Lecture 2: probability distributions and classical mechanics

Reminder: last time we defined the following quantities

$$\mu = \frac{1}{N}\sum_{i=1}^{N} x_i \quad \text{and} \quad \sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i-\mu)^2$$

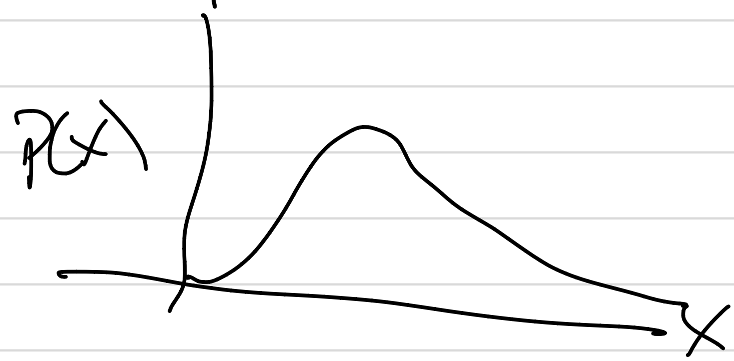
But where do these x_i come from

Sometimes they are generated by a "process" like coin flipping or dice rolling $\rightarrow$ Monte Carlo Sampling

Sometimes they come from MD (next) where $x_i \longrightarrow x_{i+1}$ is determined by Newton's equations

Sometimes they come from a series of Xpts, measurement 1, 2, 3, ...

Measurements X_i from experiments or simulations are assumed to come from an underlying probability distribution $P(X)$, eg



Properties:

① likelyhood $X \in (a,b) = \int_a^b P(x)\,dx$

② normalized, $\int_{-\infty}^{\infty} P(x)\,dx = 1$
$\leftarrow$ or range of def^n

Avg: $\langle A \rangle = \int A(x)\,P(x)\,dx$

Mean: $\mu = \langle x \rangle = \int x\,P(x)\,dx$

Var: $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = \int x^2 P(x)\,dx - \mu^2$

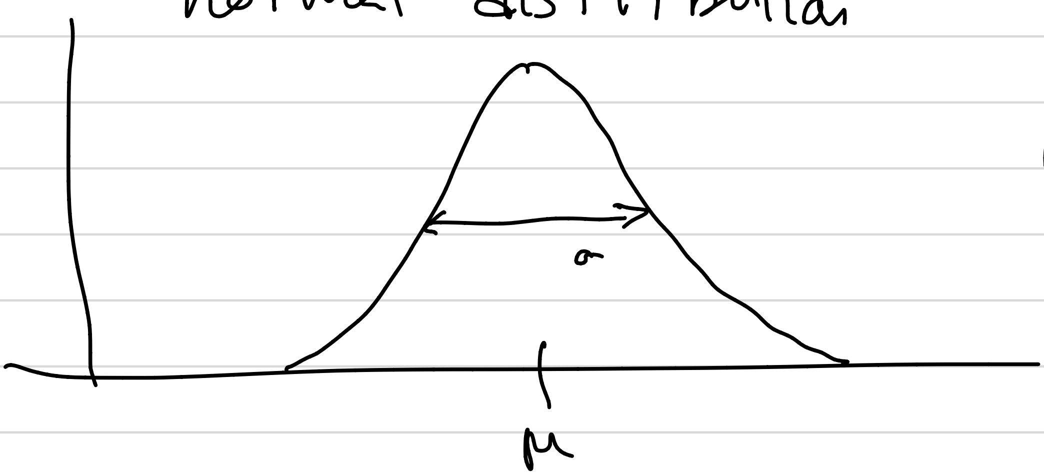
$= \int (x-\mu)^2 P(x)\,dx$

These are fixed parameters for the distribution/system

Very important distribution,

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

normal distribution



(Hw, prove normalization const)

It feels like if we sample from a distribution and measure a quantity we should get an approx to the true value

$$\underset{\text{sample mean}}{\mu_N} = \frac{1}{N}\sum_{i=1}^{N} x_i \quad \text{but what is avg } \mu_N$$

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

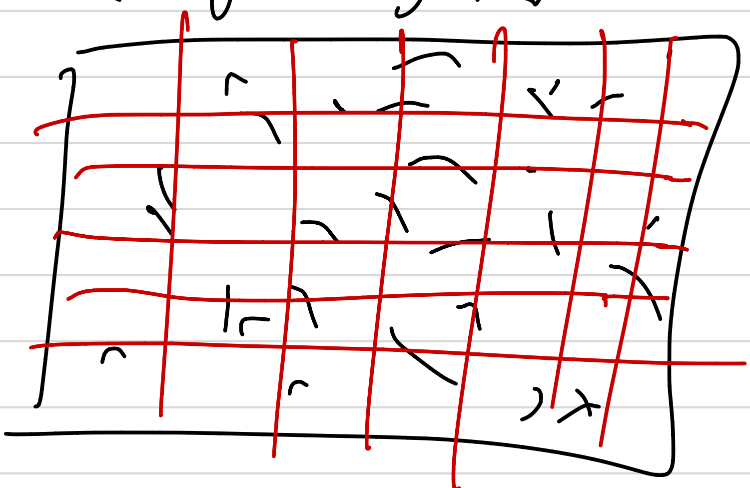
$$\mathrm{Var}(\mu_N) = \langle \mu_N^2 \rangle - \langle \mu_N \rangle^2 = \langle \mu_N^2 \rangle - \mu^2 = \left\langle \frac{1}{N^2}\sum_{ij} x_i x_j - \mu^2 \right\rangle = \frac{1}{N^2}\sum \langle x_i x_j \rangle - \mu^2$$

