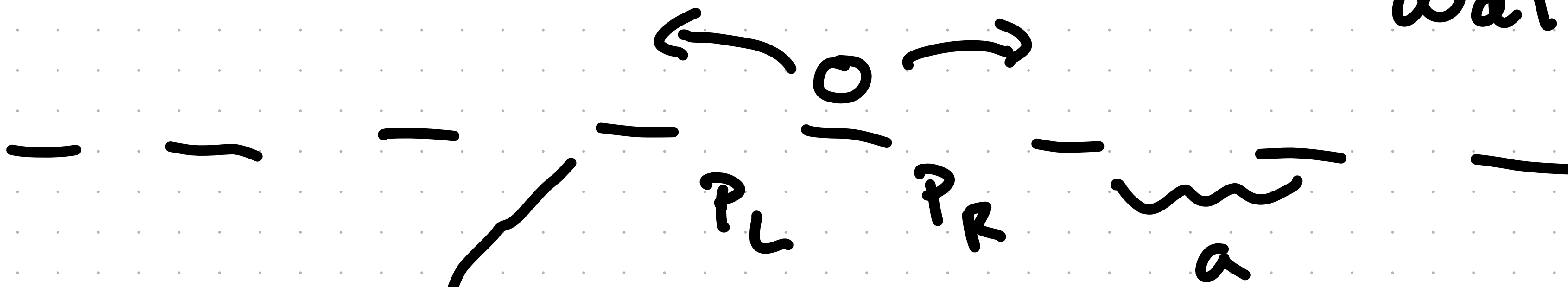
Last time: 1d ~~diffusion~~ random walk



Spreads out

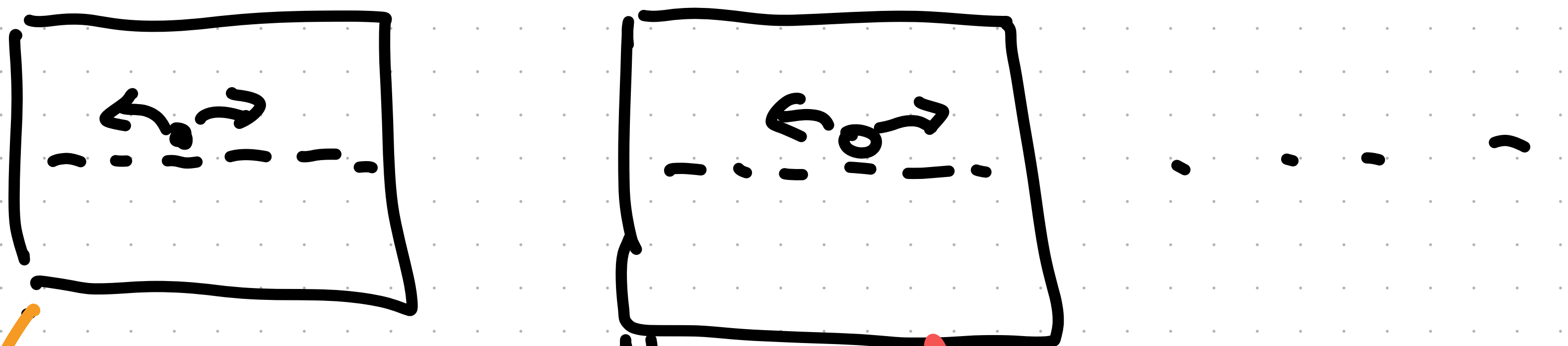
diffusion

eg position

$$\langle A \rangle_{time} = \lim_{T\to\infty} \frac{1}{T}\sum_{i=1}^{T} A_i$$

Ensemble average

many copies of system, average over all of them



N

$$\langle A\rangle = \frac{1}{N}\sum_{i=1}^{N} A_i$$

← N copies @ time t, system has state α with prob P_α ⇐ equil

$\alpha(t)$ $\beta(t)$

Random walk length M

States: $x = \{-aM, \ldots, 0, \ldots, aM\}$

will see with prob($i a$)
$i \in [-M, M]$

$$d_M = a \sum_{i=1}^{M} m_i \qquad = a(N_+ - N_-)$$

$\{+1, -1\}$

$[N_+ + N_- = M]$

$$= a(2N_+ - M)$$

$\langle d_M \rangle$

Binomial Distribution

Prob of n "successes" in m "trials" with prob of success $= p$

← 2 outcomes

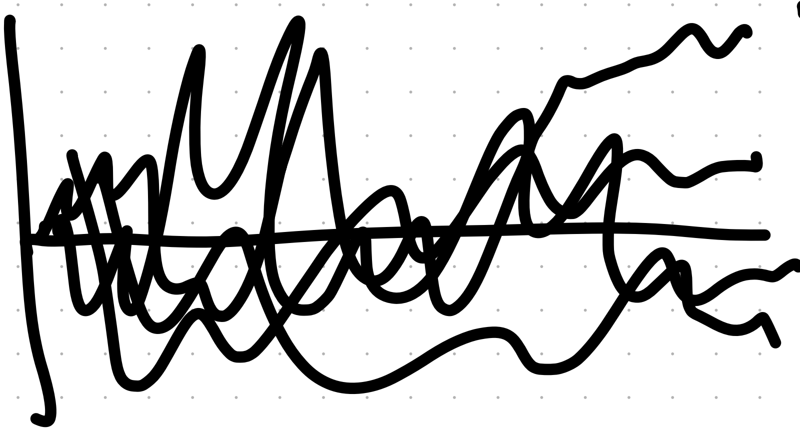
$$P(n,m) = \binom{m}{n} p^n (1-p)^{m-n}$$

binomial coeff $\dfrac{m!}{n!\,(m-n)!}$

key points

$$\langle n \rangle = mp$$

$$\langle n^2 \rangle = mp(1-p)$$



$$d_M = a(2N_+ - M)$$

spread? Variance

$$\langle d_m \rangle = \langle a(2N_+ - M) \rangle$$

$$= 2a\left(\langle N_+ \rangle - \left\langle \frac{M}{2} \right\rangle\right)$$

$$= 2a\left(\langle N_+ \rangle - \frac{M}{2}\right)$$

Mp_+

$$= 2a(Mp_+ - M/2) = \boxed{2aM(p_+ - 1/2)}$$

