Course 09/1

Random walk and diffusion

- Binomial distribution
- Random walk in 1D
- Link between random walk and diffusion
- Diffusion equation through master equation

Binomial distribution

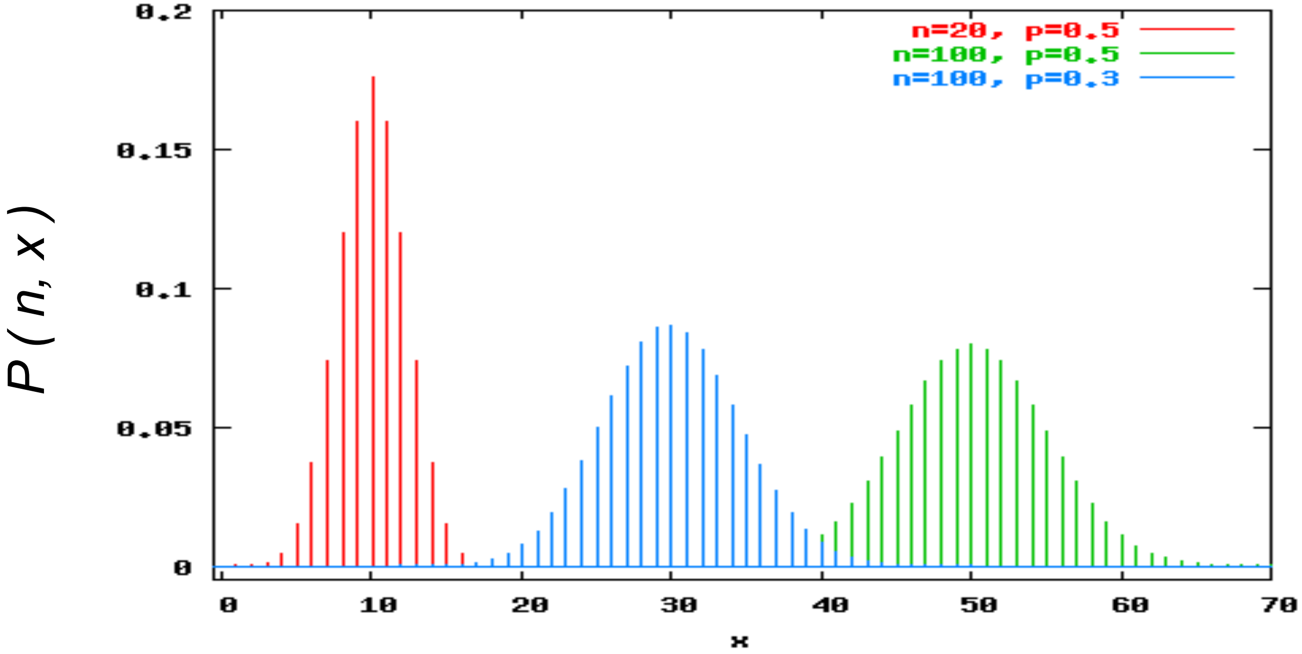
Two outcomes: (i) event A with probability p

(ii) event B with probability q

Probability: x times event A on n events

$$P(n, x) = \frac{n!}{x!\,(n-x)!}\, p^{x} q^{n-x}$$

Binomial distribution



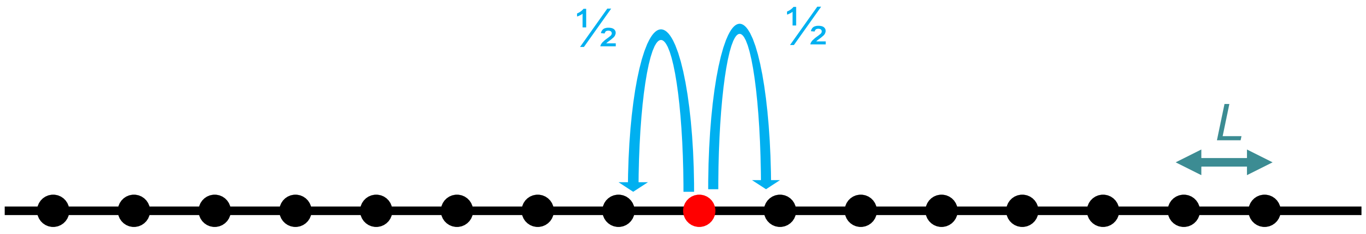
Average of x : $\mu = \langle x \rangle = n \cdot p$

Standard deviation : $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = n \cdot p \cdot q = n \cdot p \cdot (1 - p)$

