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The Hitting and Cover Times of Metropolis Walks ⋆

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Abstract

Given a finite graph $G = (V, E)$ and a probability distribution $\pi = (\pi_v)_{v \in V}$ on V, Metropolis walks, i.e., random walks on G building on the Metropolis-Hastings algorithm obey a transition probability matrix $P = (p_{uv})_{u,v \in V}$ defined by, for any $u, v \in V$,

$$p_{uv} = \begin{cases} \frac{1}{d_u} \min\{\frac{d_u \pi_v}{d_v \pi_u}, 1\} & \text{if } v \in N(u), \\ 1 - \sum_{w \neq u} p_{uw} & \text{if } u = v, \\ 0 & \text{otherwise,} \end{cases}$$

and guarantee to have π as the stationary distribution, where $N(u)$ is the set of adjacent vertices of $u \in V$ and $d_u = |N(u)|$ is the degree of u. This paper shows that the hitting and the cover times of Metropolis walks are $O(fn^2)$ and $O(fn^2 \log n)$, respectively, for any graph G of order n and any probability distribution π such that $f = \max_{u,v \in V} \pi_u/\pi_v < \infty$. We also show that there are graph G and stationary distribution π such that *any* random walk on G realizing π attains $\Omega(fn^2)$ hitting and $\Omega(fn^2 \log n)$ cover times. It follows that the hitting and the cover times of Metropolis walks are $\Theta(fn^2)$ and $\Theta(fn^2 \log n)$, respectively.

Key words: Metropolis walks, Metropolis-Hastings algorithm, Markov chain Monte Carlo, random walk Monte Carlo, hitting time, cover time

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1 Introduction

Given a finite undirected graph $G = (V, E)$ and a transition probability matrix $P = (p_{uv})_{u,v \in V}$ such that $p_{uv} > 0$ only if $(u, v) \in E$, a random walk ω on G starting at a vertex $u \in V$ under P is an infinite sequence $\omega = \omega_0, \omega_1, \cdots$ of random variables ω_i whose domain is V, such that $\omega_0 = u$ with probability 1 and the probability that $\omega_{i+1} = w$ provided that $\omega_i = v$ is p_{vw} for $i = 0, 1, \cdots$. Random walks have attracted the attention of researchers in many fields (see general surveys e.g., [3,12,15,16]).

Let $N(u)$ and $d_u = |N(u)|$ be the set of vertices adjacent to a vertex $u \in V$, and the degree of u, respectively. Also we denote the *closed neighborhood* of u by $N[u]$, that is, $N[u] = N(u) \cup \{u\}$. We define a transition probability matrix $P_0 = (p_{uv})_{u,v \in V}$ by $p_{uv} = d_u^{-1}$ for any $u, v \in V$. Standard random walks that select the vertex to be visited next at random with the same probability, i.e., random walks under P_0, are a particularly popular research target because of their simplest nature. The hitting time $H_G(P; u, v)$ from $u \in V$ to $v \in V$ is the expected number of transitions necessary for random walk ω starting at u to reach v for the first time and the hitting time $H_G(P)$ of G is defined to be $H_G(P) = \max_{u,v \in V} H_G(P; u, v)$. The cover time $C_G(P; u)$ from $u \in V$ is the expected number of transitions necessary for random walk ω starting at u to visit all vertices in V and the cover time $C_G(P)$ of G is defined to be $C_G(P) = \max_{u \in V} C_G(P; u)$. Then $C_G(P_0) \leq 2m(n-1)$ holds for any graph G of order n and size m [1,2], whose result was later refined by Feige [6,7]:

$$(1 - o(1))n \log n \leq C_G(P_0) \leq (1 + o(1))\frac{4}{27}n^3.$$

Since there is a graph L (called a Lollipop) such that

$$H_L(P_0) = (1 - o(1))\frac{4}{27}n^3,$$

both the hitting and cover times of standard random walks are $\Theta(n^3)$ [4].

However, standard random walks are by no means the only random walks that are frequently used in applications. Markov chain Monte Carlo (MCMC) methods, which have been grown explosively since early 1990, are algorithms for sampling from probability distributions using random walks that have the target probability distributions as their stationary distributions [8]. Given a probability distribution $\pi = (\pi_u)_{u \in V}$ on a set V, typical MCMC methods first consider a graph $G = (V, E)$ such that edge set E represents a natural topology among the elements in V, and next design a transition probability matrix $P = (p_{uv})_{u,v \in V}$ on G such that $\pi P = \pi$ holds. Then the vertex visited after a sufficiently long random walk under P is used as a sample from π.

