

On the Multiplicative Zagreb Indices of Bucket Recursive Trees

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ABSTRACT

Bucket recursive trees are an interesting and natural generalization of ordinary recursive trees and have a connection to mathematical chemistry. In this paper, we give the lower and upper bounds for the moment generating function and moments of the multiplicative Zagreb indices in a randomly chosen bucket recursive tree of size n with maximal bucket size $b \geq 1$. Also, we consider the ratio of the multiplicative Zagreb indices for different values of n and b . All our results reduce to the ordinary recursive trees for $b = 1$.

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1. INTRODUCTION

Trees are defined as connected graphs without cycles. Recursive trees are rooted labelled trees, where the root is labelled by 1 and the labels of all successors of any node v are larger than the label of v [8]. It is of particular interest in applications to assume the random recursive tree model and to speak about a random recursive tree with n nodes, which means that one of the $(n-1)!$ possible recursive trees with n nodes is chosen with equal probability, i.e., the probability that a particular tree with n nodes is chosen is always $1/(n-1)!$. An interesting and natural generalization of random recursive trees has been introduced in [7], and these are called bucket recursive trees. In this model the nodes of a bucket recursive tree are buckets, which can contain up to a fixed integer amount of $b \geq 1$ labels. A probabilistic description of random bucket recursive trees is given by a generalization of the stochastic growth rule for ordinary random recursive trees (which is the special instance $b = 1$). In fact, a tree grows by progressive attraction of increasing integer labels: when inserting label $n+1$ into an existing bucket recursive tree containing n

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labels (i.e., containing the labels $\{1,2,\dots,n\}$) all n existing labels in the tree compete to attract the label $n+1$, where all existing labels have equal chance to recruit the new label. If the label winning this competition is contained in a node with less than b labels (an unsaturated bucket), label $n+1$ is added to this node, otherwise if the winning label is contained in a node with b labels already (a saturated bucket), label $n+1$ is attached to this node as a new bucket containing only the label $n+1$. Starting with a single bucket as the root node containing only the label 1, after $n-1$ insertion steps, where the labels $2,3,\dots,n$ are successively inserted according to this growth rule, results in a so called random bucket recursive tree with n labels and maximal bucket size b . For an existing bucket recursive tree T with n labels, the probability that a certain node $v \in T$ with capacity $1 \leq c(v) \leq b$ attracts the new label $n+1$ is equal to the number of labels contained in v , i.e., $c(v)/n$ (see [7]). Figure 1 illustrates a bucket recursive tree of size $n=11$ with maximal bucket size $b=2$. For a connection to chemistry, suppose n atoms in a dendrimer (a repetitively branched molecule) are stochastically labelled with integers $1,2,\dots,n$, then labelled atoms in a functional group can be considered as the labels of a bucket in a bucket recursive tree. It is obvious that the number of nodes (here buckets) in a bucket recursive tree T is less than n for $b > 1$. Thus we can show the size of the tree as a function of n and b . Let $h(b)$ be a real valued function of b , where $h(1) = 0$ and $h(b) \geq 1$ for all $b \geq 2$. Now, we can write the size of the tree as $n - h(b)$, i.e., $|V(T)| = n - h(b)$. We choose the function $h(b)$ in this form for relation between the bucket recursive trees and ordinary recursive trees.

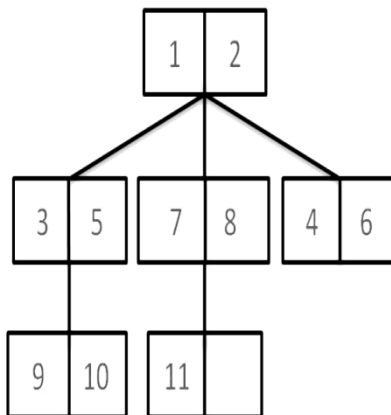


Figure 1: A bucket recursive tree of size 11 with maximal bucket size 2 [6].

