Lecture 11: MC Simulations

Wednesday, January 31, 2024 3:22 PM

Topics for today:
- Applications of Monte Carlo Method
- Ising Model
  - Metropolis algorithm
  - Site Percolation

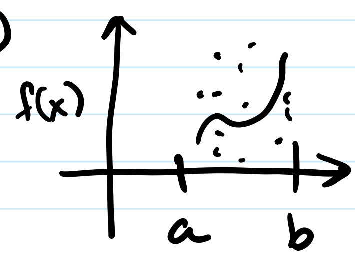
Announcements:
- HW 5: due this Friday (posted on Canvas)

Material References:
- David Landau & Kurt Binder - "A Guide to Monte Carlo Simulations in Statistical Physics", Chapter 3
- Mark Newman - "Computational Physics", Chapter 10
- Anders Sorenssen - "Percolation theory using Python"

Applications of Monte Carlo Method:

① Integrals (last week)

$$y = \int_a^b f(x)\,dx$$



② radioactive decay

$$\frac{dN}{dt} = -\lambda N$$

related to half-life

$$\Rightarrow N = N_0 e^{-\lambda t}$$

- time divided into discrete intervals
- each undecayed nuclei is 'tested' for decay during time interval
- process repeated many times to obtain series of independent 'experiments'

③ energy of ideal gas (last class)

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$$E(n_x, n_y, n_z) = \frac{\pi^2 \hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

$$\Rightarrow \Delta E = \frac{\pi^2 \hbar^2}{2mL^2}(\pm 2n_i + 1)$$

- start w/ random choice (either ±1)
- determine a random move set & calculate change in energy.
- accept or decline move & iterate

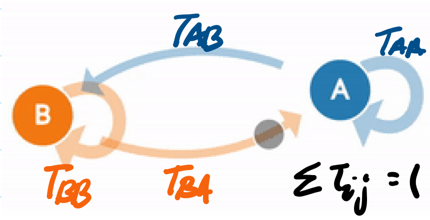
④ Ising model

- metroplis algorithm
- site percolation

Metroplis-Hastings Algorithm:

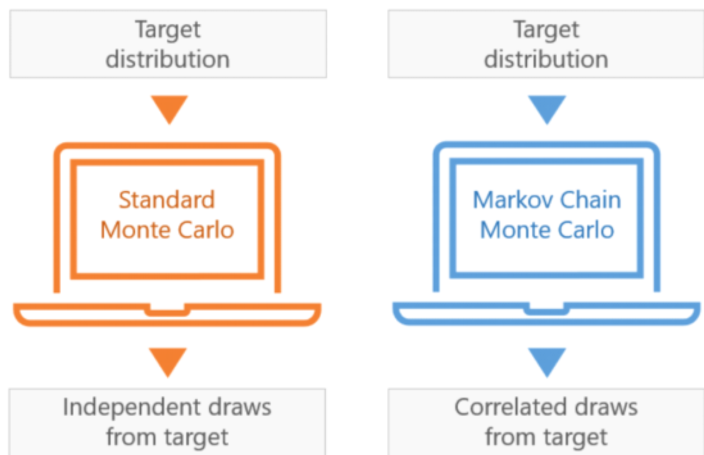
ASIDE: recap Markov Chain (last class)

- consider a move set to change the system by one degree of freedom
- start @ $i \rightarrow j$ (not random, based on i)



move set to change system by 1 degree of freedom given by transition probability T_{ij}

- Monte Carlo incorportion to marko chain
  - randomly choose many correlated draws from the "target"



☆ Metroplis   Gibbs.

- type of Markov chain MC (MCMC) method for obtaining random # from distribution where direct sampling is difficult
- random walk btwn 2 states x & y is symmetric s.t. $\underbrace{Q(x|y) = Q(y|x)}_{\text{known as hastings ratio}}$

Known as hastings ratio

- example: sample from exponential distribution

$$\pi(x) = e^{-x} \quad (x \geq 0)$$

"target" distribution

↳ choose some initial state x_i

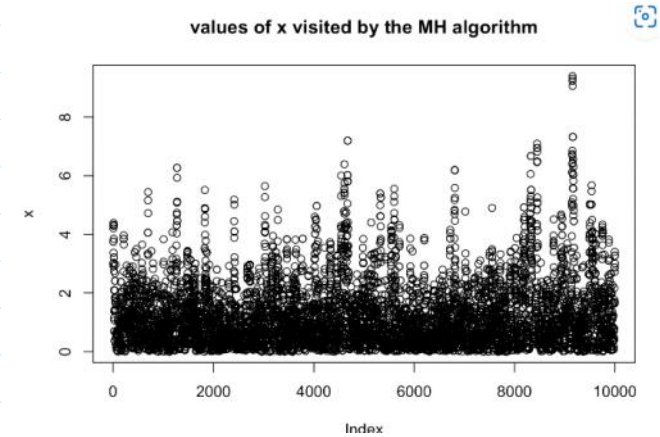
↳ as we increment time (t), sample y from $Q(y|x_t)$ where y is the "proposed" value of x_{t+1}

