i \rangle = 0 \, ; \quad \langle s_i^2 \rangle = 1 \, ; \quad \langle s_i s_j \rangle = 0 \ \text{ if } i \neq j$$

- Therefore
  - $\langle x_n \rangle = \sum_{i=1}^{n} \langle s_i \rangle = 0$
  - $\langle x_n^2 \rangle = \langle \sum_{i=1}^{n} \sum_{j=1}^{n} s_i s_j \rangle = \sum_{i=1}^{n} \langle s_i^2 \rangle + \sum_{i=1}^{n} \sum_{j>i}^{n} \langle s_i s_j \rangle = n + 0 = n$
- Assume duration of each step is Δt, $\langle x_n^2 \rangle = n = \frac{t}{\Delta t}$.

$\langle x_n^2 \rangle$ increases linearly with time, t

Random walks: Analytical analysis

- Question: how large is variation around mean, $\langle x_n^2 \rangle = n$

expect: relative variation increases with increasing n

$$
\begin{aligned}
\langle x_n^4 \rangle &= \langle \left(\sum_{i=1}^{n} s_i \right)^4 \rangle \\
&= \sum_{i=1}^{n} s_i^4 + 3 \sum_{i=1}^{n} \left[s_i^2 \sum_{j \neq i} s_j^2 \right] \\
&= n + 3n(n-1)
\end{aligned}
$$

- $\left(\langle x_n^4 \rangle - \langle x_n^2 \rangle^2 \right)^{1/2} = \left(2n^2 - 2n \right)^{1/2} \approx \sqrt{2} \cdot n$, hence
$\left(\langle x_n^4 \rangle - \langle x_n^2 \rangle^2 \right)^{1/2} / \langle x_n^2 \rangle^{1/2} \propto n^{1/2}$
$\Longrightarrow$ relative variation increases

The diffusion equation: Introduction

- Consider the continuity equation for example conservation of mass

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\nabla \mathbf{j} = -\nabla \rho \mathbf{v}$$

t is time, ρ is density, $\mathbf{v}$ is velocity, $\mathbf{j}$ is flux, ∇ is gradient

- In diffusion, flux is proportional to the *gradient* of ρ

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

diffusion from high to low density, $D > 0$

- Combining these yields the diffusion equation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = +D\nabla^2\rho$$

provided the diffusion coefficient, D, is uniform - the same everywhere in space

Random walks: Connection to diffusion

- Consider random walk on 2D lattice with spacing Δx
- Let $P_{ij}(n)$ be the probability to find the walker at lattice position ij after n steps
- At step $n-1$, there is an equal probability to find the walker at any of its 2N neighbouring sites N is the dimension, consider below $N=2$. Therefore

$$P_{ij}(n) = \frac{1}{4}\left[P_{i-1j}(n-1) + P_{i+1j}(n-1) + P_{ij-1}(n-1) + P_{ij+1}(n-1)\right]$$

- This can be re-written as

$$\begin{aligned} &P_{ij}(n) - P_{ij}(n-1) \\ = \quad &\frac{1}{4}\left[P_{i-1j}(n-1) - 2P_{ij}(n-1) + P_{i+1j}(n-1)\right. \\ &\left. + P_{ij-1}(n-1) - 2P_{ij}(n-1) + P_{ij+1}(n-1)\right] \end{aligned}$$

Random walks: Connection to diffusion

We can convert this to the diffusion equation as follows

- Define time $t = n\Delta t$ Δt is small time step

$$P(n) - P(n-1) = P(\frac{t}{\Delta t}) - P(\frac{t-\Delta t}{\Delta t}) \approx \Delta t \frac{\mathrm{d}P(t)}{\mathrm{d}t}$$

- Similarly, define position $x = i\,\Delta x$ Δx is small interval

$$P_{i-1} - 2P_i + P_{i+1} \approx (\Delta x)^2 \frac{\mathrm{d}^2 P(x)}{\mathrm{d}x^2}$$

- Combining these yields the diffusion equation,

$$\dot{P}(t) = \frac{\Delta x^2}{2N\,\Delta t} \nabla^2 P$$

the diffusion constant is $D = \frac{\Delta x^2}{2N\,\Delta t}$, where N is the dimension of the lattice. In our example, $N = 2$

The diffusion equation: Example

- Consider an initially Gaussian distribution in N-dimensions

$$\rho(\mathbf{r}, t = 0) = \left(2\pi\sigma^2\right)^{-N/2} \exp\left(-\frac{r^2}{2\sigma^2}\right)$$

where σ is a function of time, t.