Two vertices of graph G , connected by an edge, are said to be adjacent. The number of vertices of G , adjacent to a given vertex v , is the degree of this vertex, and will be denoted by $d(v)$. Todeschini *et al.* [9, 10] have suggested to consider multiplicative variants of additive graph invariants, which applied to the Zagreb indices

would lead to the multiplicative Zagreb indices of a graph G , denoted by $\Pi_1(G)$ and $\Pi_2(G)$, under the name first and second multiplicative Zagreb index, respectively. These are defined as

$$\Pi_1(G) = \prod_{v \in V(G)} (d(v))^2 \quad (1)$$

and

$$\Pi_2(G) = \prod_{uv \in E(G)} d(u)d(v), \quad (2)$$

where $V(G)$ and $E(G)$ are the vertex set and edge set of G , respectively [3].

In probability theory and statistics, the moment generating function of a random variable is an alternative specification of its probability distribution. Thus, it provides the basis of an alternative route to analytical results compared with working directly with probability density functions or cumulative distribution functions. There are particularly simple results for the moment generating functions of distributions defined by the weighted sums of random variables. Note, however, that not all random variables have moment generating functions.

Definition 1.1 The moment generating function of a random variable X is defined as

$$M_X(t) = \mathbf{E}(\exp(tX)), \quad t \in \mathbf{R},$$

wherever this expectation exists.

The reason for defining this function is that it can be used to find all the moments of the distribution. In fact,

$$M_X(t) = \sum_{k=0}^{\infty} \frac{\mu_k}{k!} t^k,$$

where μ_k ($k \geq 1$) is the k th moment of X , i.e., $\mu_k = \mathbf{E}(X^k)$ [1].

2. RESULTS

Let $d_n(v)$ denote the degree of bucket v in our model of size n with maximal bucket size b , and $Z_{1,n,b}$ be the first multiplicative Zagreb index. We also define M_n to be the sigma-field generated by the first n stages [1]. If label n is attached to an unsaturated bucket, then $Z_{1,n,b} = Z_{1,n-1,b}$. But if label n is attached to a saturated bucket, then by the stochastic growth rule of the tree and by definition of the first multiplicative Zagreb index,

$$\frac{Z_{1,n,b}}{Z_{1,n-1,b}} = \left(\frac{d_{n-1}(U) + 1}{d_{n-1}(U)} \right)^2, \quad (3)$$

where U is uniformly distributed on buckets set.

Theorem 2.1 Let $M(t) = \mathbf{E}(\exp(tZ_{1,n,b}))$ be the moment generating function of $Z_{1,n,b}$ of a bucket recursive tree of size n with maximal bucket size b . Then

$$M(t) \leq \exp \left(\left(4b^{\frac{1}{k}} \right)^{n-b-1} \left(\prod_{j=b+1}^{n-1} \frac{j-h(b)}{j} \right)^{\frac{1}{k}} t \right).$$

Proof. We have

$$M(t) = \sum_{k=0}^{\infty} \frac{\mu_{k,n,b}}{k!} t^k,$$

where $\mu_{k,n,b}$ ($k \geq 1$) is the k th moment of $Z_{1,n,b}$. For $k \geq 1$,

$$\begin{aligned} \mathbf{E}(Z_{1,n,b}^k | \mathbf{M}_{n-1}) &= \mathbf{E}(Z_{1,n,b}^k | d_{n-1}(v_j), j \leq n-1-h(b)) \\ &= \frac{Z_{1,n-1,b}^k}{n-1} \sum_{j=1}^{|\mathbf{V}(T_{n-1})|} \left(\frac{d_{n-1}(v_j) + 1}{d_{n-1}(v_j)} \right)^{2k} c(v_j), \end{aligned}$$

since $Z_{1,n-1,b}^k$ is \mathbf{M}_{n-1} -measurable and the label n is attached to any saturated bucket v of the already grown tree T_{n-1} with probability $\frac{c(v)}{n-1}$. Thus

$$\mathbf{E}(Z_{1,n,b}^k | \mathbf{M}_{n-1}) \leq \frac{n-1-h(b)}{n-1} 4^k b Z_{1,n-1,b}^k. \quad (4)$$

Taking expectation of the inequality (4):

$$\mu_{k,n,b} \leq 4^k b \frac{n-1-h(b)}{n-1} \mu_{k,n-1,b}, \quad k \geq 1. \quad (5)$$

Also $Z_{1,b+1,b} = 1$. Thus (5) leads to

$$\mu_{k,n,b} \leq (4^k b)^{n-b-1} \prod_{j=b+1}^{n-1} \frac{j-h(b)}{j} \quad (6)$$

and proof is completed.

