Markov Chains

Lecture 9

PHYS 246 class 9
Fall 2025
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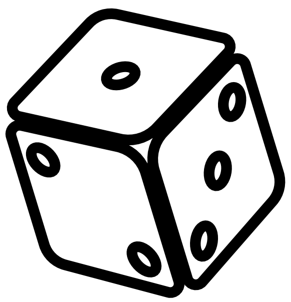
https://jnoronhahostler.github.io/IntroductionToComputationalPhysics/intro.html

Announcements

- TBD

Memory-less process

Throw (weighted) dice: odd or even number?



$P_{\text{odd}} = 0.6$

$P_{\text{even}} = 0.4$

Odd

Odd

Even

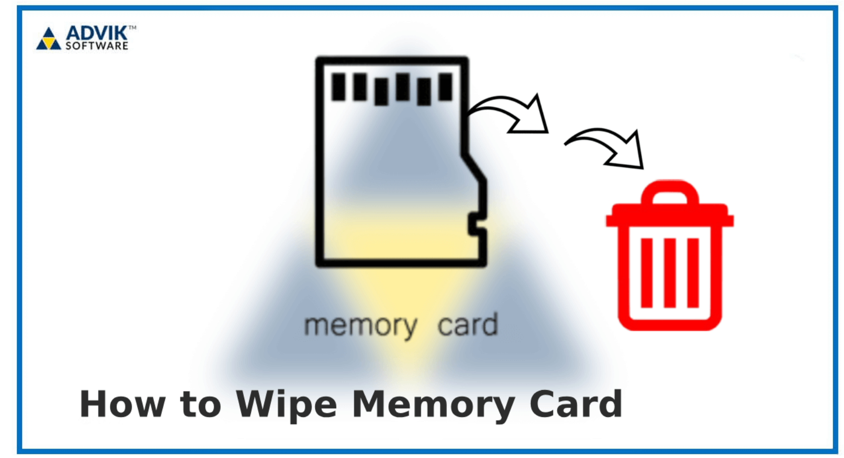
Odd

Even

Odd

Even

Sample from $0 - 1$



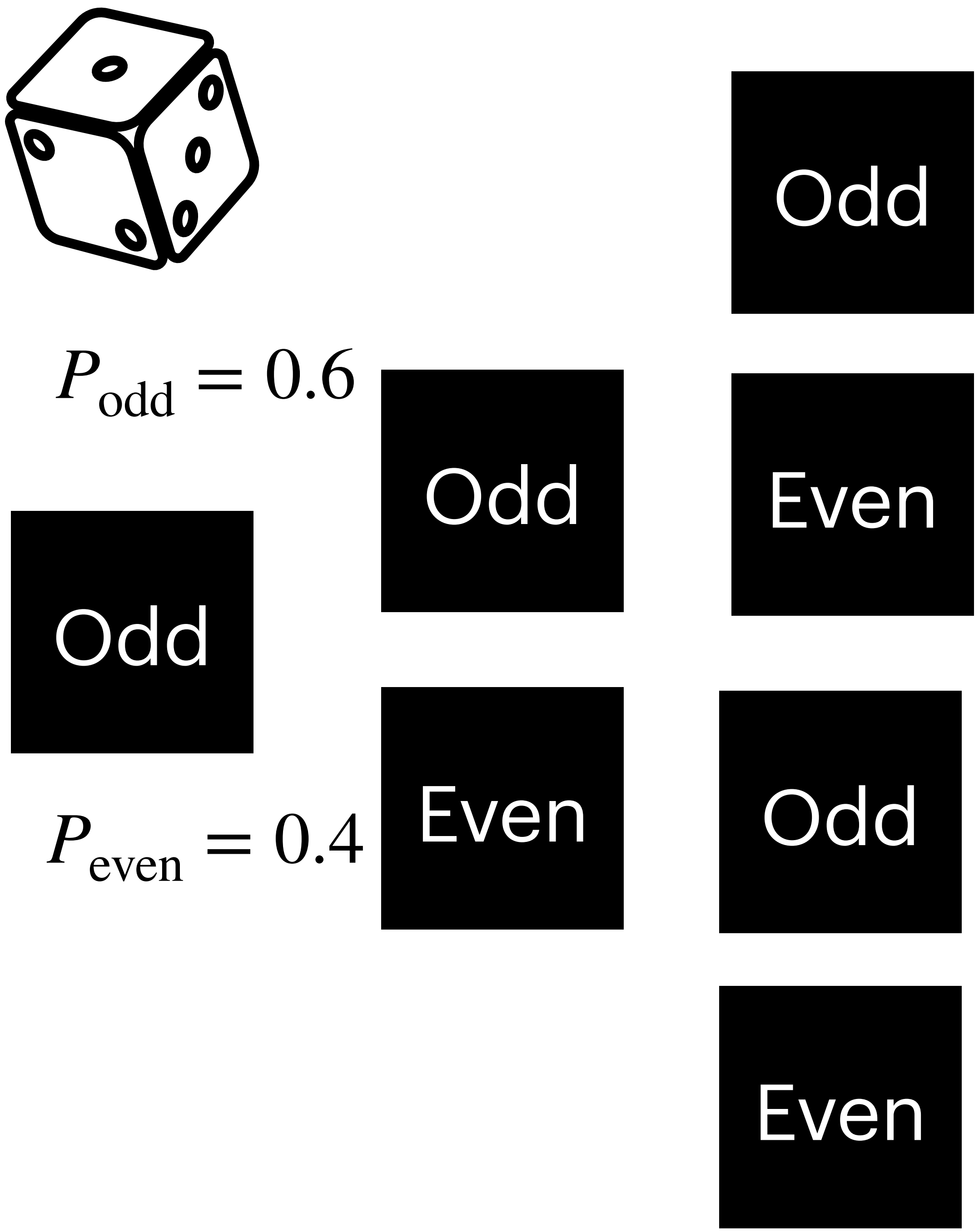
$P_{\text{odd}} = 0.6$

$P_{\text{even}} = 0.4$

What are examples of processes that depend on time, where each step does not have memory of the previous step?

Start sampling

Throw (weighted) dice: odd or even number?



Start at state x_t (odd)

For x_{t+1}, sample from $r = \text{sample}[0 - 1]$

