

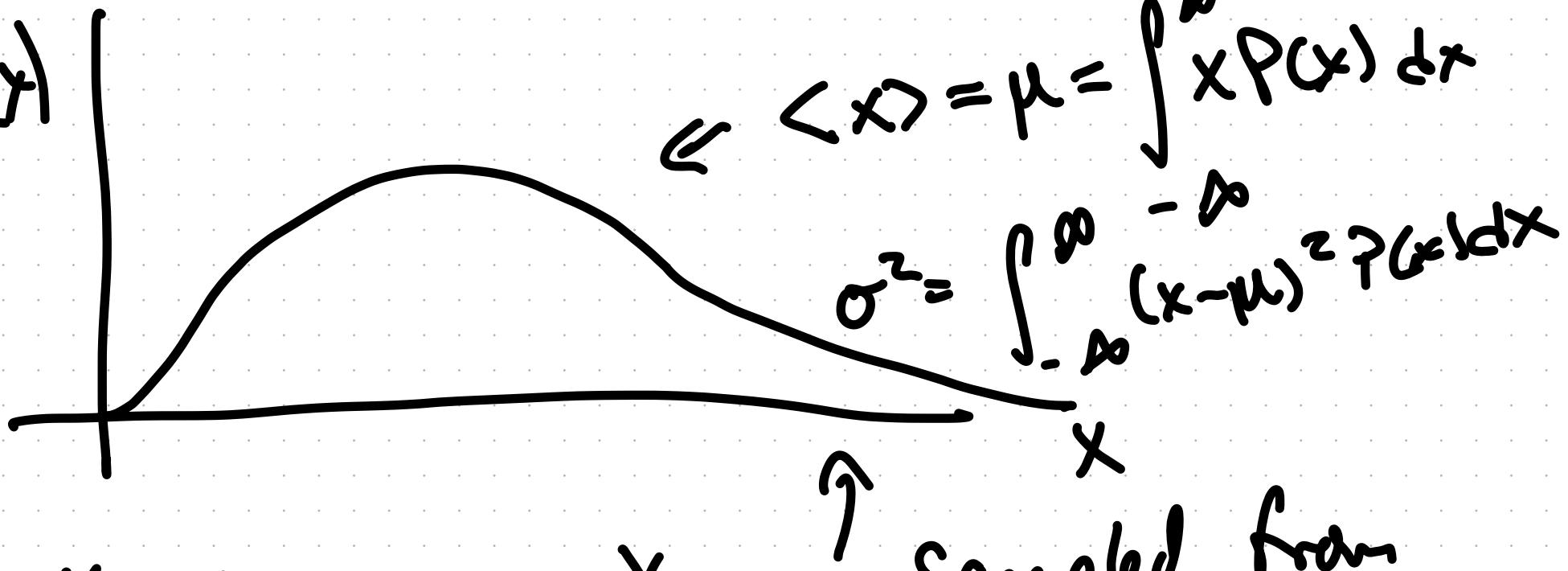
$$Q: f(x) = \int_a^x g(x) dx \quad C_{AB}(t) = \int_0^t A(t) B(0) dt$$

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

$$\text{Var } f(x) = \int_{-\infty}^{\infty} (f(x) - \langle f(x) \rangle)^2 P(x) dx$$

# Lecture 3

$P(x)$



$x_1, x_2, \dots, x_N$

sampled from  
this

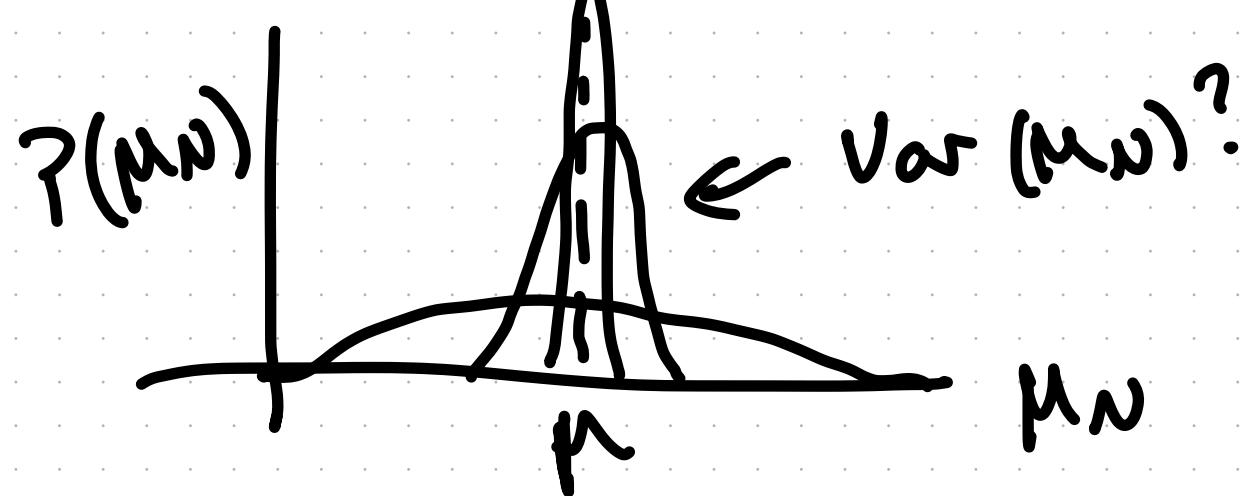
$$\mu_N = \frac{1}{N} \sum_{i=1}^N x_i$$