The Metropolis-Hastings algorithm produces such a transition probability matrix P, given π: For any $u, v \in V$,

$$p_{uv} = \begin{cases} q_{uv} \min\{\frac{q_{vu}\pi_v}{q_{uv}\pi_u}, 1\} & \text{if } v \in N(u), \\ 1 - \sum_{w \neq u} p_{uw} & \text{if } u = v, \\ 0 & \text{otherwise,} \end{cases}$$

where $Q = (q_{uv})_{u,v \in V}$ is an arbitrary transition probability matrix [9,14]. Since P satisfies the *detailed balance condition* $\pi_u p_{uv} = \pi_v p_{vu}$ for any $u, v \in V$, its stationary distribution is π.[1] When we take $Q = P_0$, the resulting transition probability matrix $P^* = (p_{uv})_{u,v \in V}$ is

$$p_{uv} = \begin{cases} \frac{1}{d_u} \min\{\frac{d_u\pi_v}{d_v\pi_u}, 1\} & \text{if } v \in N(u), \\ 1 - \sum_{w \neq u} p_{uw} & \text{if } u = v, \\ 0 & \text{otherwise,} \end{cases}$$

and random walks under P^* are called Metropolis walks, which are typical random walks used in MCMC. In what follows, we reserve symbol P^* to denote the transition probability matrix defined above.[2]

Let $f = \max_{u,v \in V} \pi_u/\pi_v$ and assume that $f < \infty$, i.e., $\pi_u > 0$ for all $u \in V$. This paper shows that the hitting and cover times of Metropolis walks are respectively $O(fn^2)$ and $O(fn^2 \log n)$, for any graph G of order n and probability distribution π such that $f < \infty$.

It is worth emphasizing that Metropolis walks use the degrees of adjacent vertices and improve the upper bounds on the hitting and cover times of standard random walks mentioned above. This impact of using local degree information was first observed by Ikeda et al. [11]. They proposed a transition probability matrix $P_1 = (p_{uv})_{u,v \in V}$ defined by, for any $u, v \in V$,

$$p_{uv} = \begin{cases} \frac{d_v^{-1/2}}{\sum_{w \in N(u)} d_w^{-1/2}} & \text{if } v \in N(u), \\ 0 & \text{otherwise,} \end{cases}$$

and showed that the hitting and cover times are respectively $O(n^2)$ and $O(n^2 \log n)$, for any graph G of order n. Metropolis walks, which are more flexible than Ikeda et al.'s walks (since their method cannot specify a target stationary distribution), still attain the same upper bounds on the hitting and cover times when $f = 1$.

[1] We can assume without loss of generality that the Markov chain defined by P is ergodic; if the chain does not include a self-loop, we can add self-loops at every vertex at a small constant probability.

[2] Since P^* depends on G and π, we could have denoted it as $P^*(G, \pi)$ for example. We however omit G and π, since they are obvious from context.

We then show that for any f, the upper bounds on the hitting and cover times of Metropolis walks are tight; Metropolis walks on a glitter star attain $\Omega(fn^2)$ hitting time and $\Omega(fn^2 \log n)$ cover time. Thus the hitting and cover times of Metropolis walks are respectively $\Theta(fn^2)$ and $\Theta(fn^2 \log n)$. It should be noted that this is shown by a much stronger result: there are stationary distributions π such that *any* random walk on a glitter star graph realizing π attains $\Omega(fn^2)$ hitting time and $\Omega(fn^2 \log n)$ cover time.

The paper is organized as follows: Section 2 shows upper bounds on the hitting and cover times of Metropolis walks, and Section 3 presents general lower bounds of random walks. Section 4 concludes the paper.

2 Upper Bounds

The following three lemmas are due to Ikeda et al [10,11]. Let $G = (V, E)$ and $P = (p_{uv})_{u,v \in V}$ be a graph and a transition probability matrix for G, respectively.

Lemma 1 [11] *For any two vertices $u \in V$ and $v \in N(u)$ adjacent each other,*

$$H_G(P; u, v) \leq (p_{vu}\pi_v)^{-1},$$

where $\pi = (\pi_u)_{u \in V}$ is the stationary distribution of P.