If $r \leq 0.6$, odd. Else even

Ex. $r = 0.27$. Odd

x_{t+2}, $r = \text{sample}[0 - 1]$ (repeat process)

...

$t = t_{end}$

Performed a Markov Chain

Now what?

- What is the probability of rolling 3 even numbers in a row?
- What is the probability of rolling odd, even, odd, even, odd?
- What is your averaged (over many, many samples) probability of getting an odd number?
- Random walks are examples of Markov chains: continuous (position) vs discrete variables (binary choices)

Equilibration time

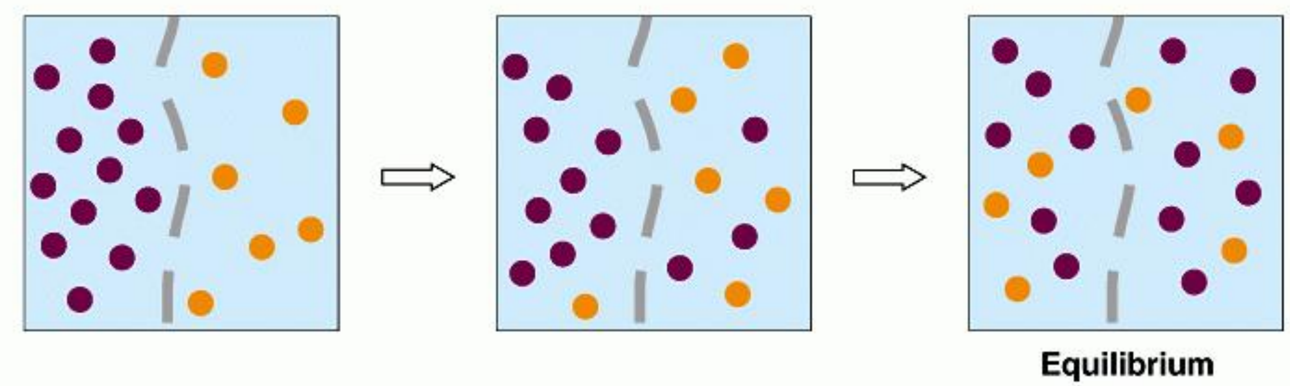
Approaching a steady state

Averages:

$$\langle O(x) \rangle = \int O(x)\rho(x)dx$$

If $P_{odd} = 0.6$ and $P_{even} = 0.4$

$$\langle \mathrm{odd}(\mathrm{t_{step}}) \rangle = \frac{1}{\mathrm{t_{step}}} \sum_{\mathrm{t}}^{\mathrm{t_{step}}} \Theta(\mathrm{P_{odd}} - \mathrm{r_t})$$



