Random Walks on Rooted Trees

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Abstract

For arbitrary positive integers h and m, we consider the family of all rooted trees of height h having exactly m vertices at distance h from the root. We refer to such trees as (h, m)-trees. For a tree T from this family, we consider a simple random walk on T which starts at the root and terminates when it visits one of the m vertices at distance h from the root. Consider the problem of finding a tree in the family on which the expected time of a random walk is minimal (an extremal tree). In this paper we present some properties of extremal trees for arbitrary h and m, completely describe extremal $(2, m)$- and $(3, m)$-trees, describe a lower bound for the expected time of any $(4, m)$-tree, and refute the conjecture that the complete binary tree is extremal in the class of all $(h, 2^h)$-trees with the degree of the root at least 2.

Introduction

All missing definitions related to probability and Markov chains can be found in [2], and those related to graph theory can be found in [8].

Let the greatest distance of any vertex from the root, the *height of* T, be h. A vertex at a distance k, $0 \le k \le h$, from the root is said to be at *tier* k. An (h, m)-tree is a rooted tree of height h having exactly m vertices at tier h. Let $\Omega(T)$ be a set of all walks $W = v_0 v_1 \ldots v_n$ in T such that v_0 is the root, v_n is at tier h, and v_i is at tier h implies $i = n$. Let $d_T(u)$ denote the *degree* of a vertex u in T, i.e., the number of edges of T incident to u. We define the probability $\Pr\{W\}$ of a walk $W \in \Omega(T)$ to be equal to the product of $[d_T(v)]^{-1}$ for all vertices of a walk W, excluding the last.

Let X be a random variable representing the length of a walk in $\Omega(T)$, and let $E[X]$ be the expected value of X, i.e., $E[X] = \sum_{W \in \Omega(T)} \ell(W) \Pr\{W\}$, and we will refer to it as the *expected time* of a random walk. In this paper, we are concerned with the following:

Problem *Given two positive integers h and m, we wish to find an (h, m)-tree on which the expected time of a random walk is minimal. We refer to such a tree as being* extremal.

The above was considered by Lee [3] for the class of "spherically symmetric trees," that is, trees in which the degrees of all vertices at the same tier are the same. This reduces the analysis of the problem to that of a Markov process on a path of length h. Let us describe the case in which a complete solution (for spherically symmetric (h, m)-trees) was obtained. Suppose there exists a

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positive integer k such that $m = (k-1)^2 k^{h-3}$. Then the unique extremal tree (Lee tree) has the degree of the root and of vertices at tier h equal to 1, the degree of the vertices at tiers 1 and $h-1$ equal to k, and all other vertices of degree $k+1$. If such k does not exist, the expected time for the path still can be calculated for all m and this expected time provides a lower bound for the expected time for all spherically symmetric trees. It was shown that this bound is achieved if and only if $m = (k-1)^2 k^{h-3}$ and k is an integer. Problems related to random walks on various families of graphs were considered by many authors. Here we mention just [1] and references therein.

In this paper we present some properties of extremal trees for the class of *all* (h, m)-trees and *arbitrary* positive integers h and m (Section 1) as well as descriptions of the extremal tree for $h = 2, 3$ and all integer values of m (Section 2). Then we discuss the relationship between the expected time of the Lee tree and the expected time of any rooted tree of height 4 (Section 2).

In Section 3 we provide a counterexample to a conjecture which motivated our research (see [3] and references therein). A particular case of this conjecture, which we disprove, can be stated as follows: Among all $(h, 2^h)$-trees with the degree of the root at least two, the complete binary tree is the unique extremal tree. We close by stating a new conjecture.

1 General Results

We begin by exhibiting a simple operation on a tree that strictly decreases the expected time.