For any subset $U \subseteq V$ and vertex $u \in U$, let $C_G(P; U, u)$ be the expected number of transitions necessary for a random walk obeying P to visit all vertices in U starting at u, and let $C_G(P; U) = \max_{u \in U} C_G(P; U, u)$. By definition $C_G(P; u) = C_G(P; V, u)$ and $C_G(P) = C_G(P; V)$. The following lemma is thus a generalization of a famous theorem by Matthews, which relates the hitting and cover times [13].

Lemma 2 [10]

$$h(\ell - 1) \min_{u,v \in U, u \neq v} H_G(P; u, v) \leq C_G(P; U) \leq h(\ell - 1) \max_{u,v \in U, u \neq v} H_G(P; u, v),$$

where $\ell = |U|$ and $h(k)$ denotes the k-th harmonic number, i.e., $h(k) = \sum_{i=1}^{k} i^{-1}$.

Lemma 3 [11] *For any two vertices $u, v (u \neq v) \in V$, let $x_0 (= u), x_1, \cdots, x_\ell (= v)$ be a shortest path connecting u and v. Then*

$$\sum_{i=0}^{\ell} \deg(x_i) \leq 3n.$$

Let $\pi_{\min} = \min_{u \in V} \pi_u$ and $\pi_{\max} = \max_{u \in V} \pi_u$. Since $1 = \sum_{u \in V} \pi_u \le \sum_{u \in V} f\pi_{\min} = fn\pi_{\min}$, $\pi_u^{-1} \le fn$ for any $u \in V$.

Theorem 4 *For any graph $G = (V, E)$ with order n and probability distribution π on V, 1) $H_G(P^*) = O(fn^2)$, and 2) $C_G(P^*) = O(fn^2 \log n)$, where $f = \max_{u,v \in V} \pi_u/\pi_v$.*

PROOF. If $H_G(P^*) = O(fn^2)$ then $C_G(P^*) = O(fn^2 \log n)$ by Lemma 2. We thus concentrate on showing $H_G(P^*) = O(fn^2)$. That is, for any graph $G = (V, E)$, two vertices u_0 and v_0 in V, and probability distribution π on V, we show $H_G(P^*; u_0, v_0) = O(fn^2)$.

Let $u \in V$ and $v \in N(u)$. By the definition of P^*, $p_{vu}^{-1} = \max\{\frac{d_u \pi_v}{\pi_u}, d_v\}$. By Lemma 1, $H_G(P^*; u, v) \le \max\{\frac{d_u}{\pi_u}, \frac{d_v}{\pi_v}\}$. Since $\pi_u^{-1} \le fn$ and $\pi_v^{-1} \le fn$ as observed, $H_G(P^*; u, v) \le fn \max\{d_u, d_v\}$. Let $x_0 (= u_0), x_1, \cdots, x_\ell (= v_0)$ be any shortest path connecting u_0 and v_0. Then

$$H_G(P^*; u_0, v_0) \le \sum_{i=0}^{\ell-1} H_G(P^*; x_i, x_{i+1}) \le fn \sum_{i=0}^{\ell-1} \max\{d_{x_i}, d_{x_{i+1}}\},$$

which implies

$$H_G(P^*; u_0, v_0) \le 6fn^2 = O(fn^2)$$

by Lemma 3. □

3 Lower Bounds

A glitter star (see Figure 1) is a graph constructed from a star by inserting a vertex in each of the edges. Formally, a glitter star $S = (V, E)$ of order $n = 2\ell + 1$ is defined by $V = \{v^{(0)}\} \cup \{v_i^{(1)} : i = 1, 2, \cdots, \ell\} \cup \{v_i^{(2)} : i = 1, 2, \cdots, \ell\}$, and $E = \{(v^{(0)}, v_i^{(1)}) : i = 1, 2, \cdots, \ell\} \cup \{(v_i^{(1)}, v_i^{(2)}) : i = 1, 2, \cdots, \ell\}$.

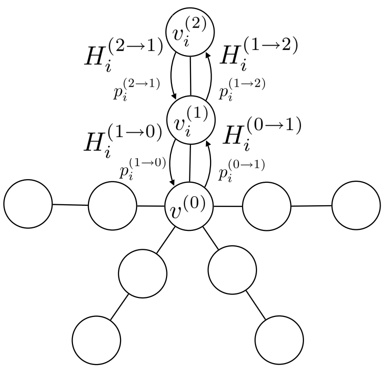

Fig. 1. Glitter-Star

We show that a glitter star graph S has $\Omega(fn^2)$ hitting time and $\Omega(fn^2 \log n)$ cover time for any transition probability (i.e., it is not necessarily to be the one of Metropolis walks) of some probability distribution π on V with $f = \max_{u,v \in V} \pi_u/\pi_v$.

