

Lecture 7

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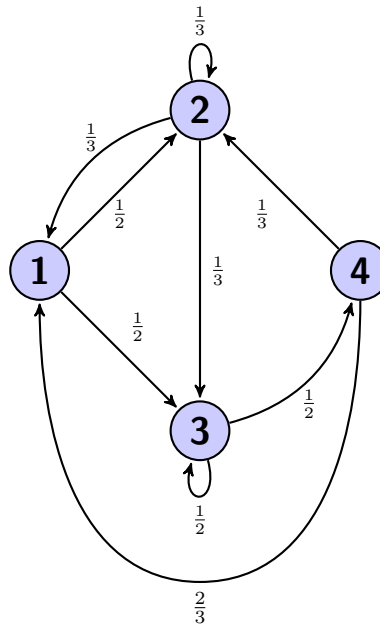
In this lecture we introduce Markov Chains and prove their property, mainly existence of unique stationary distribution. Then we present Metropolis-Hastings algorithm used for sampling vertices from graph using Markov Chains.

1 Markov Chains

A Markov Chain has a finite set of states and associated with them transition matrix P , such that P_{xy} is a probability of moving from x to y , where for each x $\sum_y P_{xy} = 1$. Markov Chains are often represented as a directed graph with each vertex representing a state and edge from x to y having weight P_{xy} .

Let $\pi \in [0, 1]^{|V|}$, $\pi^T \mathbf{1} = 1$ be initial probability distribution. Then πP^t is a probability distribution after t steps. It can be easily seen that πP^t is indeed a distribution, because it is non-negative and using induction $\pi P^t \mathbf{1} = \pi P^{t-1} P \mathbf{1} = \pi P^{t-1} \mathbf{1} = \pi \mathbf{1} = 1$.

1.1 Example of Markov Chain



The transition matrix associated with this Markov chain is:

$$P = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{2}{3} & \frac{1}{3} & 0 & 0 \end{pmatrix}$$

1.2 Properties of Markov Chains

Definition 1 Let $p^{(0)}$ be any initial distribution and let $p^{(t)}$ denote distribution after t steps, so $p^{(t)} = pP^{(t)}$. Then a long-term probability distribution is: $a^{(t)} = \frac{1}{t} (p^{(0)} + \dots + p^{(t-1)})$.

Definition 2 Markov Chain is connected if for each pair of states i, j there is a path from i to j .

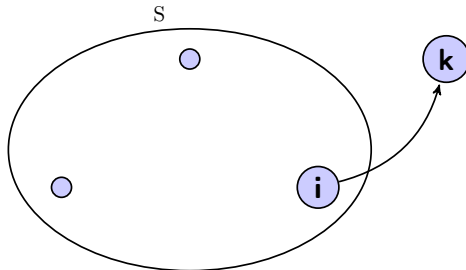
Definition 3 π is a stationary distribution if $\pi P = \pi$.

If π is a stationary distribution then π is left eigenvector of P with eigenvalue 1. P has no eigenvalue λ such that $|\lambda| > 1$, because otherwise let v be an eigenvector of P , so $vP^{(t)} = \lambda^{(t)} v$. Then $\|\lambda^{(t)}v\|_{\infty}$ is large, whereas all entries in $P^{(t)}$ are at most 1.

1.3 Fundamental theorem of Markov Chains

Lemma 4 Let P be a transition matrix of connected Markov Chain and let $A = [P - I, \mathbf{1}]$. Then $\text{rank}(A) = n$, where n is number of states in Markov Chain.

Proof $Ax = 0$ has a solution $\begin{pmatrix} \mathbf{1} \\ 0 \end{pmatrix}$. Let's assume that $\text{rank}(A) < n$. Then there is another solution $\begin{pmatrix} x \\ \alpha \end{pmatrix}$ which is orthogonal to $\begin{pmatrix} \mathbf{1} \\ 0 \end{pmatrix}$, in particular $\sum_i x_i = 0, x \neq \mathbf{0}$. Let's consider set S of largest entries in x . Because Markov Chain is connected, then there is some $i \in S, k \notin S$ such that there is an edge from i to k .



From $Ax = 0$ follows that $x_i = \sum_j P_{ij}x_j + \alpha$, so x_i is a convex combination of neighbour states of i . Because $x_k < x_i$ and $P_{ik} > 0$, then α must be greater than 0.

From similar argument for smallest entries in x follows that $\alpha < 0$, which is a contradiction. ■

Corollary 5 $\{\pi : \pi P = \pi\}$ has dimension at most 1.

Proof π such that $\sum_i \pi_i = 1$ is an eigenvector of P with eigenvalue 1 if and only if it is a solution of $\pi A = (0, 0, \dots, 0, 1)$. Because this system has $n + 1$ equations of rank n , then if there is any solution, it is unique. ■

Theorem 6 (Fundamental theorem of Markov Chains) *For a connected Markov Chain there exists a unique probability distribution π such that $\pi P = \pi$. Moreover for any initial distribution p^0 long-term probability distribution satisfies $\lim_{t \rightarrow \infty} a^{(t)} = \pi$.*

Proof Let $b^{(t)} = a^{(t)}P - a^{(t)} = \frac{1}{t}(p^{(1)} + \dots + p^{(t)}) - \frac{1}{t}(p^{(0)} + \dots + p^{(t-1)}) = \frac{1}{t}(p^{(t)} - p^{(0)})$. Because $|b^{(t)}| \leq \frac{2}{t}$, $a^{(t)}P - a^{(t)} = b^{(t)}$ converges to $\mathbf{0}$, so $a^{(t)}$ converges to such π that $\pi P = \pi$.

Uniqueness of this solution follows from Corollary 5. ■

1.4 Time-reversible Markov Chains

Definition 7 *Markov Chain is time-reversible if there exists $\pi, \sum \pi_i = 1$ such that $\forall_{i,j} \pi_i P_{ij} = \pi_j P_{ji}$.*

Theorem 8 *A connected time reversible Markov Chain has stationary distribution π , where π is a distribution from the definition of time-reversible Markov Chains.*

Proof π is a stationary distribution if $\forall_i \pi P^i = \pi_i$. But $\pi_i = \sum_j \pi_j P_{ij} = \sum_j \pi_j P_{ji} = \pi P^i$, so π is indeed a stationary distribution. ■

2 Application of Markov Chains

2.1 Metropolis Hastings

Let G be a huge graph and vol some weight function on vertices of G . We want to sample vertices from G with respect to vol , so the probability of choosing vertex i is $\pi_i = \frac{\text{vol}(i)}{\sum_j \text{vol}(j)}$. Because G is too big to calculate probabilities and

directly sample vertices, we need to create Markov Chain for walking through G .

Let d be largest degree of vertex in G . The transition matrix of Markov Chain will be as follows. The probability of going from i to neighbour j is $\frac{1}{d} \min\{1, \frac{\pi_j}{\pi_i}\} = \frac{1}{d} \min\{1, \frac{\text{vol}(j)}{\text{vol}(i)}\}$, and the probability of staying in i is $1 - \frac{1}{d} \sum_{j \in N(i)} \min\{1, \frac{\text{vol}(j)}{\text{vol}(i)}\}$.

This is a time-reversible Markov Chain, because $\pi_i P_{ij} = \frac{1}{d} \min\{\pi_i, \pi_j\} = \pi_j P_{ji}$. From Theorem 8 follows that π is a stationary distribution of Markov Chain, so random walk will converge to sampling vertices with respect to π .