how close is  
 $\mu_N$  to  $\mu$

$$\mu_N = \frac{1}{N} \sum_{i=1}^N x_i; \quad x_i \text{ are samples} \\ \text{independent}$$

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

$$\text{Var}(\mu_N) = \langle \mu_N^2 \rangle - \langle \mu_N \rangle^2$$



$$\text{Var}(\mu_N) = \langle \mu_N^2 \rangle - \underbrace{\langle \mu_N \rangle^2}_{\sim \mu^2}$$

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

$$\begin{aligned} \langle \mu_N^2 \rangle &= \left\langle \left( \frac{1}{N} \sum_{i=1}^N x_i \right) \left( \frac{1}{N} \sum_{j=1}^N x_j \right) \right\rangle \\ &= \left\langle \frac{1}{N^2} \sum_{i,j=1}^N x_i x_j \right\rangle = \frac{1}{N^2} \sum_{i,j} \underbrace{\langle x_i x_j \rangle}_{\sim} \end{aligned}$$

$$\langle x_i x_j \rangle = \begin{cases} \langle x_i \rangle^2 & i=j \\ \underbrace{\langle x_i \rangle \langle x_j \rangle}_{\mu^2} & i \neq j \end{cases} \leftarrow \text{independent}$$

$$\langle \mu_N \rangle = \frac{1}{N^2} \sum_{i,j} \langle x_i x_j \rangle \stackrel{?}{=} \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N \underbrace{\langle x_i x_j \rangle}_{\mu^2}$$

$$\begin{aligned} &= \frac{1}{N^2} \sum_{i=1}^N (\langle x_i \rangle^2 + \underbrace{(N-1)\mu^2}_{N\mu^2 - \mu^2}) \\ &= \frac{1}{N^2} \sum_{i=1}^N (\underbrace{\langle x_i \rangle^2 - \mu^2}_{\text{Var}(x_i)}) + \frac{1}{N^2} \sum_{i=1}^N N\mu^2 \end{aligned}$$

$$\text{Var}(\bar{\mu}_N) = \langle \mu_N^2 \rangle - \mu^2$$

$$= \left[ \left( \frac{1}{N^2} \sum_{i=1}^N \text{Var}(x_i) \right) + \mu^2 \right] - \mu^2$$

$$\sigma_N^2 = \frac{1}{N^2} \sum_{i=1}^N \sigma^2 = \frac{1}{N} \sigma^2$$

$$\boxed{\sigma_N = \sigma / \sqrt{N}}$$

"Standard error of the mean"