For large n :

Take $p = q = ½$ $\Rightarrow$ $\mu = n / 2$ and $\sigma^2 = n / 4$ $\Rightarrow$ $\dfrac{\sigma}{\mu} = \dfrac{1}{\sqrt{n}}$

Random walk in 1D



Binomial

steps to the right

steps to the left

$$P\,(\,n_\mathrm{R},\,n_\mathrm{L}\,) = \frac{(n_\mathrm{R}+n_\mathrm{L})!}{n_\mathrm{R}!\;n_\mathrm{L}!}\;p^{\,n_\mathrm{R}}\,q^{\,n_\mathrm{L}} \;=\; \left(\frac{1}{2}\right)^{n_\mathrm{R}+n_\mathrm{L}} \frac{(n_\mathrm{R}+n_\mathrm{L})!}{n_\mathrm{R}!\;n_\mathrm{L}!}$$

Average $\quad \langle\, n_\mathrm{R} \rangle = n \cdot p = \dfrac{n}{2} = \langle\, n_\mathrm{R} \rangle$

Variance $\quad \mathrm{Var}\; n_\mathrm{R} = \langle\, (n_\mathrm{R} - \langle n_\mathrm{R} \rangle)^2 \,\rangle = npq = \dfrac{n}{4}$

$n = n_R + n_L$

Displacement $\quad x = (n_\mathrm{R} - n_\mathrm{L})\, L = m\, L$

$m = n_R - n_L$

Random walk in 1D

Change of variables

$$\begin{cases} n = n_R + n_L \\ m = n_R - n_L \end{cases} \quad \Longrightarrow \quad \begin{cases} n_R = (n + m)/2 \\ n_L = (n - m)/2 \end{cases}$$

Binomial probability

$$P(n, m) = \left(\frac{1}{2}\right)^n \frac{n!}{\left(\frac{n+m}{2}\right)! \left(\frac{n-m}{2}\right)!}$$

Average $\langle m \rangle = \langle n_R - n_L \rangle = \langle n_R \rangle - \langle n_L \rangle = 0$

Variance

$$\text{Var } m = \langle (m - \overbrace{\langle m \rangle}^{=0})^2 \rangle = \langle m^2 \rangle = \langle (2n_R - n)^2 \rangle$$

$$= 4 \langle (n_R - \underbrace{\frac{n}{2}}_{\langle n_R \rangle})^2 \rangle = 4 \text{ Var } n_R = 4 \cdot \frac{n}{4} = n$$

Standard deviation $\sigma = \sqrt{\text{Var } m} = \sqrt{n}$

NB $m \ll n$, for $n \to \infty$

Root mean square displacement $d_{rms} = \sqrt{n} \cdot L$

Random walk in 1D: from binomial to normal

Binomial distribution

$$P(n, m) = \left(\frac{1}{2}\right)^n \frac{n!}{\left(\frac{n+m}{2}\right)!\left(\frac{n-m}{2}\right)!}$$

Approximations in the limit of large n

1. Stirling approximation: $$n! \cong \sqrt{2\pi n}\ e^{n \ln n - n}$$
2. First-order expansion for small ε: $$\ln(1 \pm \varepsilon) \cong \pm\, \varepsilon$$

Result: normal distribution

$$P(n, m) = \sqrt{\frac{2}{\pi n}}\ e^{-\frac{m^2}{2n}}$$

Link between random walk and diffusion

From discrete to continuum spatial variables

We define a continuous variable: $x = m \cdot L$

We define the probability of finding x in the interval $[\,x, x+\Delta x\,]$:

$$p\,(\,x, n\,) \cdot \Delta x \;=\; \sum P\,(n, m) \;=\; P\,(n, m) \cdot \Delta N_m$$

probability density

all $m \mid x \in [\,x, x+\Delta x\,]$
$x = m \cdot L$

number of
$m \in [\,x, x+\Delta x\,]$

ΔN_m

Example: (x_L, x_R)

For $n = 2$: (2,0) (1,1) (0,2)

$m = 2$ $m = 0$ $m = -2$

For $n = 3$: (3,0) (2,1) (1,2) (0,3)