Theorem 5 *There exists a stationary distribution π such that for any transition probability P realizing π, $H_S(P) = \Omega(fn^2)$ and $C_S(P) = \Omega(fn^2 \log n)$ hold.*

Before proving this theorem, we first show reversibility of a random walk on a tree. For a transition probability P of a random walk on a graph, its stationary distribution π is called *reversible* if it satisfies the detailed balanced condition:

$$p_{uv}\pi_u = p_{vu}\pi_v$$

holds for any $u, v \in V$. Also, a random walk is called *reversible* if its stationary distribution is reversible for its transition probability. It is known that a reversible random walk is characterized by *conductance* $(c_{uv})_{(u,v)\in E}$, where $c_{uv} = c_{vu}$ holds for each $(u, v) \in E$, as follows: Given a conductance $(c_{uv})_{(u,v)\in E}$, a random walk defined by $p_{uv} = c_{uv}/c_u$ has stationary distribution $\pi_u = c_u/c$, where $c_u = \sum_{w\in N[u]} c_{uw}$ and $c = \sum_{u\in V} c_u$ [5]. Conversely, a random walk defined by $p_{uv} = c_{uv}/c_u$ for some conductance $(c_{uv})_{(u,v)\in E}$ is reversible.

We show the following lemma.

Lemma 6 *Any random walk on a tree is reversible.*

PROOF. We show that, from any transition probability matrix P on a tree, a conductance $(c_{uv})_{(u,v)\in E}$ satisfying $p_{uv} = c_{uv}/c_u$ is constructed, which proves the lemma. For an arbitrary vertex r, suppose that T is rooted at r, which defines parent-child relations through the tree structure. We define a conductance $(c_{uv})_{(u,v)\in E}$ as follows: First let $c_{rv} := p_{rv}$ for every $v \in N[r]$. We define the other conductance values along the rooted tree structure. For a vertex v and its parent u, let us assume that c_{uv} has been determined. We then define the other conductance values on v by $c_{vw} = c_{uv}p_{vw}/p_{vu}$ for every $w \in N[v] \setminus \{u\}$. By going down to child vertices and continuing this procedure until reaching leaves, we obtain conductance $(c_{uv})_{(u,v)\in E}$. It is easy to see that $p_{uv} = c_{uv}/c_u$ holds for any $(u, v) \in E$ indeed. □

PROOF of Theorem 5. Suppose that a transition probability matrix $P = (p_{uv})_{u,v\in V}$ for S. Let us introduce the following abbreviations. For any $u = v^{(0)}$ and $v = v_i^{(1)}$, p_{uv} (resp. p_{vu}) is denoted by $p_i^{(0\to1)}$ (resp. $p_i^{(1\to0)}$) and $H_S(P; u, v)$ (resp. $H_S(P; v, u)$) by $H_i^{(0\to1)}$ (resp. $H_i^{(1\to0)}$). For any $u = v_i^{(h)}$ and

$v = v_i^{(k)}$ $(h \neq k)$, p_{uv} is denoted by $p_i^{(h\to k)}$ and $H_S(P; u, v)$ by $H_i^{(h\to k)}$. By definition, we have the following equalities.

$$
\begin{aligned}
H_i^{(2\to1)} &= p_i^{(2\to1)} + (1 - p_i^{(2\to1)})(1 + H_i^{(2\to1)}),\\
H_i^{(1\to0)} &= p_i^{(1\to0)} + p_i^{(1\to2)}(1 + H_i^{(2\to1)} + H_i^{(1\to0)}) + (1 - p_i^{(1\to0)} - p_i^{(1\to2)})(1 + H_i^{(1\to0)}),\\
H_i^{(0\to1)} &= p_i^{(0\to1)} + \sum_{j\neq i} p_j^{(0\to1)}(1 + H_j^{(1\to0)} + H_i^{(0\to1)}) + (1 - p_i^{(0\to1)} - \sum_{j\neq i} p_j^{(0\to1)})(1 + H_i^{(0\to1)}),\\
H_i^{(1\to2)} &= \frac{1}{p_i^{(1\to2)}}(1 + p_i^{(1\to0)} H_i^{(0\to1)}).
\end{aligned}
$$