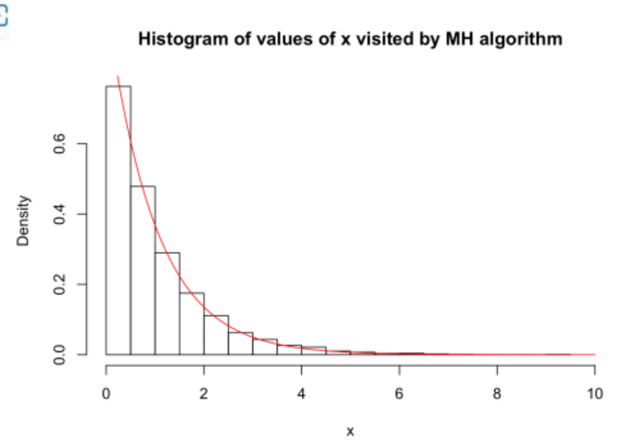
↳ calculate acceptance probability

$$A = \min\left(1, \frac{\pi(y)}{\pi(x_t)}\right)$$

$$\begin{cases} \text{accept w/ probability } A & x_{t+1} = y \\ \text{reject}, & x_{t+1} = x_t \end{cases}$$

```
x = x0
trajectory = [x0]
for i in range(1,N):
    y = prop(x)
    ratio = pi(y,V)*g(x,y)/pi(x,V)/g(y,x)
    a = np.min([1.,ratio])
    r = np.random.rand()
    if r < a:
        x = y
    trajectory += [x]
```



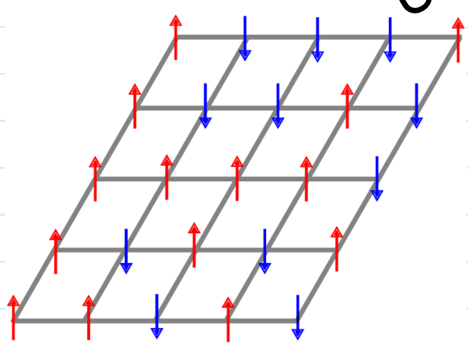


Basics of Ising Model:

- model used in condensed matter physics
- mathematical model of ferromagnetism
- consists of atomic spins of magnetic dipole moments

either +1 or −1
(↑) (↓)

- spins are arranged on lattice



ground state: all ↑
all ↓

where ferromagnetism arises

⇒ net magnetic moment that is macroscopic

- consider interactions w/ nearest neighbors (NN)

$$H = \underbrace{-\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j}_{\text{sum over adjacent spins}} \underbrace{- \mu \sum_j h_j \sigma_j}_{\text{external magnetic field interactions}}$$

$\sigma_k \in \{-1, +1\}$
J_{ij} = NN interaction
h_j = external magnetic field

average for any observable X:

$$\langle X \rangle = \frac{1}{Z}\sum_{\{\sigma\}} X e^{-H/T} \quad \text{where } Z = \sum_{\{\sigma\}} e^{-H/T}$$

- incorporate metropolis algorithm into ising model
  ↳ probability of appearing in a given configuration j is $\propto$ to Boltzmann weight
  $e^{-E_j/T}$
  ↳ condition for acceptance of random spin flip given by the ratio of transition probabilities

↳ condition for acceptance of random spin flip given by the ratio of transition probabilities

$$\frac{P(j)}{P(i)} = \frac{e^{-E_j/T}}{e^{-E_i/T}}$$

$$A = \min\left(1, e^{E_i/T - E_j/T}\right)$$

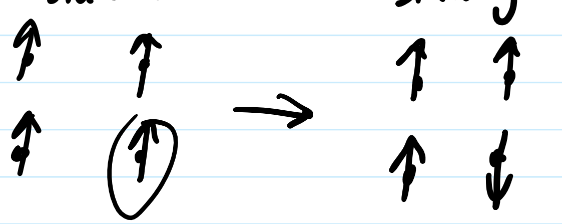
$$\begin{cases} \text{accept w/ probability } A \\ \text{reject, try another spin flip} \end{cases}$$

