Lecture 2
Statistics & Classical Mech

Office Hours:

130-230 Thursday and 10-11 friday?

Statistics Reminder

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

$Var(x) \equiv \sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i-\mu)^2$, σ is std dev

Sometimes adjusted

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

$$Var(x) \geq 0 \Rightarrow \langle x^2\rangle \geq \langle x\rangle^2$$

Lets look back at our random walks

$$disp = \sum_{i=1}^{M} m_i \quad (+a, -a) \text{ for each } m_i$$
$$= a(N_+ - N_-) = a(2N_+ - M)$$

$$\langle d\rangle = a\langle N_+\rangle - a\langle N_-\rangle \xrightarrow[M\to\infty]{} aM(p_+ - p_-)$$
$$aM(2p-1)$$

$= 0$ for $p_+ = p_- = 1/2$

$\langle d\rangle^2 = a^2M^2(4p^2-4p+1)$

$$Var(d) = \langle d^2\rangle - \langle d\rangle^2$$
$$\langle d^2\rangle = a^2\langle(2N_+-M)^2\rangle = a^2\langle 4N_+^2 - 4N_+M + M^2\rangle$$
$$Var(N_+) = Mp(1-p) = \langle N_+^2\rangle - \langle N_+\rangle^2$$
$$\Rightarrow \langle N_+^2\rangle = Mp(1-p) + M^2p^2$$

$$Var(d) = a^2\left[4(Mp(1-p) + M^2p^2) - 4M^2p + M^2\right]$$
$$= a^2\left[4Mp(1-p)\right] \underset{p=1/2}{=} Ma^2$$

$$\text{RMS } D = \sqrt{\langle d^2\rangle} \to a\sqrt{M}$$

We saw for a real example how we can get a series of X_i from a coin flip process.

Could also get X_{i+1} from X_i by some rule, EG in MD equations of motion (next)

X_i could also come from a series of measurements

Assumed that X_i come from underlying prob dist $P(x)$

eg $P(x)$ 

P has properties

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

Normalized $\int_{-\infty}^{\infty} P(x)\,dx = 1$ ← or proper range

For this continuous distribution

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

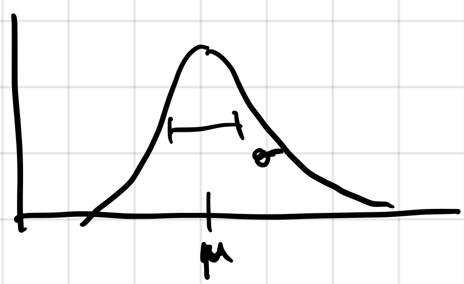
$$\mu = \langle x \rangle = \int x P(x)\,dx$$

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

μ & σ are fixed properties of dist

Name probability distributions?

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



If we sample from a dist and measure a quantity, feels like we should approx the true value

$$\overset{\text{sample mean}}{\mu_N} = \frac{1}{N}\sum_{i=1}^{N} x_i \quad , x_i \text{ independent measurements}$$

$$\langle \mu_N \rangle = \frac{1}{N}\sum \langle x_i \rangle = N\mu / N = \mu$$

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

$$\langle \mu_N^2 \rangle = \frac{1}{N^2}\sum_i \sum_j \langle x_i x_j \rangle = \frac{1}{N^2}\sum_i \left(\langle x_i^2 \rangle + (N-1)\mu^2\right)$$

$$= \frac{1}{N^2}\sum_i \underbrace{(\langle x_i^2 \rangle - \mu^2)}_{\mathrm{Var}(x_i)} + \frac{N^2\mu^2}{N^2}$$

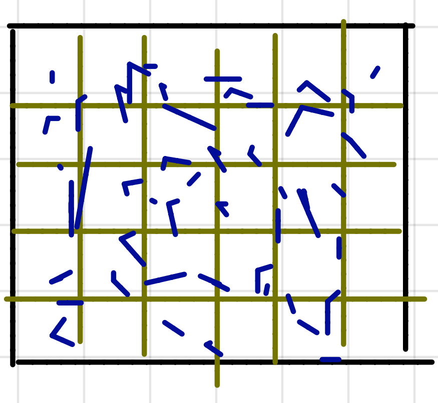
$$\langle x_i x_j \rangle = \langle x_i^2 \rangle \quad , i = j$$

$$\langle x_i \rangle \langle x_j \rangle = \mu^2 \quad i \neq j$$

$$\Rightarrow \mathrm{Var}(\mu_N) = \frac{1}{N^2}\sum_{i=1}^{N} \mathrm{Var}(x_i) = \frac{1}{N}\mathrm{Var}(x) = \sigma^2/N$$