From these equalities, we obtain the following:

$$
\begin{aligned}
H_i^{(2\to1)} &= \frac{1}{p_i^{(2\to1)}},\\
H_i^{(1\to0)} &= \frac{1}{p_i^{(1\to0)}}\left(1 + \frac{p_i^{(1\to2)}}{p_i^{(2\to1)}}\right),\\
H_i^{(0\to1)} &= \frac{1}{p_i^{(0\to1)}}\left(1 + \sum_{j\neq i}\frac{p_j^{(0\to1)}}{p_j^{(1\to0)}}\left(1 + \frac{p_j^{(1\to2)}}{p_j^{(2\to1)}}\right)\right),\\
H_i^{(1\to2)} &= \frac{1}{p_i^{(1\to2)}}\left(1 + \frac{p_i^{(1\to0)}}{p_i^{(0\to1)}}\left(1 + \sum_{j\neq i}\frac{p_j^{(0\to1)}}{p_j^{(1\to0)}}\left(1 + \frac{p_j^{(1\to2)}}{p_j^{(2\to1)}}\right)\right)\right).
\end{aligned}
\tag{1}
$$

We denote $\pi_{v^{(0)}}$ by $\pi^{(0)}$, and $\pi_{v_i^{(k)}}$ by $\pi_i^{(k)}$ for $i = 1, \dots, \ell$ and $k = 1, 2$. We prove this theorem by showing that the following stationary distribution π attains the lower bounds $\Omega(fn^2)$ and $\Omega(fn^2 \log n)$ on the hitting and cover times, respectively: $\pi^{(0)} = \pi_{\min}$ and $\pi_w = \pi_{\max}$ for any other vertices $w \in V \setminus \{v^{(0)}\}$.

As shown in Lemma 6, for any transition probability P of a random walk on glitter star S, its stationary distribution π is reversible. Thus from the detailed balanced condition and (1), we obtain

$$
H_i^{(0\to1)} = \frac{1}{p_i^{(0\to1)}}\left(1 + \sum_{j\neq i}\frac{\pi_j^{(1)}}{\pi^{(0)}}\left(1 + \frac{\pi_j^{(2)}}{\pi_j^{(1)}}\right)\right).
$$

Then, we have

$$
H_i^{(0\to1)} = \frac{1}{p_i^{(0\to1)}}\left(1 + \sum_{j\neq i} 2f\right) = \frac{1}{p_i^{(0\to1)}}\left(1 + 2f(\ell - 1)\right). \tag{2}
$$

Here, let us consider $U = \{v_i^{(1)} \mid p_i^{(0\to1)} \leq 2/\ell\}$. Note that U is not empty, and actually $|U| > \ell/2$ holds, otherwise $\sum_{i=1}^{\ell} p_i^{(0\to 1)} > 1$. Thus, for any $v_i^{(1)} \in U$, (2) is estimated as

$$H_i^{(0\to 1)} \geq \frac{\ell}{2}(1+2f(\ell-1)) \geq \frac{f(n-3)^2}{4} = \Omega(fn^2),$$

which shows the first part of the theorem.

As for the cover time, we consider $C_S(P;U)$. By Lemma 2, we have

$$C_S(U;P) \geq \min_{v_i^{(1)},v_j^{(1)}\in U} H(v_i^{(1)},v_j^{(1)})h(|U|-1).$$

Since $|U| > \ell/2$ and $H(v_i^{(1)},v_j^{(1)}) \geq H(v^{(0)},v_j^{(1)}) = f(n-3)^2/4$, we have

$$C_S(U;P) \geq \frac{f(n-3)^2}{4} h\left(\frac{\ell}{2}-1\right) = \Omega(fn^2 \log n),$$

which completes the proof. □

By combining Theorems 5 with Theorem 4, we obtain the following corollary.

Corollary 7 *$H_G(P^*) = \Theta(fn^2)$ and $C_G(P^*) = \Theta(fn^2 \log n)$.*

4 Conclusion

In this paper, we have shown that for any graph $G = (V,E)$ and probability distribution $\pi = (\pi_u)_{u\in V}$ on V, Metropolis walks, i.e., random walks obeying the transition probability matrix P^*, guarantee that the hitting time is $\Theta(fn^2)$ and the cover time is $\Theta(fn^2 \log n)$, where $f = \max_{u,v\in V} \pi_u/\pi_v$. Also we show that a glitter star graph has $\Omega(fn^2)$ hitting time and $\Omega(fn^2 \log n)$ cover time for any random walk realizing the stationary distribution π.

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