$$\bar{\mu}_N \rightarrow \mu$$

like  $\frac{1}{\sqrt{N}}$

# Central Limit Theorem

$x_i$  points sampled from  $P(x)$

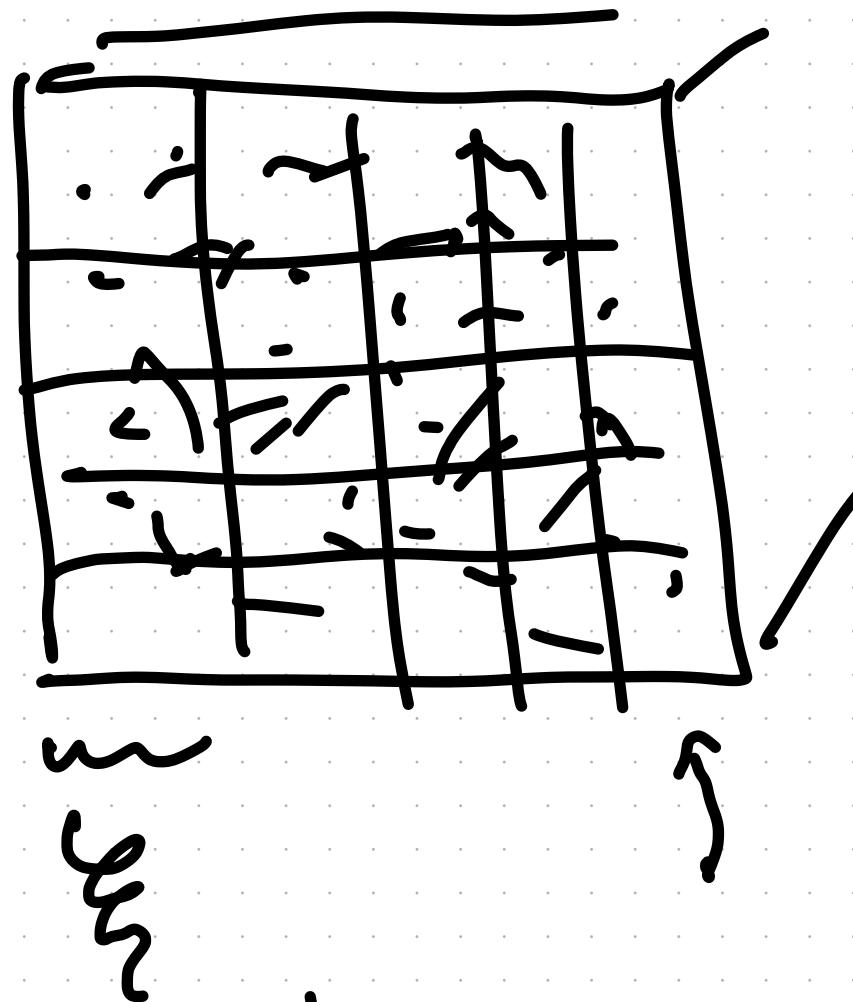
$$\mu_N = \frac{1}{N} \sum_{i=1}^N x_i$$

near zero  
var

$$P(\mu_N - \mu) \xrightarrow[N \rightarrow \infty]{} N(\underline{\mu}, \sigma^2/N)$$
$$= \frac{1}{A} e^{-\frac{(\mu_N - \mu)^2}{2(\sigma^2/N)}}$$

# Statistical Mechanics

$$N_{\text{boxes}} = \frac{V}{\xi^d}$$



Calculate  $A_i$  in each box

$\langle A_i \rangle = \langle A \rangle$  for system

$$\text{Var } A_i \sim \frac{1}{\sqrt{N_{\text{boxes}}}}$$

# Classical Mechanics

$$\vec{r} = (\vec{r}_1, \dots, \vec{r}_N)$$

$$\vec{v} = (\vec{v}_1, \dots, \vec{v}_N)$$

$$\vec{a} = \frac{d\vec{v}}{dt} = \frac{d^2\vec{r}}{dt^2}$$

$$\vec{\ddot{a}} = \vec{\ddot{v}} = \vec{\ddot{r}}$$

Newton's Equation says  $\vec{F} = m \vec{a}$

N differential equations

$$m_i \vec{\ddot{r}}_i = \vec{F}_i (\vec{r}_1, \dots, \vec{r}_N)$$

if we know  $\vec{r}(0)$ ,  $\vec{v}(0)$  and  $\vec{F}(\vec{r})$   
then everything is determined

If no friction, and know

$$U(\vec{r})$$

$$\vec{F}(\vec{r}) = -\nabla U(\vec{r}) \text{ ie}$$

$$F_i(\vec{r}) = -\frac{\partial U(\vec{r})}{\partial \vec{r}_i} \quad (\text{no veloc.})$$

$$\nabla A = \left( \frac{\partial A}{\partial \vec{r}_1}, \frac{\partial A}{\partial \vec{r}_2}, \dots, \frac{\partial A}{\partial \vec{r}_N} \right)$$

$$E(\vec{r}, \vec{v}) = \sum_{i=1}^n \frac{1}{2} m v_i^2 + \underbrace{U(r)}_{\text{potential}}$$