$$= \frac{1}{N^2}\sum (\langle x_i x_j \rangle - \mu)$$

$$\langle x_i x_j \rangle = \begin{cases} \langle x_i^2 \rangle & i = j \\ \langle x_i \rangle \langle x_j \rangle = \mu^2 & i \neq j \end{cases}$$

$$= \frac{1}{N^2}\sum_i \langle x_i^2 \rangle - \mu^2 = \frac{1}{N^2}\sum_i \langle x_i^2 \rangle - \mu^2 = \frac{1}{N^2}\sum_i \mathrm{Var}(x_i) = \frac{1}{N^2}\sum_i \sigma^2 = \underline{\underline{\sigma^2/N}}$$

In stat mech, we imagine taking our large system



$\sim \xi$

$N_{boxes} = V/\xi^d$

$\propto N_{molecules}$

Compute A_i on avg subsystem

Then $\sqrt{\langle A - \langle A \rangle \rangle^2} \sim 1/\sqrt{N}$

Hence for a large system we always measure the avg quantity

(if ξ can be sufficiently small)

Central limit theorem!

Suppose X_i from any $P(x)$

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

$P(\mu_N - \mu) \xrightarrow[N \to \infty]{} \mathcal{N}(0, \sigma^2/N)$

HW, test on data

which means avg error on mean

$\langle (\mu_N - \mu)^2 \rangle = \sigma^2/N \to$ std dev of mean $\propto 1/\sqrt{N}$

Classical Mechanics

We will assume for now that our system obeys classical mechanics,

The positions of all the atoms are given by $\vec{r} = (\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$

and $\vec{v} = d\vec{r}/dt = \dot{r}$, $\vec{a} = \frac{d\vec{v}}{dt} = \ddot{r}$

Newton's equations say that $F = ma$ or

$$m_i \ddot{\vec{r}}_i = F_i(\vec{r}_1, \ldots, \vec{r}_N), \quad 3N \text{ diff. eqns.}$$

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

So what is F? If there is no friction or dissipation in the system, and we know the potential energy of the system $U(\vec{r})$, then

$$F(\vec{r}) = -\nabla U(r) \quad \text{i.e.}$$

$$F_i(r) = -\frac{dU(r)}{dr_i}$$

(no dep. on velocities)

The total energy $\mathcal{E}(r)$ is kinetic + potential energy,

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

where $p_i = m_i v_i$ is the momentum

If $F = -\nabla u$, then these are conservative forces, b/c the total energy is const

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

(chain rule)

$$\left[\text{identity} \quad \frac{dX(l_1, l_2, \ldots, l_N)}{dt} = \sum_{i=1}^{N} \frac{\partial X}{\partial l_i}\frac{\partial l_i}{\partial t} = \sum_{i=1}^{N} \frac{\partial X}{\partial l_i}\dot{l}_i \right]$$

$$= \vec{m}\vec{v}\vec{a} + \underbrace{\sum \frac{\partial u}{\partial r_i}}_{-F}\dot{r}_i$$

$$= \vec{v}\cdot\vec{F} + (-\vec{F}\cdot\vec{v}) = 0$$

Lagrangian mechanics

for conservative systems, there is another way to solve classical problems called Lagrangian mechanics

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

The Euler Lagrange eqn says

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{r}_1}\right) - \frac{\partial \mathcal{L}}{\partial r_1} = 0$$

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

This is of course

$$m\ddot{r} = -\nabla U = F$$

Why is this helpful? It applies In other coordinates ie

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

where $q_i = f_i(\vec{r})$ diff f^n for each coord

(see homework? / sect 1.6)

Lagrangian mechanics is useful later for formulating certain methods, but it also leads to a second generalized method, Hamiltonian mechanics

Here there will be a function $\mathcal{H}(\vec{r}, \vec{p})$

$\vec{p}$ are "conjugate" momenta. In cartesian $\vec{p} = \vec{m}\vec{v}$, but now we generalize to

$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$ (of course, if $K(\dot{q}) = \frac{m\dot{q}^2}{2}$ same)

$K = \sum \frac{p_i^2}{2m_i}$, $\mathcal{H} = K + U(q)$

Hamilton's eqns $\boxed{\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i} \\ \dot{p}_i &= -\partial H / \partial r_i \end{aligned}}$

$\mathcal{H}$ generates dynamics in any coord system
The $\mathcal{H}$ and $\mathcal{L}$ are connected by a
Legendre transform (book 1.5)
(later)

$$H(p,q) = \sum p_i \dot{q}_i - \mathcal{L}(q,\dot{q})$$

(for cartesian, "obvious")

$$\sum m v^2 - (\tfrac{1}{2} m v^2 - U)$$
$$= \tfrac{1}{2} m v^2 + U$$

Since $H = E_{total}(r)$, expect $\frac{dH}{dt} = 0$

chain rule

$$\frac{dH(q,p)}{dt} = \sum_i \frac{\partial H}{\partial q_i}\frac{\partial q_i}{\partial t} + \frac{\partial H}{\partial p_i}\frac{\partial p_i}{\partial t}$$

$$= \sum_i -\dot{p}_i \dot{q}_i + \dot{q}_i \dot{p}_i = 0$$