Lemma 1.1 *Let T be an (h, m)-tree. Let the tree T' be constructed by adding a vertex v at tier h and joining any vertex w at tier $h-1$ in T to v. Then, T' is an $(h, m+1)$-tree and $E[X'] < E[X]$.*

Proof. Let $d = d_T(w)$, then $d+1 = d_{T'}(w)$. Our proof is based on an idea known as coupling (see, e.g., [5]). We introduce a tree T^* that "couples" T and T'. T^* is created from T' by pruning v. The probabilities of moving from one vertex to another, however, will not change. In other words, in T^*, if u is a neighbor of w distinct from v, then the probability $p(w, u)$ of moving from vertex w to vertex u in one step is $\frac{1}{d+1}$. We would like to point out that a tree in the context of the coupling method is not just viewed as a graph but as a graph together with a probability distribution on its walks.

Let W be a walk in T' that does not visit v. It must have the exact same probability in T^* because these transition probabilities have not changed. So, what about walks that *do* visit v in T'? Such walks visit v only once, when they reach tier h. Let W be such a walk in T'. In order to have W correspond to a walk in T^*, we must distribute the remaining $\frac{1}{d+1}$ among the transition probabilities of exiting vertex w in T^*. We can distribute them in any way we choose to create a new tree T^{**}. As long as we increase the probability $p(w, u)$ where u is at tier h, then the expected time in tree T^{**} is less than the expected time in tree T'.

The validity of this point can be seen by traversing W in T' and its counterparts in T^{**} simultaneously. The walk W in T' must split into walks in T^{**} instead of visiting v. According to the distribution of the transition probabilities in T^{**}, some walks will conclude with one more step traversing some wu (where u is at tier h) instead of traversing wv. These walks will not change the expected time. But, some walks will return to the parent of w. This means that these walks will take at least 3 steps to complete after visiting w.

Without loss of generality, we choose to create T^{**} by equally distributing $\frac{1}{d+1}$ among the transition probabilities of exiting w. So, if u is one of the d neighbors of w in T^{**}, then $p(w,u) = \frac{1}{d+1} + \frac{1}{d(d+1)} = \frac{1}{d}$. Therefore, if X^{**} is a random variable representing the length of a simple random walk in T^{**}, $E\left[X^{**}\right] < E[X]$. It is clear, though, that $T^{**} = T$. Then, $E[X'] < E[X]$. □

By repeated application of this lemma, we obtain the following:

Corollary 1.2 *For a fixed h, let T_{m_i} be an extremal (h, m_i)-tree and X_{m_i} the length of a walk in $\Omega\left(T_{m_i}\right)$ for $i = 1, 2$. If $m_1 > m_2$, then $E\left[X_{m_1}\right] < E\left[X_{m_2}\right]$.*

We consider the class of all (h,m)-trees. A *leaf* in any graph is a vertex of degree 1, and an *internal leaf* in a rooted tree is a leaf at a tier other than 0 or h. The following lemma states that any random walk which enters an internal leaf is "wasting time."

Lemma 1.3 *An extremal tree has no internal leaves.*

Proof. The original proof of this lemma (see [6]) did not make use of the coupling method. As was suggested by David Wilson [7] we can again utilize coupling.

Let T be a tree with an internal leaf v with neighbor u and $T' = T \setminus \{v\}$. Let X be the random variable representing the length of a random walk on T and Y be the random variable representing the length of a random walk on T'. We wish to couple X and Y appropriately to show that $E[X] > E[Y]$. Let $W = w_0 w_1 w_2 \cdots w_L$ be a walk in $\Omega(T)$ and let W' be a walk in $\Omega(T')$. We say W "is coupled to" W' if the following procedure results in W': Whenever $w_i = v$ and $w_{i+1} = u$ then we delete both w_i and w_{i+1}.

It is trivial to observe that every walk in $\Omega(T)$ is coupled to exactly one walk in $\Omega(T')$. So we create a joint probability density function

$$\Pr{}_{X,Y}\{W, W'\} = \begin{cases} \Pr{}_X\{W\}, & \text{if } W \text{ is coupled to } W' \\ 0, & \text{otherwise.} \end{cases}$$