$$\langle aX + b \rangle = \langle aX \rangle + \langle b \rangle = a\langle X \rangle + b$$

a, b constants, X is a random vars.

<u>Note:</u>

$$\langle A \rangle_{time} = \lim_{T\to\infty} \frac{1}{T} \sum_{i=1}^{T} A_i$$

1 long traceetory

$$\langle A \rangle = \frac{1}{N} \sum_{i=1}^{N} A_i$$

N things to average

$$\langle A \rangle_{ensemble} = \sum_{n \in \underline{states}} A_n P_n$$

Example: $n=2$ —— E_2 $\uparrow \downarrow$

$n=1$ —— E_1

Prob of state n, $P_n = \dfrac{e^{-\varepsilon_n/k_BT}}{Z}$

Example dist. Boltzmann

$$\langle \varepsilon \rangle_{eq} = \sum_n P_n \varepsilon_n = \frac{\varepsilon_1 e^{-\varepsilon_1/k_BT}}{Z} + \frac{\varepsilon_2 e^{-\varepsilon_2/k_BT}}{Z}$$

@ equilibrium

Statistics Reminder

Mean $\langle x \rangle = \mu = \frac{1}{N}\sum_{i=1}^{N} x_i$

$$\mathrm{Var}(x) = \sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i-\mu)^2 = \langle (x-\mu)^2 \rangle$$

σ is standard deviation

$$\langle (x-\mu)^2 \rangle = \langle (x^2 - 2x\mu + \mu^2) \rangle$$

$$= \langle x^2 \rangle - 2\mu \underbrace{\langle x \rangle}_{\mu} + \mu^2$$

$$= \langle x^2 \rangle - \mu^2 = \langle x^2 \rangle - \langle x \rangle^2$$

$$\mathrm{Var}(x) = \langle (x-\mu)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