- This distribution has verify as an exercise

$$\begin{aligned} \frac{\mathrm{d}\rho}{\mathrm{d}t} &= -\left(N - \frac{r^2}{\sigma^2}\right)\frac{\dot{\sigma}}{\sigma}\rho \\ \nabla^2\rho &= -\left(N - \frac{r^2}{\sigma^2}\right)\frac{1}{\sigma^2}\rho \end{aligned}$$

and hence is a solution to the diffusion equation, provided

$$\sigma^2(t) = \sigma^2(t = 0) + 2D\,t\,.$$

The diffusion equation: Example

- Special case of Gaussian distribution: start all random walkers at $\mathbf{r} = 0$

  A Gaussian with dispersion $\sigma^2 = 0$ corresponds to a Dirac delta-function

- The previous analysis shows that $\sigma^2(n) = \Delta x^2 n/N$

  standard deviation of the Gaussian after n steps in case dimensionality of grid is N. This is what you might have expected: for n random steps in N dimensions, on average n/N will be in the x-direction. Therefore the walker will have travelled a typical distance of $(n/N)^{1/2}$ in the x-direction (and similarly in every other dimension). Hence the standard deviation is $(n/N)^{1/2}$.

The diffusion equation: Application

- Consider a drop of milk in a cup of hot tea
- Sufficiently many 'milk particles' in solution
- Goal: Calculate spatial distribution as function of time
- Obstacle: Complicated dynamics on a molecular level (e.g. collisions), ignore and use random processes.

  we are not really interested in computing the position of each and every 'milk' particle
- Coarse graining: divide volume of tea cup in large number of smaller volumes, and count number of 'milk' particles in each sub-volume. Count / volume is density, ρ, of 'milk' particles
- Connection to random walk: Identify density $\rho(x, y, z, t)$ with probability $P(x, y, z, t)$ to find a particle in the respective sub-volume: $\rho \to P$

The diffusion equation: Solutions

- No general solution known
- See previous slides

The Gaussian distribution $\rho(\mathbf{r}, t) = \frac{1}{(2\pi\sigma)^{N/2}} \exp\left[-\frac{r^2}{2\sigma^2}\right]$ solves the diffusion equation, provided $\sigma^2(t) = \sigma_0^2 + 2Dt$.

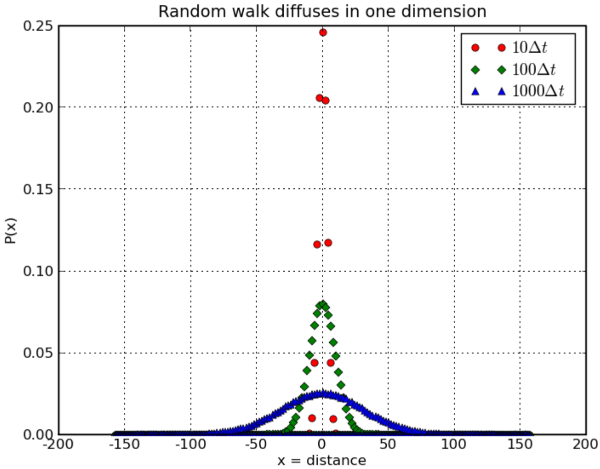
in N dimensions

- Gaussian distribution in space with time-dependent width $\Longleftrightarrow$ striking connection with random walks