↳ update site of random spin flip

PYTHON IN-CLASS PROBLEM

start w/ random state then plot the configuration for square lattice (NxN) & no external field & pbc

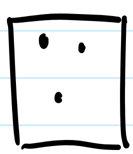
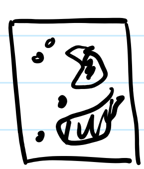
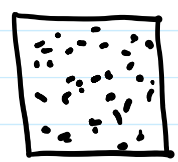
state: i   state: j



$$A = \min\left(1, e^{(E_i - E_j)/T}\right)$$

$$E_i - E_j = (\sigma_i - \sigma_j)\sum_{\langle ij \rangle} \sigma_{ij}$$

- Phase transition of ising model

$T < T_c$	$T = T_c$	$T > T_c$
low temp	critical temp	high temp
		
- dominance of one spin w/ some fluctuations of other spin - long range correlation	- no clear dominance - fluctuations at all scales - long range correlations	- no dominance of either spin - no obvious patterns - short range correlations

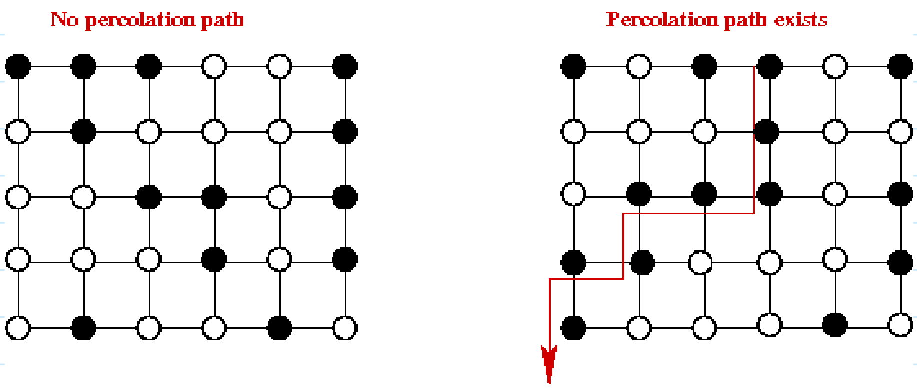
T_c : critical temp where we transition from one phase to another

$T < T_c$: spontaneous magnetization

$T > T_c$: loses its magnetization

Percolation Problem:

- geometric problem where a random addition of objects forms a contiguous path that spans the entire system
- suppose we have a lattice, composed of a periodic array of potential occupation sites



- sites are randomly occupied w/ some probability p
- clusters are formed by bonds that are drawn btwn NN

- calculate quantities

① P_{span} : probability of having ∞ cluster

$$\left.\begin{array}{l} \text{if } p < 0.5,\ P_{span} = 0 \\ \text{if } p > 0.5,\ P_{span} = 1 \end{array}\right\} \text{in 2D}$$

② $\pi(p, L)$: percolation probability

- probability there is a connected path btwn one side to another
- measure:
  - generate lattice $L \times L$
  - roll dice @ each bond
  - find clusters
  - check if spanning

probability of

- check if spanning

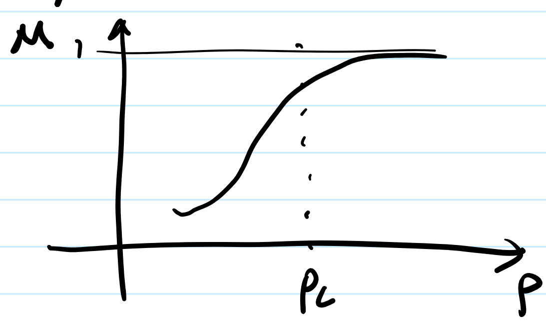
$$\Pi(p,L) = \sum_c \underbrace{\Pi(p, L, c)}_{\text{value of } \Pi \text{ for given config}} P(c)$$

probability of this config

(3) $M(p,L)$: if site belongs to a spanning cluster

- also known as order parameter
- measure:
  - count # sites in spanning cluster
  - for each site, see if part of spanning cluster

- if lattice is sparsely occupied, $M=0$ but as p increases, we reach percolation threshold, $\boxed{p_c}$.



- p_c : can be thought of a mathematical phase transition
  - back to P_{span}:

    if $p \le p_c$, $P_{span} = 0$
    if $p > p_c$, $P_{span} = 1$

- incorporate MC methods
  - begin w/ empty lattice, randomly fill lattice w random #s btwn 0 & 1
  - if # > p, then draw bond btwn NN
  - for large p, easier to start w/ full lattice & then remove bonds
  - calculate quantities