$$\mathrm{Var}(x) \geq 0$$

$$\langle x^2 \rangle - \langle x \rangle^2 \geq 0$$

$$\langle x^2 \rangle \geq \langle x \rangle^2$$

$$\sqrt{\langle x^2 \rangle} \geq \mu$$

$$d_M = a(2N_+ - M)$$

$$\langle N_+ \rangle = p_+ M$$

$$\langle d_M \rangle = aM(2p-1)$$

$$\mathrm{Var}(N_+) = \underline{M p_+ (1-p_+)}$$

$$\mathrm{Var}(d_M) = \langle d_M^2 \rangle - \langle d_M \rangle^2$$

$$\langle a^2 (2N_+ - M)^2 \rangle = a^2 \langle 4N_+^2 - 4N_+ M + M^2 \rangle$$

$$= a^2 \left[4\langle N_+^2 \rangle - 4\langle N_+ \rangle M + M^2 \right]$$

pM

$$\langle N_+^2 \rangle - \langle N_+ \rangle^2 = M p_+ (1-p_+)$$

$$\langle N_+^2 \rangle = Mp(1-p) + p^2 M^2$$

$$\mathrm{Var}(d) = \langle d_m^2 \rangle - \langle d_m \rangle^2$$

prev

← check

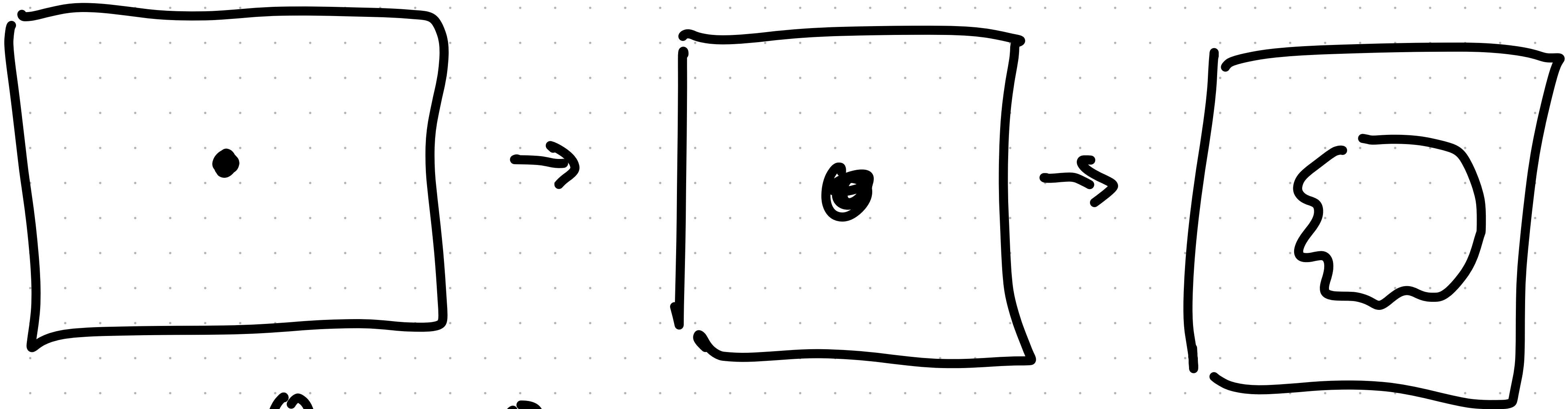
$$= a^2 \left[4M p(1-p) \right]$$

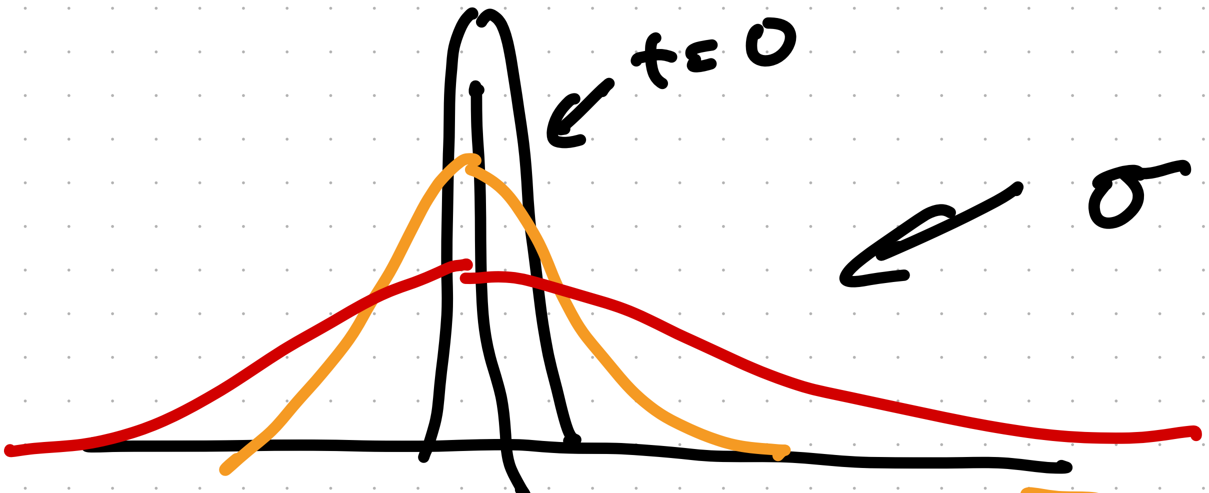
$$= \underline{a^2 M}$$

if $p = \frac{1}{2}$

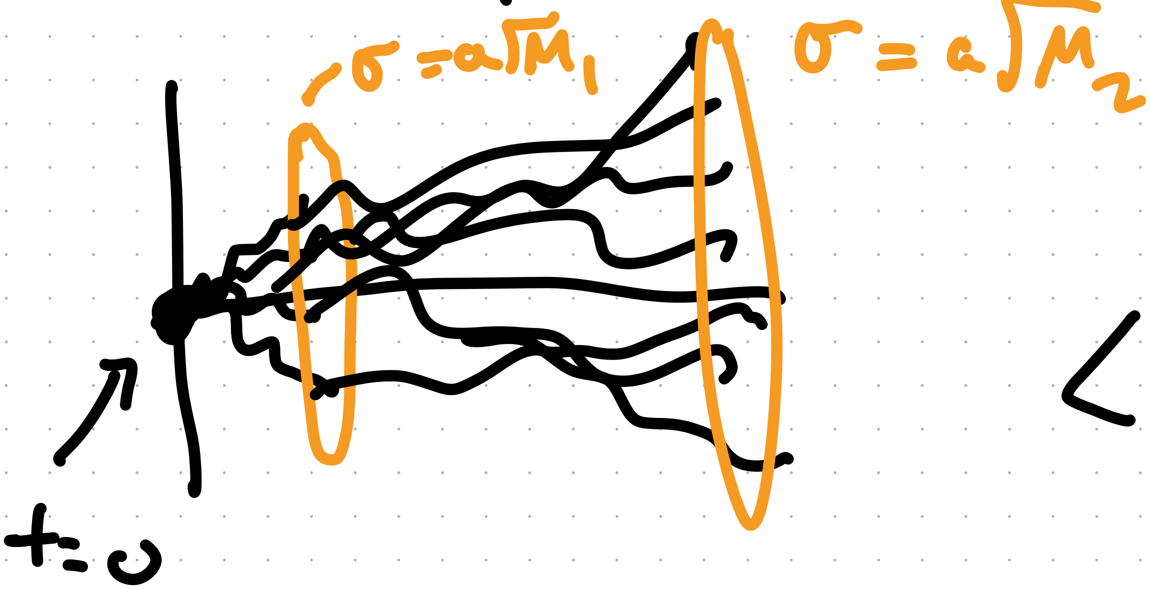
σ = root mean squared disp =

$$= a\sqrt{M}$$





$\sigma \propto \sqrt{T}$



diffusion

$\langle x^2 \rangle \propto t$

Einstein relation

Distributions of samples

1d random walk

① produces samples X_i from coin flips

$$X_i \xrightarrow{} X_{i+1}$$

coin flip

Could get $X_i \to X_{i+1}$ other rules

