Monte Carlo Integration

Root equation

$$I = \int a(x)\,dx$$

designed

$$= \int \underbrace{\boxed{\frac{a(x)}{f(x)}}}_{h(x)} f(x)\,dx = E_{X\sim f(x)}\left[\frac{a(X)}{f(X)}\right]$$

memorize

$$X_1, X_2, \ldots, X_n \overset{iid}{\sim} f(x)$$

$$\hat{I} = \frac{1}{n}\sum_{i=1}^{n} \frac{a(X_i)}{f(X_i)}$$

Unnormalized Density

$$f(x) = \frac{1}{Z}\tilde{f}(x)$$

$$Z = \int \tilde{f}(x)\,dx$$

$$\int f(x)\,dx = 1$$

Physics: Gibbs Distribution (Boltzman)

$$f(x) = \frac{1}{Z} e^{-\frac{\mathcal{E}(x)}{T}}$$

$\mathcal{E}(x) \rightarrow$ energy function

$T \rightarrow$ temperature

$Z \rightarrow$ (also called partition function)

Last time: $f(x) = \frac{1}{Z} e^{-\frac{x^2}{2}}$

Special case: Unif(A)

$$P(x) = \begin{cases} \frac{1}{|A|} & x \in A \\ 0 & x \notin A \end{cases}$$

$$= \frac{1(X \in A)}{|A|}$$

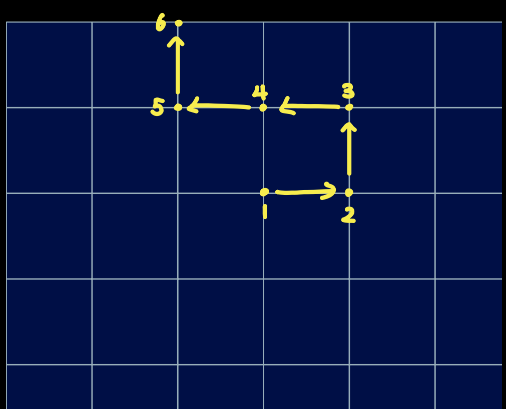
$1(X \in A) \rightarrow \hat{f}(x)$

$|A| \rightarrow Z$

unnormalized function

can approximate Z using root equation

Self avoiding walk



$$A = \left\{ \begin{matrix} \text{Paths of length } N \text{ that} \\ \text{are self-avoiding} \end{matrix} \right\}$$

$$P(X) = \frac{1(X \in A)}{|A|}$$

$$x = (X_1, X_2, X_3, \ldots X_N)$$

E.g. A = molecule configuration

$$x = (x_1, x_2, \dots, x_N)$$ input X are all coordinates

$$E_p = (|X_N - X_1|^2)$$ Euclidean distance

Suppose we want : $$|A| = \sum_{x \in \Omega} 1(x \in A)$$

$$(A \subset \Omega)$$

$$= \sum_{x \in \Omega} \frac{1(x \in A)}{q(x)} q(x)$$

each step is uniform
also includes shorter paths
where $x \notin A$

$$= E_{x \sim q(x)} \left[\frac{1(x \in A)}{q(x)} \right]$$

How do we generate $q(x)$?

$q(x)$ = Self-avoiding random walk.

Each x_i is sampled uniformly from available positions.

(stop if we get N points or there's no position available)

for $x \in A$, $x = (x_1, x_2, \dots, x_N)$

$$q(x) = \frac{1}{m_1} \cdot \frac{1}{m_2} \cdot \frac{1}{m_3} \cdots \frac{1}{m_{N-1}}$$

m_t is the # of available positions at time t

e.g. $m_1 = 4$

$m_2 = 3$

...... until $t = N-1$ or $m_t = 0$

Monte Carlo

- Repeatedly do self-avoiding random walk n times (1000) includes early stops
- Collect n_1 (800) paths of length N.

$$\{ \vec{x}^{(i)}, i = 1, \dots, n_1 \}$$

$$|\hat{A}| = \frac{1}{n} \sum_{i=1}^{n_1} \frac{1}{\frac{1}{m_1^{(i)}} \frac{1}{m_2^{(i)}} \cdots \frac{1}{m_{N-1}^{(i)}}}$$

$$= \frac{1}{n} \sum_{i=1}^{n_1} m_1^{(i)} m_2^{(i)} \dots m_{N-1}^{(i)}$$

(1) Discrete Case

$$I = \sum_{x \in \Omega} a(x)$$

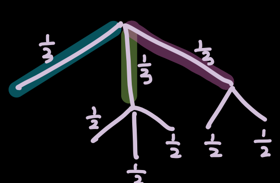
$$= \sum_{x \in \Omega} \frac{a(x)}{q(x)} q(x)$$

$$= E_{X \sim q(x)} \left[\frac{a(X)}{q(X)} \right]$$

How come different paths have different probabilities?
Because m is different for different paths