$\sigma_N = \sigma/\sqrt{N}$, increasing ind samples gets μ_N closer to μ by factor $\sqrt{N}$

In stat mech, imagine taking a large system



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

Compute A_i on any subsystem

Then $\mathrm{Var}(A_i) \sim 1/\sqrt{N}$

Bigger the system, the more a single measurement is reflective of true $\langle A \rangle$

Central limit theorem: If X_i taken from any $P(x)$

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

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

Classical Mechanics

Assume our systems will be classical

$$\vec{r} = (\vec{r}_1, \vec{r}_2, \dots \vec{r}_N) \qquad \vec{a} = \frac{d\vec{v}}{dt} = \frac{d^2\vec{r}}{dt^2}$$

$$\vec{v} = (\vec{v}_1, \vec{v}_2, \dots, \vec{v}_N) \qquad \vec{a} = \dot{\vec{v}} = \ddot{\vec{r}}$$

Newton's Equations say $F = ma$ ie

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

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

If no friction, or dissipation, and know potential energy $U(\vec{r})$ then $F(\vec{r}) = -\nabla U(\vec{r})$ ie

$$F_i(\vec{r}) = -dU(r)/dr_i \quad \text{(no dep on vel)}$$

The total $\mathcal{E}$ is kinetic + pot energy

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

momentum $p_i = v_i m_i$

If $F = -\nabla U$, say these are conservative forces because $\mathcal{E}$ is const

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

chain rule $\left[\frac{dX}{dt} = \sum_{i=1}^{N} \left(\frac{\partial X}{\partial l_i} \right) \frac{dl_i}{dt} = \sum \left(\frac{\partial X}{\partial t} \right) \dot{l}_i \right]$

$$= m\vec{v}\vec{a} + \sum \frac{\partial U}{\partial r_i} \dot{r}_i = \vec{v} \cdot \vec{F} - \vec{F} \cdot \vec{v} = 0$$

Lagrangian Mechanics

For conservative systems, there is another way to solve classical problems called Lagrangian Mechanics:

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

Euler-Lagrange equations:

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{r}_i}\right) - \partial \mathcal{L}/\partial r_i = 0$$ (Sec 1.6)

For $\vec{K} = \frac{1}{2} m \dot{r}_i^2$, equiv to

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

Why is this helpful? It applies for other coordinates, ie where $q_i = f_i(\vec{r})$, could be diff func for each coord

Lagrangian Mech. is useful for some methods, but also leads to a second generalized set of EOMs, Ham. Mech.

$\mathcal{H}(\vec{r}, \vec{p})$ is Hamiltonian and $\vec{p}$ are "conj. mom."

In cartesian, $\vec{p} = m\vec{v}$, but generalize to

$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$ [Same for $K(\dot{q}) = m\dot{q}_i^2/2$]

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

$$\boxed{\begin{aligned}\dot{q}_i &= \partial \mathcal{H}/\partial p_i \\ \dot{p}_i &= -\partial \mathcal{H}/\partial r_i\end{aligned}}$$

$\mathcal{H}$ generates dynamics in any coord system

The $\mathcal{H}$ and $\mathcal{L}$ are connected by a "Legendre transform" [sec 1.5]

$$\mathcal{H}(p,q) = \sum_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i}\dot{q}_i - \mathcal{L} = \sum_i \dot{q}_i p_i - \mathcal{L}$$ [for cartesian, $\sum m_i v_i^2 - (\frac{1}{2}\sum m_i v_i^2 - U) = U + K$]

$$\frac{d\mathcal{H}(q,p)}{dt} = \sum \frac{\partial \mathcal{H}}{\partial q_i}\dot{q}_i + \frac{\partial \mathcal{H}}{\partial p_i}\dot{p}_i = \sum -\dot{p}_i \dot{q}_i + \dot{q}_i \dot{p}_i = 0$$