② Molecular dynamics "rule" newtons equations

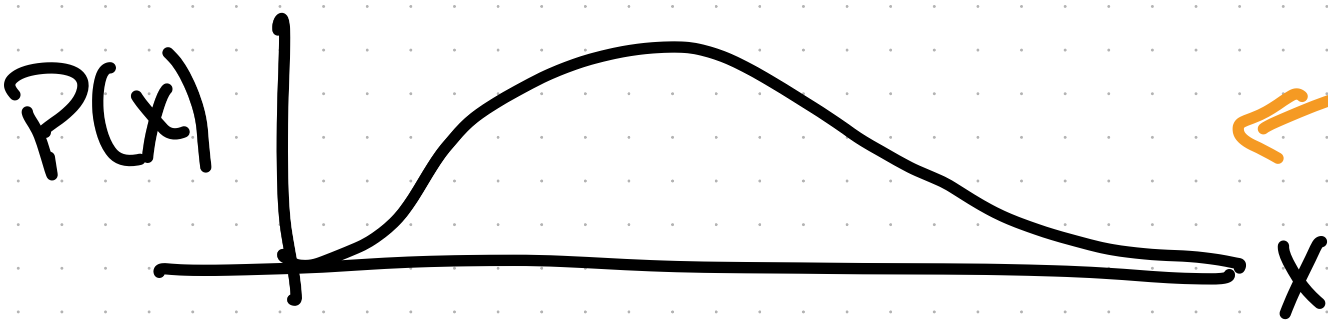
③ Make measurements

generate a set of $\{x_i\}$

1, 2, 3 examples of a process

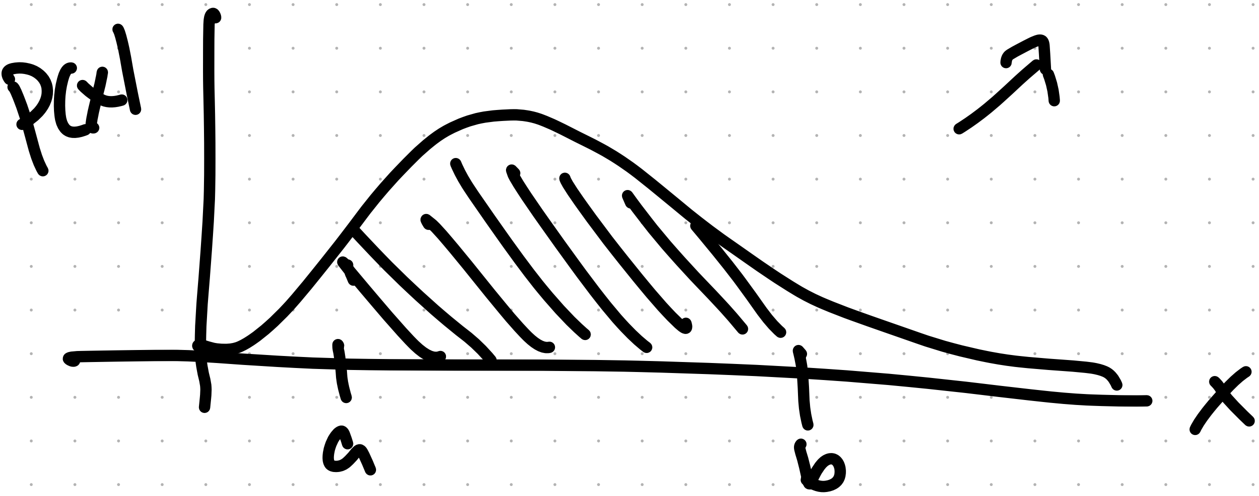
x_i samples from a distribution

x_i come from e.g.



eg Maxwell-Boltzmann $P(v) \propto v^2 e^{-v^2}$

Prob $x \in (a,b) = \int_a^b P(x)\,dx$



Normalized $\int_{-\infty}^{\infty} P(x)\,dx = 1$ all possible x

full range

$$\langle A \rangle = \int_{-\infty}^{\infty} A(x)\,P(x)\,dx$$

$$\langle x \rangle = \mu = \int_{-\infty}^{\infty} x\,P(x)\,dx$$

$$\sigma^2 = \langle (x-\mu)^2 \rangle = \int_{-\infty}^{\infty} (x-\mu)^2\,P(x)\,dx$$