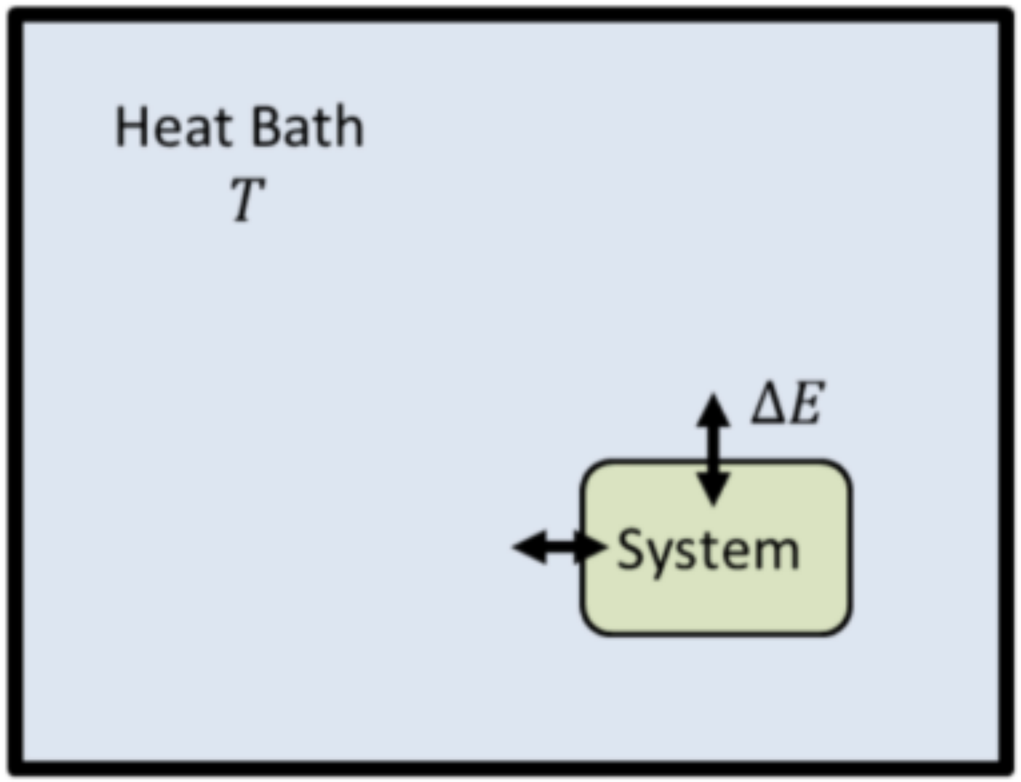
(b) Diffusion of two solutes

For $t_{step} \to \infty$, $\langle \mathrm{odd}(\infty) \rangle = 0.6$

Equilibration time t_{eq}, time when t_{step} reaches a steady state of $\langle \mathrm{odd}(\mathrm{t_{step}}) \rangle \sim 0.6$

Statistical Mechanics

Thermal Equilibrium



Boltzmann:

$$P(x) = \frac{e^{-\frac{E(x)}{kT}}}{\int e^{-\frac{E(x)}{kT}} dx} \equiv \frac{e^{-\frac{E(x)}{kT}}}{Z}$$

Where x is the states of the system

Monte Carlo integration

Expectation values

Boltzmann:

$$P(x) = \frac{e^{-\frac{E(x)}{kT}}}{\int e^{-\frac{E(x)}{kT}} dx} \equiv \frac{e^{-\frac{E(x)}{kT}}}{Z}$$

Averages:

x might be very high dimensional!

