I. DIFFUSION AS A MIXING PROCESS

Diffusion equation:

$$J = -D_{12}\frac{\partial \rho}{\partial y} \tag{1}$$

Divergence theorem (continuity equation)

$$\frac{\partial \rho}{\partial t} + \nabla J = 0 \tag{2}$$

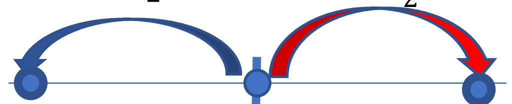
Combine the two to get the partial differential equation for diffusion:

$$\frac{\partial \rho}{\partial t} + D_{12}\frac{\partial^2 \rho}{\partial y^2} = 0 \tag{3}$$

Starting with particles in $y = 0$ at time $t = 0$: $\rho(t = 0, y) = \delta(y)$, where δ is the Kroeneker delta function the diffusion equation has solution (you may easily verify this):

$$\rho(t, y) = \frac{1}{\sqrt{4\pi D_{12} t}} \exp(-\frac{y^2}{4D_{12}t}) \tag{4}$$

1D Random walk



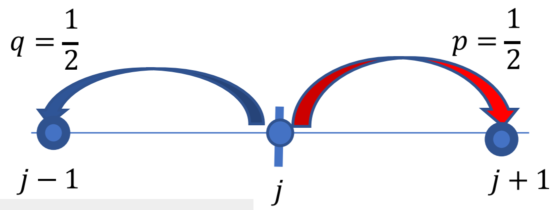
- Random motion of a walker along a line
  - Discrete time steps $N = 0,1,2 \cdots$ in units of $\Delta t = 1$
  - Discrete space: lattice index $j = 0, \pm 1, \pm 2 \cdots$ with increments $\Delta x = 1$

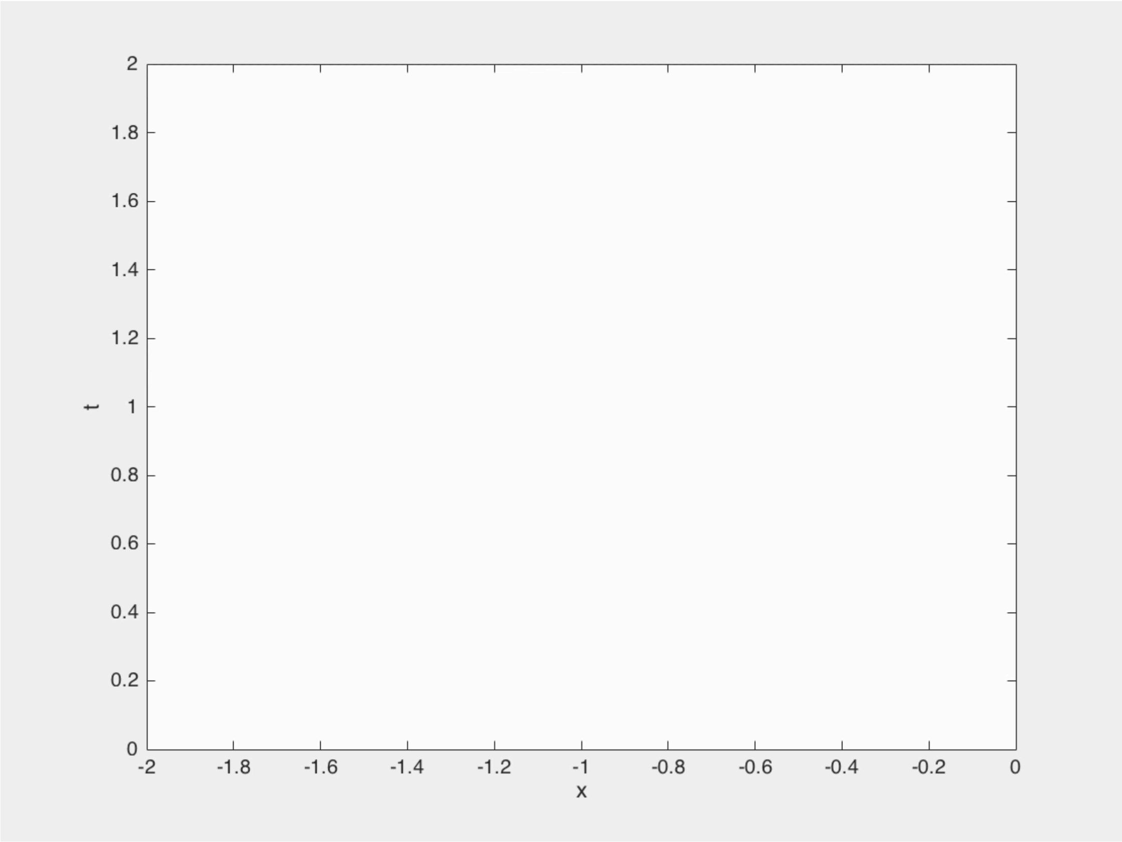
- **At each timestep**, the walker has probability $p = \frac{1}{2}$ to the right $j \rightarrow j+1$