var

expand

$$= \langle x^2 \rangle - \langle x \rangle^2$$

μ, σ are fixed properties

Eg: Bolzmann $P(\varepsilon) = \dfrac{e^{-\varepsilon/k_BT}}{Z}$

$$\int P(E)\, d\varepsilon = 1$$

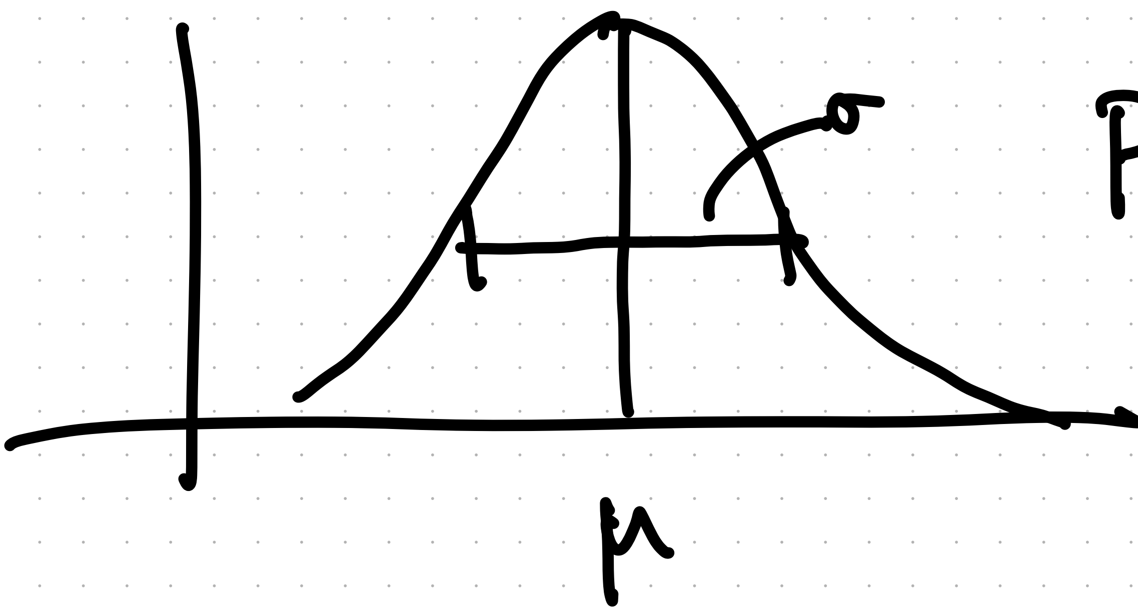
$$\frac{1}{Z}\int e^{-\varepsilon/k_BT}\, d\varepsilon = 1$$

$$\Rightarrow \quad Z = \frac{1}{\int e^{-\varepsilon/k_BT}\, d\varepsilon}$$

$$P(\varepsilon) = e^{-\varepsilon/k_BT} \Big/ \int e^{-\varepsilon/k_BT}\, d\varepsilon$$

Eg 2 M-B → $P(v) \propto v^2 e^{-v^2/k_BT}$

Eg 3: Gaussian, normal dist



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

$\langle x \rangle = \mu$

$\langle (x-\mu)^2 \rangle = \sigma^2$

$$\langle e^x \rangle \stackrel{?}{=} e^{\langle x \rangle}$$

$$1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \cdots$$

$$= \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

$$\langle e^x \rangle = \sum_{n=0}^{\infty} \frac{\langle x^n \rangle}{n!}$$

$$e^{\langle x \rangle} = \sum_{n=0}^{\infty} \frac{\langle x \rangle^n}{n!}$$

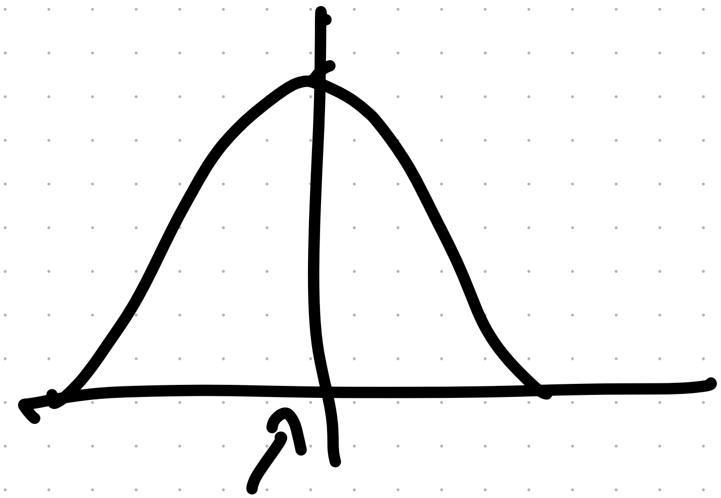
Next time

measurements

N values for x_i

$$\mu_N = \frac{1}{N}\sum_{i=1}^{N} x_i$$

0 ± 1



$-0.53, \ 0.68, \ -.71 \ldots$

$\mu_N \to \mu$ distribution N gets big

also ... classical mechanics