Diffusion: Connection to random walks

- Start 40000 walkers at $x = 0$ for $t = 0$

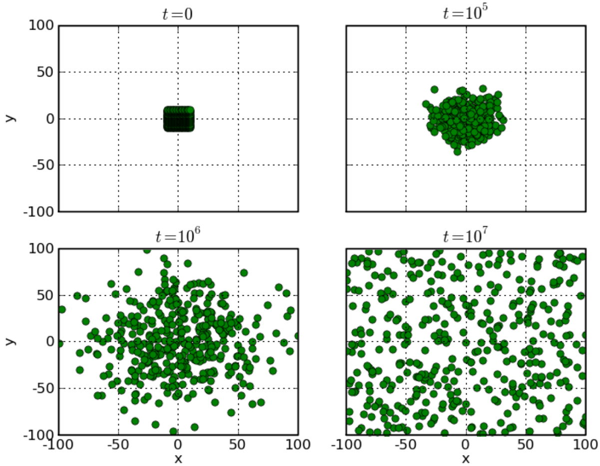
run each for 1000 steps



Diffusion: Connection to random walks

- Start many walkers close to $(x, y) = (0, 0)$ for $t = 0$.

Notice how they 'diffuse' away from the origin



Diffusion: Connection to random walks

- Lab session: try this out in N-dimensions
- Find relation between σ of the Gaussian, n, the number of steps, N the dimension of the problem, and the typical distance that a particle walks.

Random walks: Connection to Entropy

- Our walks are random: it is equally likely for a particle to travel back in time, 'exactly' tracing its track back in time!
  - On a microscopic level: yes!
  - On a macroscopic level: no!

  milk particles do not spontaneously collect back from where they were started - ever!
- What introduces the arrow of time here?
- To describe: define the entropy: $S = k_B \ln \Omega$

  Entropy is a measure of the likelihood of a given micro-state
  - Suppose the total number of sub-volumes is N
  - Let there be n_i particles in cell i for a given micro-state
  - The likelihood Ω for this configuration is provided particles are indistinguishable

$$\Omega = \frac{N!}{\prod_{i=1}^{N} n_i!}$$

Random walks: Connection to Entropy

- Examples
  - All N_T particles are in one cell unlikely!

$$\Omega_1 = \frac{N!}{N_T!}$$

  - Each cell has the same, N_T/N, number of particles likely!

$$\Omega_2 = \frac{N!}{((N_T/N)!)^N}$$

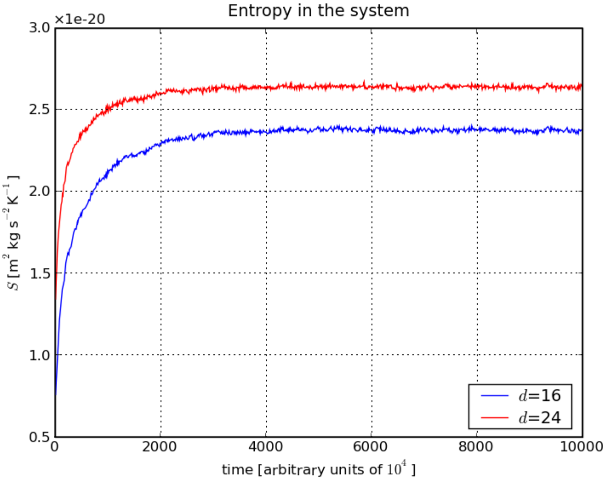
- Use Stirling's approximation, $\ln(N!) \approx N\ln(N) - N$ for large N
- Then demonstrate as an exercise

$$\ln\left(\frac{\Omega_2}{\Omega_1}\right) \approx N_T \ln(N) \gg 1$$

disordered state 2 has *much* larger entropy than ordered state 1, and is *much* more likely

Random walks: Connection to Entropy

- Example: compute entropy as a function of time as 'milk' particles diffuse



Random walks: Connection to Entropy

- Entropy increases with time, until plateau is reached, system evolves to reach signals equilibrium state
- Fluctuations are due to finite cell size - unimportant artefact.
- Particles spread to fill all states (lattice sites, cells) uniformly, maximising the entropy.
- This is not build in: the random walkers do not know about entropy.
- So, obvious question: Why does this happen?
  Answer: System spends time, exploring **all** possibilities
  Ultimately system spends more time in more likely states
- This insight goes under the name of the ergodic hypothesis, a central assumption of statistical mechanics

ensemble average and time average are ‘equivalent’

Summary

- Studied properties of random walks
- Made link to diffusion
- Made link to entropy and arrow of time
- Illustration of how to use numerical simulations to explore physics