$m = 3$ $m = 1$ $m = -1$ $m = -3$

$$\Longrightarrow \quad \Delta N_m = \frac{\Delta x}{2L}$$

Link between random walk and diffusion

From a discrete to a continuous spatial variable

$$p\,(\,x, n\,) = P\,(n, m) \cdot \frac{\Delta N_m}{\Delta x}$$

$$x = m \cdot L$$

$$P\,(n, m) \;=\; \sqrt{\frac{2}{\pi n}}\;\mathrm{e}^{-\frac{m^2}{2n}}$$

$$\Delta N_m = \frac{\Delta x}{2L}$$

$$p\,(\,x, n\,) = \frac{1}{\sqrt{2\pi n L^2}}\;\mathrm{e}^{-\frac{x^2}{2nL^2}}$$

Normal distribution

with $\mu = 0$ and $\sigma = \sqrt{n} \cdot L$

Link between random walk and diffusion

From a discrete to a continuous temporal variable

$$t = n\,\Delta t$$

$$p(x, n) = \frac{1}{\sqrt{2\pi n L^2}}\, e^{-\frac{x^2}{2nL^2}}$$

$$p(x, n) = \frac{1}{\sqrt{2\pi L^2\, t\,/\,\Delta t}}\, e^{-\frac{x^2}{2L^2 t\,/\,\Delta t}}$$

$$= \frac{1}{\sqrt{4\pi D t}}\, e^{-\frac{x^2}{4Dt}}$$

Diffusion coefficient

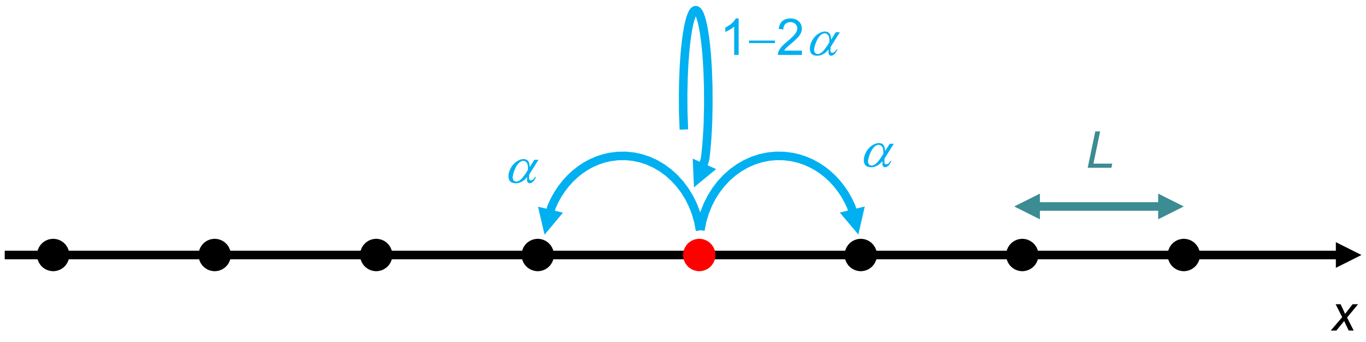
$$D = \frac{L^2}{2\Delta t}$$

$[\,D\,]$ = unit of D = m^2/s

$$\mu = \langle\, x \,\rangle = 0$$

$$\sigma = d_{rms} = \sqrt{2Dt}$$

Diffusion equation through master equation



Master equation

$$\rho(x, t+\Delta t) = \alpha\,\rho(x+L, t) + \alpha\,\rho(x-L, t) + (1-2\alpha)\,\rho(x, t)$$

$$\rho(x, t+\Delta t) - \rho(x, t) = \alpha\,[\,\rho(x+L, t) + \rho(x-L, t) - 2\,\rho(x, t)\,]$$

Diffusion equation through master equation

Master equation

$$\rho(x, t+\Delta t) - \rho(x, t) = \alpha\,[\,\rho(x+L, t) + \rho(x-L, t) - 2\,\rho(x, t)\,]$$

Left-hand side

$$= \Delta t\,\frac{\partial \rho}{\partial t}(x, t)$$

Right-hand side

$$\rho(x+L) = \rho(x) + L\,\rho'(x) + \frac{L^2}{2}\rho''(x)$$

$$+\quad \rho(x-L) = \rho(x) - L\,\rho'(x) + \frac{L^2}{2}\rho''(x)$$

$$\rho(x+L) + \rho(x-L) = 2\rho(x) + L^2\rho''(x)$$

This gives ...

$$\Delta t\,\frac{\partial \rho}{\partial t}(x, t) = \alpha L^2\,\frac{\partial^2 \rho}{\partial x^2}(x, t) \quad \Rightarrow$$

… the diffusion equation

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

where the diffusion coefficient $D = \dfrac{\alpha L^2}{\Delta t}$

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