Kinetic

Momenta  $\vec{p}_i = m_i \vec{v}_i$

If  $\vec{F} = -\nabla U$ , forces are  
"conservative"

total energy is conserved

$$\mathcal{E} = \frac{1}{2}mv^2 + U(r) = \frac{p^2}{2m} + U(r)$$

$$\frac{d\mathcal{E}}{dt} = \frac{1}{2}m(v\dot{v} + \dot{v}v) + \frac{dU(r)}{dt}$$

$$= mva + \frac{dU(r)}{dt}$$

$$= VF + \frac{dU(r)}{dt} = VF + \left(\frac{\partial U}{\partial r}\right) \frac{\partial r}{\partial t} = 0$$

Chain rule

$$\frac{dX}{dt} = \sum_{i=1}^n \left( \frac{\partial X}{\partial x_i} \right) \frac{\partial x_i}{\partial t} = \sum_{i=1}^n \frac{\partial X}{\partial x_i} \dot{x}_i$$

$$\frac{d\epsilon}{dt} = \vec{v} \cdot \vec{F} - (\nabla u) \cdot \dot{\vec{r}}$$
$$= \vec{v} \cdot \vec{F} - \vec{F} \cdot \vec{v} = 0$$

in higher  
dimensions

Energy is conserved

# Lagrangian Mechanics

for conservative systems

$$L(\vec{r}, \dot{\vec{r}}) = K(\dot{\vec{r}}) - U(\vec{r})$$

Euler-Lagrange Equation

$$\frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{r}_i} \right) - \frac{\partial \mathcal{L}}{\partial r_i} = 0$$

(sec 1.6)  
Tuckerman

$$K = \frac{1}{2} m \dot{r}_i^2$$

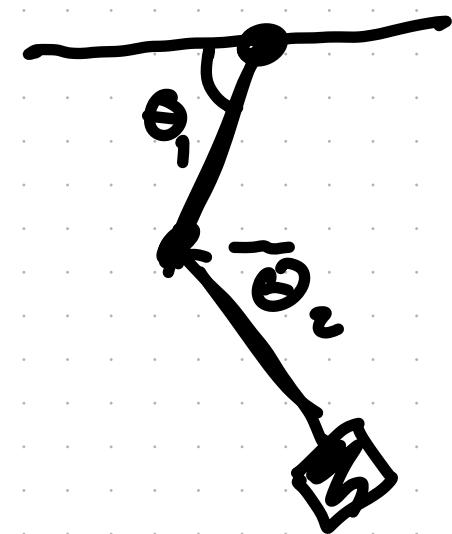
$$\frac{d}{dt} (m \dot{r}_i) = - \frac{\partial U}{\partial r_i}$$

$$m \ddot{r}_i = F_i$$

Why is this helpful?

Other coordinates

$$q_i = f_i(\vec{r})$$



# Hamiltonian Mechanics

$\mathcal{H}(\vec{q}, \vec{p})$       in    xyz  
 $\vec{p} = m\vec{v}$

In general  $p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$

↓ total energy

$$K(q_i) = \frac{1}{2}m\dot{q}_i^2$$

$$\frac{\partial \mathcal{L}}{\partial q_i} = M\ddot{q}_i \approx m\ddot{v}_i \\ = p_i$$

$$\mathcal{H}(\vec{q}, \vec{p}) = K + U(q), K = \sum_{i=1}^n \frac{p_i^2}{2m}$$

total energy

$$H(\vec{q}, \vec{p}) = K + U(q), K = \sum_{i=1}^n p_i^2 / 2m$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$
$$\dot{p}_i = - \frac{\partial H}{\partial q_i}$$

← equations of motion

$H$  and  $\mathcal{L}$  are connected  
by a "Legendre transform"

[Sec 1.5]

$$\begin{aligned} H(\vec{p}, \vec{q}) &= \sum_{i=1}^n \frac{\partial \mathcal{L}}{\partial q_i} \dot{q}_i - \mathcal{L} \\ &= \sum_{i=1}^n \dot{q}_i p_i - \mathcal{L} \end{aligned}$$


$\mathcal{H}$  is total energy

$$\frac{d\mathcal{H}}{dt} = \sum_{i=1}^N \left( \frac{\partial \mathcal{H}}{\partial q_i} \right) \left( \frac{\partial q_i}{\partial t} \right) + \left( \frac{\partial \mathcal{H}}{\partial p_i} \right) \left( \frac{\partial p_i}{\partial t} \right)$$

$$\begin{aligned} \mathcal{H}(\vec{q}, \vec{p}) &= \sum_{i=1}^N (-\dot{p}_i) q_i + (\dot{q}_i)(\dot{p}_i) \\ &= \sum_{i=1}^N [q_i p_i - \dot{p}_i q_i] \\ &= 0 \end{aligned}$$