If we replace t by $\ln t$, then we obtain the upper bound for the probability generating function [1].

Let $Z_{2,n,b}$ be the second multiplicative Zagreb index of a bucket recursive tree of size n with maximal bucket size b . Then by definition of the second multiplicative Zagreb index,

$$\frac{Z_{2,n,b}}{Z_{2,n-1,b}} = \left(\frac{d_{n-1}(U)+1}{d_{n-1}(U)} \right)^{d_{n-1}(U)} \times (d_{n-1}(U)+1). \quad (7)$$

Theorem 2.2 Let $N(t) = \mathbf{E}(\exp(tZ_{2,n,b}))$ be the moment generating function of $Z_{2,n,b}$ of a bucket recursive tree of size n with maximal bucket size b . Then

$$N(t) \geq \exp \left(\left(4b^{\frac{1}{k}} \right)^{n-b-1} \left(\prod_{j=b+1}^{n-1} \frac{j-h(b)}{j} \right)^{\frac{1}{k}} t \right).$$

Proof. Let $\gamma_{k,n,b}$ ($k \geq 1$) be the k th moment of $Z_{2,n,b}$ of a bucket recursive tree of size n with maximal bucket size b . For $k \geq 1$, similar to the first multiplicative Zagreb index,

$$\begin{aligned} \mathbf{E}(Z_{2,n,b}^k | M_{n-1}) &= \mathbf{E}(Z_{2,n,b}^k | d_{n-1}(v_j), j \leq n-1-h(b)) \\ &= \frac{Z_{2,n,b}^k}{n-1} \sum_{j=1}^{n-1-h(b)} \left(\frac{d_{n-1}(v_j)+1}{d_{n-1}(v_j)} \right)^{d_{n-1}(v_j)} \\ &\quad \times (d_{n-1}(v_j)+1)c(v_j). \end{aligned}$$

Thus

$$\mathbf{E}(Z_{2,n,b}^k | M_{n-1}) \geq \frac{n-1-h(b)}{n-1} 4^k b Z_{2,n-1,b}^k. \quad (8)$$

Taking expectation of the inequality (8):

$$\gamma_{k,n,b} \geq 4^k b \frac{n-1-h(b)}{n-1} \gamma_{k,n-1,b}, \quad k \geq 1.$$

Now, proof is completed just similar to the proof of Theorem 2.1.

In passing, we consider the ratio of the multiplicative Zagreb indices for different values of n and b .

Theorem 2.3 Suppose

$$Z_{t_1, t_2, n, b; k}^* = \frac{Z_{t_1, n, b}^k}{Z_{t_2, n, b}^k}, \quad t_i \in \{1, 2\}, t_1 \neq t_2$$

and

$$P_{t_1, t_2, n, b; k} = \mathbf{E}(Z_{t_1, t_2, n, b; k}^*).$$

Then

$$P_{2, 1, n, b; k} \geq \frac{4^k}{b^{n-b-1}} \prod_{j=b+1}^{n-1} \frac{j}{j-h(b)}$$

and

$$P_{1, 2, n, b; k} \leq \frac{b^{n-b-1}}{4^k} \prod_{j=b+1}^{n-1} \frac{j-h(b)}{j}.$$

Proof. We have $Z_{2, n, b}^k \geq Z_{2, n-1, b}^k$. Let $g(x) = x^{-1}$ for $x > 0$. Then g is convex because $g''(x) = 2x^{-3} \geq 0$ and by Jensen's inequality $\mathbf{E}\left(\frac{1}{X}\right) \geq \frac{1}{\mathbf{E}(X)}$. Thus