Note that

$$\begin{aligned} \sum_{W \in \Omega(T)} \Pr{}_{X,Y}\{W, W'\} &= \Pr{}_Y\{W'\} \\ \sum_{W' \in \Omega(T')} \Pr{}_{X,Y}\{W, W'\} &= \Pr{}_Y\{W\} \left(\frac{1}{1 - (\deg_T(u))^{-1}}\right)^{\eta_W(u)} = \Pr{}_X\{W\}, \end{aligned}$$

where $\eta_W(u)$ denotes the number of times that W visits u. So, we use this idea to compare the expectations of X and Y

$$\begin{aligned} E[X] &= \sum_{W \in \Omega(T)} \Pr{}_X\{W\} \ell(W) \\ &= \sum_{W \in \Omega(T)} \sum_{W' \in \Omega(T')} \Pr{}_{X,Y}\{W, W'\} \ell(W) \\ &\geq \sum_{W' \in \Omega(T')} \sum_{W \in \Omega(T)} \Pr{}_{X,Y}\{W, W'\} \ell(W') \end{aligned}$$

The inequality occurs because if W is not coupled to W', $\Pr_{X,Y}\{W, W'\} = 0$ and if W is coupled to W', $\ell(W) \geq \ell(W')$. So we have

$$E[X] \geq \sum_{W' \in \Omega(T')} \Pr_Y\{W'\}\ell(W') = E[Y].$$

And, in fact this inequality is strict because for each W' there exists at least one W (with positive probability) which is coupled to W' with $\ell(W) > \ell(W')$. $\square$

As a result, we shall from this point forward only consider trees without internal leaves. Our goal now is to prove Theorem 1.4.

Theorem 1.4 *The root of an extremal tree has degree 1.*

Proof. Suppose there is an extremal tree T where the root has degree d. T can be decomposed into d trees T_i, $1 \leq i \leq d$, each of height h and each with a root of degree 1. Let X_i be the random variable measuring the length of a walk in T_i. Without loss of generality, these indices can be chosen such that $E[X_1] \leq E[X_2] \leq \ldots \leq E[X_d]$.

We define $p_i^{0\to 0}$ to be the probability that a walk in $\Omega(T_i)$ returns to the root. In the tree T_i, let $E^{0\Rightarrow h}[X_i]$ denote the expected length of a walk given that the walk does not return to the root, and $E^{0\to 0}[X_i]$ denote the expected length of the first return to the root given that the walk does indeed return to the root. Then, by the law of total probability, we have

$$E[X_i] = \left(1 - p_i^{0\to 0}\right) E^{0\Rightarrow h}[X_i] + p_i^{0\to 0}\left(E^{0\to 0}[X_i] + E[X_i]\right) \tag{1}$$

We now turn our attention to the entire tree T. By the law of total probability according to the tree T_i in which the walk begins, we obtain

$$E[X] = \frac{1}{d}\sum_{i=1}^{d}\left[\left(1 - p_i^{0\to 0}\right) E^{0\Rightarrow h}[X_i] + p_i^{0\to 0}E^{0\to 0}[X_i] + p_i^{0\to 0}E[X]\right] \tag{2}$$

Solving the above equation for $E[X]$ and using (1), we get

$$E[X] = \frac{\sum_{i=1}^{d}\left[\left(1 - p_i^{0\to 0}\right) E^{0\Rightarrow h}[X_i] + p_i^{0\to 0}E^{0\to 0}[X_i]\right]}{\sum_{i=1}^{d}\left(1 - p_i^{0\to 0}\right)} = \frac{\sum_{i=1}^{d}\left[\left(1 - p_i^{0\to 0}\right) E[X_i]\right]}{\sum_{i=1}^{d}\left(1 - p_i^{0\to 0}\right)}, \tag{3}$$

which is a weighted average of the $E[X_i]$'s.

This implies that the expected time on one of the subtrees is at most that of the original tree if the root of the original tree is not a leaf. Adding vertices in the manner described by Corollary 1 strictly lessens the time. $\square$

2 Results for $h = 2, 3, 4$

In this section we collect our results on the problem in cases when $h = 2, 3, 4$.