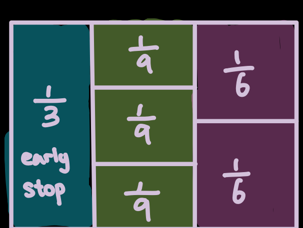
(2) Probability of path $q(x)$

q



\# of branches of length $2 = 5$

$P(\text{each branch of length } 2) = \frac{1}{5}$



$q(x)$

each block is a branch

$$E_p(|X_N - X_1|^2)$$

$$= \sum_{x \in A} |X_N - X_1| \, p(x)$$

$$= \sum_{x \in A} |X_N - X_1| \frac{1}{|A|}$$

$$= \frac{1}{|A|} \sum_{x \in A} |X_N - X_1|$$

$$= \frac{1}{|A|} \sum_{x \in A} \frac{|X_N - X_1|}{q(x)} \cdot q(x)$$

$$= \frac{1}{|A|} \cdot E_q \left[\frac{|X_N - X_1|}{q(x)} \right]$$

$\frac{1}{n}$ is cancelled

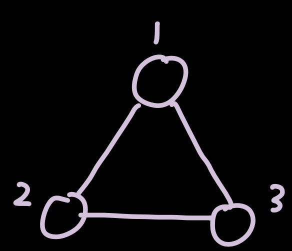
$$\approx \frac{1}{\sum_{i=1}^{n} m_1^{(i)} \cdots m_{N-1}^{(i)}} \sum_{i=1}^{n} |X_N^{(i)} - X_1^{(i)}| \, m_1^{(i)} m_2^{(i)} \cdots m_{N-1}^{(i)}$$

Part 3: MCMC

Markov Chain Monte Carlo

Markov chain / random walk

State space e.g.



Transition Probability

$$K_{ij} = P(X_{t+1} = j \mid X_t = i) \quad \text{(conditional prob.)}$$

X_{t+1}: state at t+1

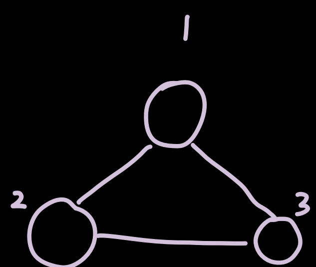
X_t: state at time t

Markov Property

future — Present — Past

$$P(X_{t+1} = j \mid X_t = i, X_{t-1}, X_{t-2}, \dots X_0)$$
$$= P(X_{t+1} = j \mid X_t = i)$$
$$X_{t+1} = h(X_t, U_t)$$

Example:



At each state, randomly flip a fair coin.

- head ⟶ stay
- tail ⟶ flip again
  - head ⟶ clockwise
  - tail ⟶ counter-clockwise

$$K = \begin{array}{c|ccc} i \backslash j & 1 & 2 & 3 \\ \hline 1 & \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ 2 & \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ 3 & \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \end{array}$$

transition matrix

Example:

$$X_0 = 1 \rightarrow X_1 \rightarrow X_2 \rightarrow \cdots$$

$$p_i^{(t)} = P(X_t = i)$$

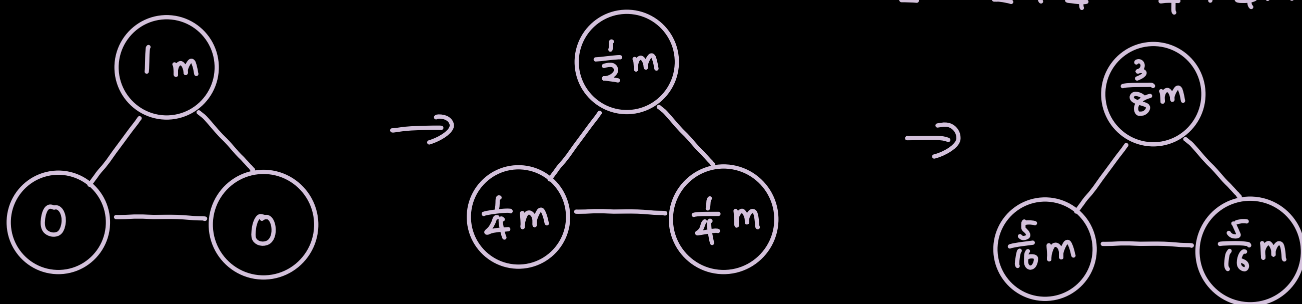
e.g. $p_3^{(2)} = P(X_2 = 3)$

Marginal Probability

Population migration

1 million people

$\frac{1}{2}m \times \frac{1}{2} + \frac{1}{4}m \times \frac{1}{4} + \frac{1}{4}m \times \frac{1}{4}$

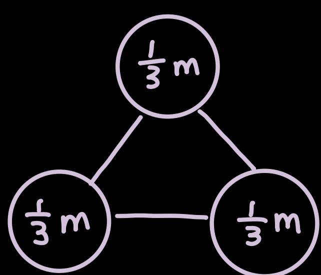


$t=0$ $t=1$ $t=2$

$p_3^{(t)} = P(X_2 = 3) = \frac{5}{16}$

eventually

$\cdots\cdots \longrightarrow$



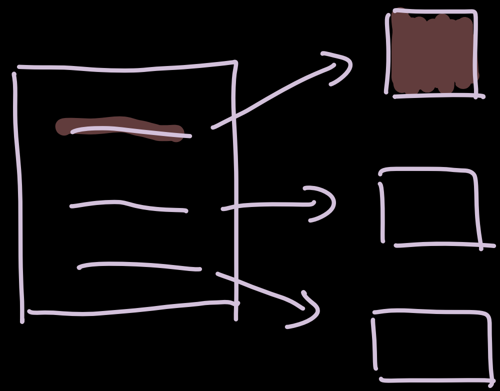
stationary distribution (equilibrium) π

$$p^{(t)} = (p_1^{(t)}\ p_2^{(t)}\ p_3^{(t)}) \rightarrow \pi = (\underset{\frac{1}{3}}{\pi_1}\ \underset{\frac{1}{3}}{\pi_2}\ \underset{\frac{1}{3}}{\pi_3})$$

Example: Google Page Rank

Each page is a state

Random Server



more popular

K_{ij}

$p^{(t)} \to \pi$ popularity

Page Rank : given K, calculate π

vs.

MCMC : given π, design K

(card shuffling)