

Markov Chain Monte Carlo (MCMC)

— Monte Carlo (Explain bio-math project)

Goal: Estimate $\mathbb{E}h(X)$

↑ ↑
function of interest high dimensional random vector.

Challenge • h is hard to compute and/or
• X has many states so

$\mathbb{E}h(X) = \sum_j h(x_j) \cdot P(X=x_j)$ is computationally prohibitive.

Soln: "simulate" several copies of $h(X)$

$$\mathbb{E}h(X) \approx \text{sample mean} = \frac{1}{n} \sum_{i=1}^n h(X_i)$$

↑
law of large #'s

↑
indep copy of X

Challenge: Sometimes producing a high-dim random vector is computationally infeasible.

Soln: MCMC Find an ^{irreducible} Markov chain w/ stationary dist π where $\pi_j = P(X=x_j)$. Take

$$\mathbb{E}h(X) \approx \frac{1}{n} \sum_{i=1}^n h(X_i) \quad (*)$$

↑
state of MC. after i steps

$$\pi_j = \lim_{n \rightarrow \infty} \left(\begin{array}{l} \text{proportion of time} \\ \text{state spends in state } j \end{array} \right)$$

$$\text{Thus, } \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n h(X_i) = \sum_j \pi_j \cdot h(x_j) = \sum_j P(X=x_j) \cdot h(x_j) = \mathbb{E}h(X)$$

i.e. RHS of $(*) \rightarrow \mathbb{E}h(X)$.

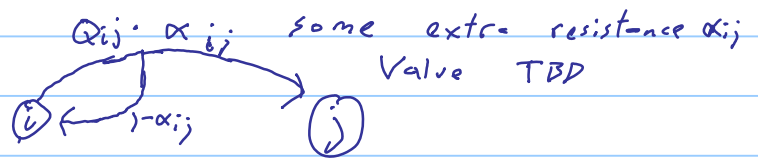
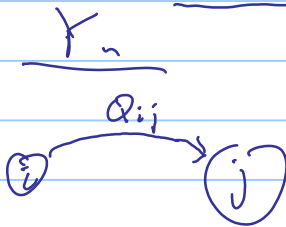
Key challenge: Given a stationary dist π ,
find a MC with that stationary dist.

Soln: Hastings-Metropolis algorithm.

Input: π , Q
non-zero entries \nearrow trans. matrix for some irreducible m.c. w/ commensurate state space. $(Y_n)_{n \geq 0}$

Output: Irreducible MC (X_n) w/ transition matrix P satisfying $\pi P = \pi$.

Works by adding "chute" to Y_n



$$P_{ij} = \begin{cases} Q_{ij} \cdot \alpha_{ij} \\ Q_{ii} + \sum_{j \neq i} Q_{ij} (1 - \alpha_{ij}) \end{cases}$$

Desire: $\pi_i P_{ij} = \pi_j P_{ji}$

$$\pi_i \cdot Q_{ij} \alpha_{ij} = \pi_j Q_{ji} \alpha_{ji} \quad (*)$$

Soln: $\alpha_{ij} = \min\left(\frac{\pi_j Q_{ji}}{\pi_i Q_{ij}}, 1\right)$

Indeed, if $\pi_j Q_{ji} \leq \pi_i Q_{ij}$

then $\alpha_{ij} = \frac{\pi_j Q_{ji}}{\pi_i Q_{ij}}$, $\alpha_{ji} = 1$ & (*) is satisfied.

Similarly if $\pi_j Q_{ji} > \pi_i Q_{ij}$.