Theorem 2.1 *(i) The extremal tree for $h = 2$ and any m is a star with $m + 2$ vertices, with the center of the star at tier 1. The expected time for this tree is $2 + \frac{2}{m}$.*

(ii) Let $h = 3$ and $m = k^2 + \alpha$, where $0 \leq \alpha \leq 2k$. Let t be the number of vertices at tier 2. If $0 \leq \alpha \leq k - 1$, $E[X]$ achieves its minimum only when $t = k$. If $k + 1 \leq \alpha \leq 2k$, $E[X]$ achieves its minimum only when $t = k + 1$. If $\alpha = k$, $E[X]$ achieves its minimum if and only if $t = k$ or $t = k + 1$. The minimum is

$$E[X] = \begin{cases} 3 + \frac{4}{k} + 2\frac{(k-\alpha)\left(1+\frac{2}{k}\right)}{k^3+2k^2+\alpha} & 0 \leq \alpha \leq k \\ 3 + \frac{4}{k} + 2\frac{(k-\alpha)\left(1+\frac{2}{k}\right)}{k^3+3k^2+k+\alpha} & k \leq \alpha \leq 2k. \end{cases}$$

Proof. The proof of (i) is a much shorter version than that of (ii) which we present below. By Theorem 1.4, the extremal tree has one vertex at tier 1. Its degree is denoted to be $t + 1$. If v_i is a vertex at tier 2, $1 \leq i \leq t$, then let the degree of v_i be d_i. Therefore, $\sum_{i=1}^{t} d_i = m + t$.

Let E_0 be the expected time of the walk initiated from the root of the tree. Let E_1 be the expected time of the walk initiated from the vertex at tier 1. Let $E_{2,i}$ be the expected time of the walk initiated from v_i at tier 2, $1 \leq i \leq t$. We have the following system of equations:

$$\begin{cases} E_0 &= 1 + E_1 \\ E_1 &= 1 + \frac{1}{t+1}E_0 + \frac{1}{t+1}\sum\limits_{i=1}^{t} E_{2,i} \\ E_{2,i} &= 1 + \frac{1}{d_i}E_1. \end{cases} \tag{4}$$

Solving these equations gives us the following expression for $E_0 = E[X]$:

$$E[X] = 1 + 2\left(\frac{t+1}{t - \sum_{i=1}^{t}\frac{1}{d_i}}\right).$$

For a fixed t, the sum $\sum_{i=1}^{t} d_i$ is fixed. Since each d_i is a positive integer, by Jensen's inequality, $\sum_{i=1}^{t}\frac{1}{d_i}$ is a minimum if and only if $\max\limits_{1\leq i\leq t}\{d_i\} - \min\limits_{1\leq i\leq t}\{d_i\} \leq 1$ and that this set of values of d_i's is unique. If we let $s = \lfloor\frac{m}{t}\rfloor$, then we obtain that an extremal graph contains $ts + t - m$ vertices of degree $s + 1$ and $m - ts$ vertices of degree $s + 2$ at tier 2.

Thus the minimum $E[X]$ is of the form $E[X] = 1 + 2\left(\frac{(t+1)(s+1)(s+2)}{m+ts(s+1)}\right)$, which for a fixed m is a function of t only. It can be shown that the minimum for $E[X]$ occurs when $t = k$ if $0 \leq \alpha \leq k - 1$, when $t = k + 1$ if $k + 1 \leq \alpha \leq 2k$, and when $t = k$ or $t = k + 1$ if $\alpha = k$. The proof is elementary. See Chapter 3 in [6] for all details. □

In the case of $h = 4$ and arbitrary m we fail to describe extremal $(4, m)$-trees, but if $m = (k-1)^2k$, where k is a positive integer, it can be shown that the Lee tree defined in Section 1 is the only extremal tree. Its expected time is $4 + \frac{6k-4}{(k-1)^2}$. It can also be shown that the function of k in the expression of the expected time on Lee tree serves as a lower bound for the expected time on an arbitrary $(4,(k-1)^2k)$-tree. This is achieved using elementary methods such as Jensen's inequality and Lagrange multipliers. The details can be found in [6].

3 Counterexample and Conjecture

The counterexample to the conjecture described at the end of Introduction was constructed in the following three steps.