$$\langle O(x) \rangle = \int O(x) P(x) dx$$

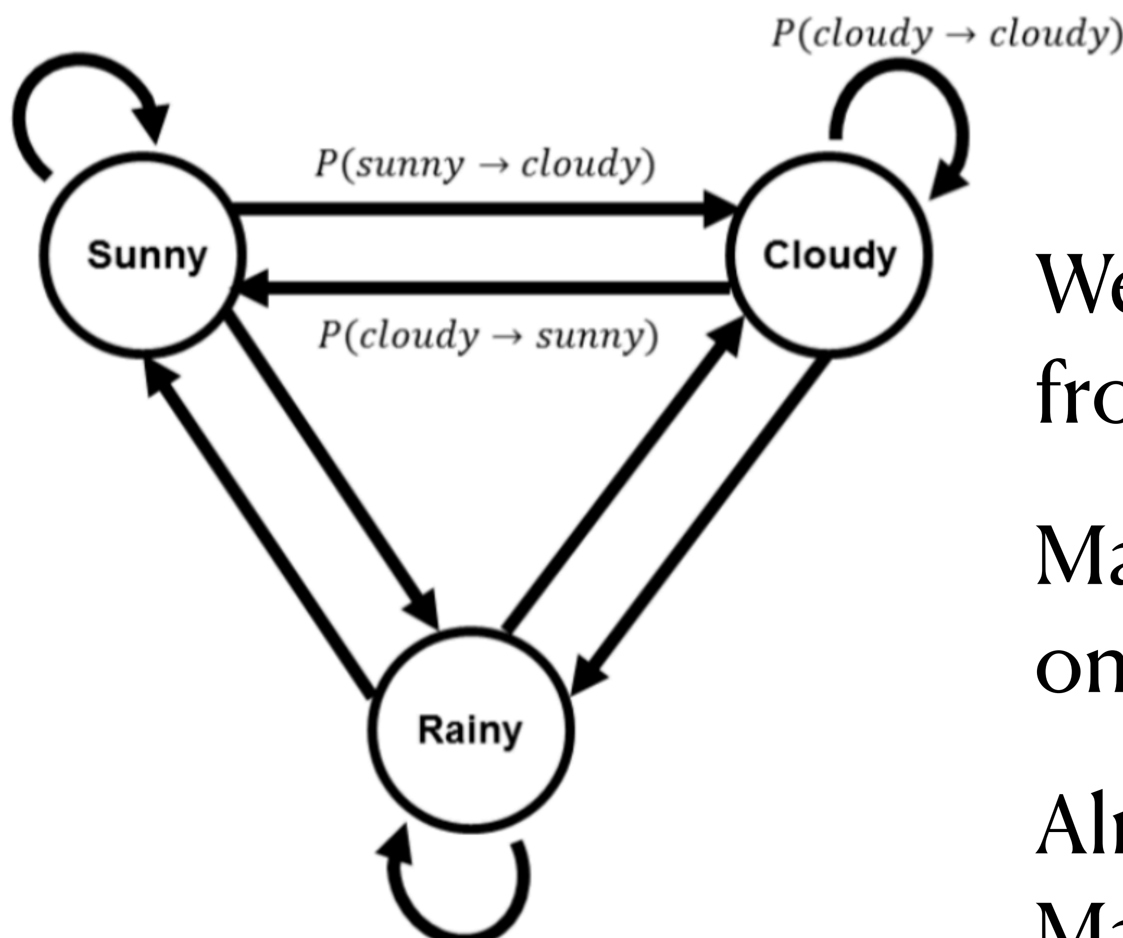
Expectation value

$$\langle O(x) \rangle = \int O(x) P(x) dx = \langle O(x) \rangle_{x \sim P}$$

Sample average where x is drawn from $P(x)$

Markov Chains

Solving the weather



We will use Markov chains to generate x from the Boltzmann distribution.

Markov chains are random processes that only depend on the current state.

Almost everything can be written as a Markov chain..

Metropolis algorithm: simple case

If you are in state A:

With probability 0.5, move to state B

With probability 0.5, stay in state A

If you are in state B:

With probability 1, move to state A

Question: what is the probability distribution we will sample?

Metropolis: general case

Looping over i

1. Start at point x_i

2. Choose point t at random (note some caveats)

3. x_{i+1} is set to t with probability $\min\left(1, \frac{P(t)}{P(x_i)}\right)$, otherwise $x_{i+1} = x_i$

Notes and tricks

We work with unitless numbers $h = \dfrac{\mu B}{kT}$ and $\dfrac{\epsilon}{kT}$, which are the only things that change the physics. High temperature is small h and low temperature is large h.

Make sure that if you reject a move, you average the old position again.