and probability $q = \frac{1}{2}$ to the left $j \rightarrow j-1$

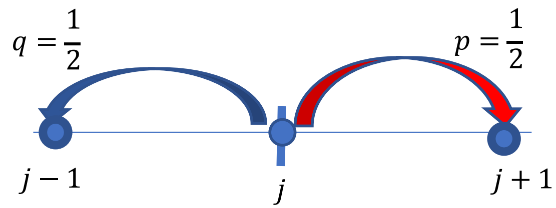
  - *What is the probability distribution for R steps to the rightN steps, $P(N,R)$?*
  - *What is the mean displacement $\langle S \rangle$ after N steps?*

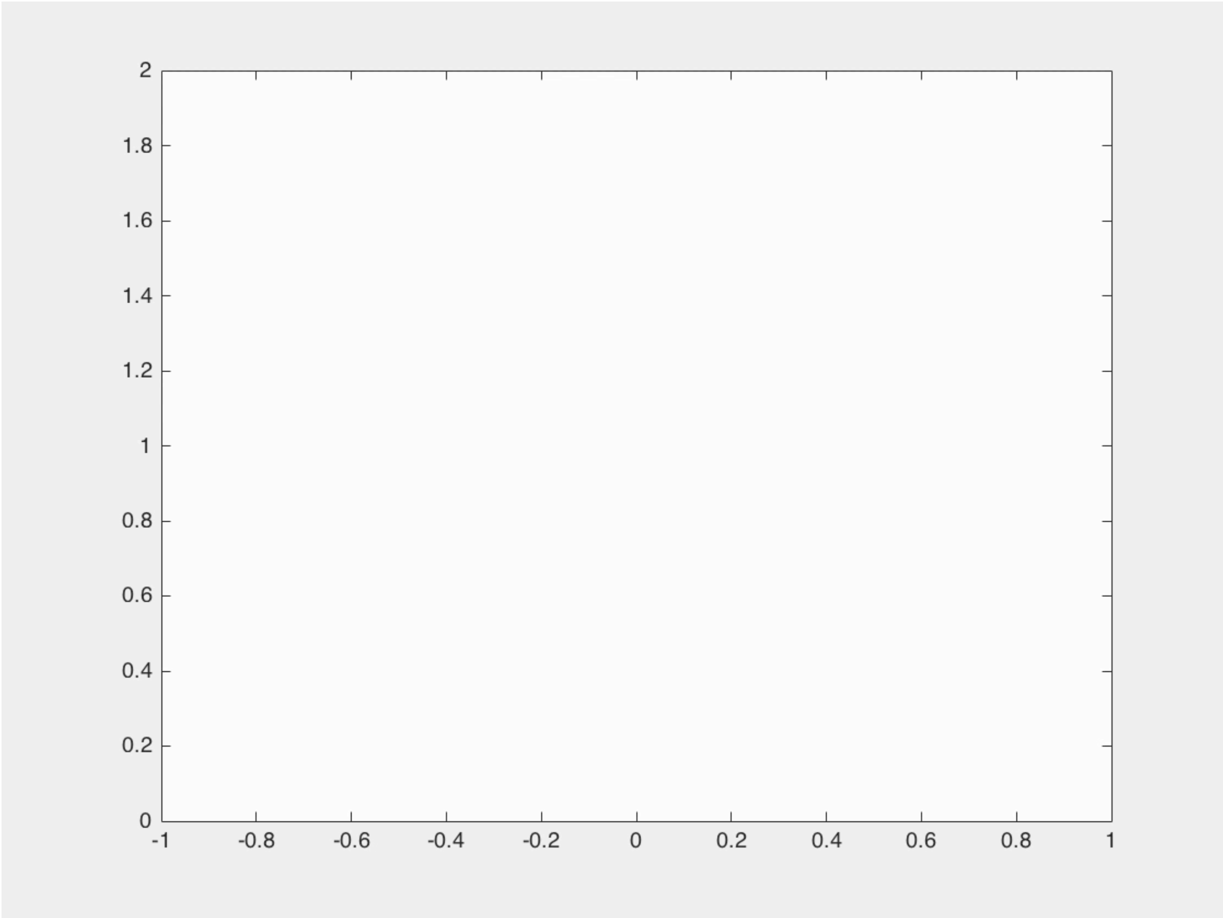
1D Random Walk
1 walker



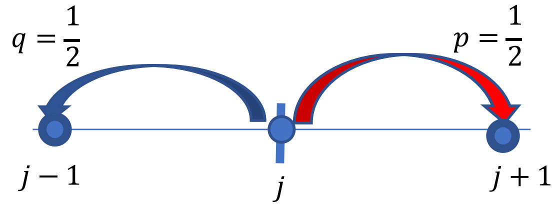


1D Random Walk many walkers





1D Random walk



- Particle moves on a grid
- Equal probability for left and right step
- After N steps: R steps right, L steps left
  - $R + L = N,$
  - $S = R - L$ (net displacement)
- Number of configurations (multiplicity) which have R right steps out of N steps

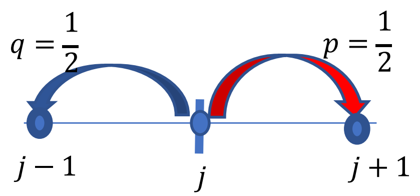
$$\Omega(N, R) = \frac{N!}{R!\,(N-R)!}$$

- Probability for R steps to the right out of N steps

$$P(N, R) = 2^{-N} \frac{N!}{R!\,(N-R)!}$$

Average displacement from the origin

$$P(N,R) = 2^{-N}\frac{N!}{R!\,(N-R)!}$$



Distribution is symmetrical => most probable = mean value:

$$\langle R\rangle = \frac{N}{2}$$

Mean displacement $\langle S\rangle = \langle R\rangle - (N - \langle R\rangle) = 2\langle R\rangle - N$

$$\langle S\rangle = 0$$

$$\sigma^2 = \langle S^2 - \langle S\rangle^2\rangle = \frac{N}{4}$$

(p 89 in compendium)

Binomial distribution in continuum limit => diffusion

$$P(N,n) = 2^{-N}\frac{N!}{n!\,(N-n)!}$$

(n= steps to right)

$\boldsymbol{N! \approx N^N e^{-N}\sqrt{2\pi N}}$ or $\boldsymbol{\ln N! \approx N\ln N - N}$

Lots of algebra $=> P(N,n) \approx \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-\left(\frac{N}{2}-n\right)^2}{\frac{N}{2}}} = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-\left(\frac{n-<n>}{\sigma}\right)^2}{2}}$

Gaussian distribution

Compare with solution to diffusion equation: $\sigma^2 = 2Dt, \;\; N = 8Dt$

Measure

- Width of distribution: σ
- Second moment of distribution: $\sum y^2 \rho(y)$
- Mean square displacement: $\frac{d\sigma^2}{dt} = 2D$