1. Let H_1 and H_2 be two identical $(h,2^{h-1})$-trees with the degree of the root being 1. Let H be a tree obtained from H_1 and H_2 by identification of their roots. Then H is an $(h,2^h)$-tree with the root of degree 2. If $p_i^{0\to 0}$, $i=1,2$, denotes the probability that a walk in $\Omega(H_i)$ returns to the root, then $p_1^{0\to 0}=p_2^{0\to 0}$, $E[H_1]=E[H_2]$, and (2) implies

$$E[H]=\frac{(1-p_1^{0\to 0})E[H_1]+(1-p_2^{0\to 0})E[H_2]}{(1-p_1^{0\to 0})+(1-p_2^{0\to 0})}=E[H_1].$$

2. Consider an $(8,2^7)$-tree B_0 in which the root has degree 1 and each vertex at tiers 1 to 7 has exactly two children. By identifying roots of two copies of such tree, we obtain the complete binary $(8,2^8)$-tree B. From step 1, $E[B]=E[B_0]$.

3. Let C_0 be an $(8,2^7)$-tree given by Figure 1, and C be the tree obtained from two copies of C_0 by identifying their roots. From step 1, $E[C]=E[C_0]$. By direct computation, we have $E[B_0]=\frac{1281}{64}\approx 20.0156$ and $E[C_0]=\frac{176073}{8800}\approx 20.0083$, which implies $E[C]<E[B]$. Hence C is a counterexample.

The following new conjecture was motivated by the discussion in the last section, numerical evidence and [3].

Conjecture 3.1 *If k is a positive real root of the polynomial $f(x)=(x-1)^2x^{h-3}-m$, then*

$$E[X]\geq\frac{k+1}{k-1}h+\frac{4-2k}{(k-1)^2},$$

and this bound is achieved if and only if k is an integer.

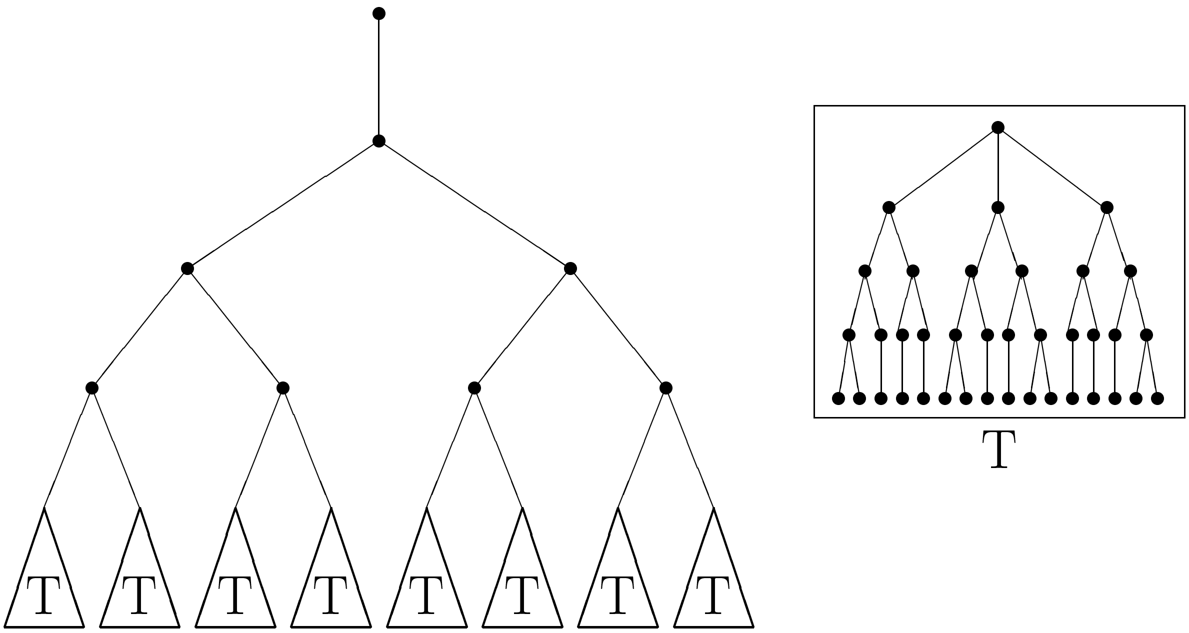

Figure 1: The tree C_0

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