$$\begin{aligned} P_{2, 1, n, b; k} &= \mathbf{E}\left(\mathbf{E}\left(\frac{Z_{2, n, b}^k}{Z_{1, n, b}^k} \mid M_{n-1}\right)\right) \\ &\geq \mathbf{E}\left(\mathbf{E}\left(\frac{Z_{2, n-1, b}^k}{Z_{1, n, b}^k} \mid M_{n-1}\right)\right) \\ &\geq \mathbf{E}\left(Z_{2, n-1, b}^k \mathbf{E}\left(\frac{1}{Z_{1, n, b}^k} \mid M_{n-1}\right)\right) \\ &\geq \mathbf{E}\left(4^k Z_{2, n-2, b}^k \mathbf{E}\left(\frac{1}{Z_{1, n, b}^k} \mid M_{n-1}\right)\right) \\ &\geq \dots \geq 4^{k(n-b)} \mathbf{E}\left(\frac{1}{Z_{1, n, b}^k}\right) \\ &\geq 4^{k(n-b)} \frac{1}{\mu_{n, b, k}} \\ &\geq \frac{4^k}{b^{n-b-1}} \prod_{j=b+1}^{n-1} \frac{j}{j-h(b)}. \end{aligned}$$

With the same manner, we can obtain the upper bound for $P_{1, 2, n, b; k}$.

Theorem 2.4 Suppose

$$Z_{1, 2, n, b_1, b_2; k}^* = \frac{Z_{1, n, b_1}^k}{Z_{2, n, b_2}^k}, \quad Z_{2, 1, n, b_1, b_2; k}^* = \frac{Z_{2, n, b_1}^k}{Z_{1, n, b_2}^k}, \quad b_1 \neq b_2,$$

and

$$K_{1,2,n,b_1,b_2;k} = \mathbf{E}(Z_{1,2,n,b_1,b_2;k}^*), \quad S_{2,1,n,b_1,b_2;k} = \mathbf{E}(Z_{2,1,n,b_1,b_2;k}^*).$$

Then

$$K_{1,2,n,b_1,b_2;k} \leq 4^{k(b_2-b_1-1)} b_1^{n-b_1-1} \prod_{j=b_1+1}^{n-1} \frac{j-h(b_1)}{j},$$

and

$$S_{2,1,n,b_1,b_2;k} \geq \frac{4^{k(b_2-b_1+1)}}{b_2^{n-b_2-1}} \prod_{j=b_2+1}^{n-1} \frac{j}{j-h(b_2)}.$$

Proof. By definition of the conditional expectation,

$$\begin{aligned} K_{1,2,n,b_1,b_2;k} &= \mathbf{E} \left(\mathbf{E} \left(\frac{Z_{1,n,b_1}^k}{Z_{2,n,b_2}^k} \mid M_{n-1} \right) \right) \\ &\leq \mathbf{E} \left(\mathbf{E} \left(\frac{Z_{1,n,b_1}^k}{Z_{2,n-1,b_2}^k} \mid M_{n-1} \right) \right) \\ &\leq \dots \leq \frac{1}{4^{k(n-b_2)}} \mu_{n,b_1,k} \\ &\leq 4^{k(b_2-b_1-1)} b_1^{n-b_1-1} \prod_{j=b_1+1}^{n-1} \frac{j-h(b_1)}{j}. \end{aligned}$$

With the same manner, we can obtain the lower bound for $S_{2,1,n,b_1,b_2;k}$.

Corollary 2.5 The presented results in Theorem 4 reduce to the previous results in Theorem 2 for $b_1 = b_2 = b$.

Theorem 2.6 Suppose

$$Z_{t,i,b}^* = \frac{Z_{t,i,b}^k}{Z_{t,i-1,b}^k}, \quad t = 1, 2, \quad Z_{t,i,b} \neq Z_{t,i-1,b}$$

and

$$\mathbf{E}_{t,i,j,b} = \mathbf{E}(Z_{t,i,b}^* Z_{t,j,b}^*), \quad i < j.$$

Then

$$\mathbf{E}_{1,i,j,b,k} \leq \frac{(i-1-h(b))(j-1-h(b))}{(i-1)(j-1)} (4^k b)^2$$

and

$$\mathbf{E}_{2,i,j,b,k} \geq \frac{(i-1-h(b))(j-1-h(b))}{(i-1)(j-1)} (4^k b)^2.$$

Proof. From (4),

$$\begin{aligned}
\mathbf{E}_{1,i,j,b,k} &= \mathbf{E}(\mathbf{E}(Z_{1,i,b}^* Z_{1,j,b}^* \mid \mathbf{M}_{j-1})) \\
&= \mathbf{E}(Z_{1,i,b}^* \mathbf{E}(Z_{1,j,b}^* \mid \mathbf{M}_{j-1})) \\
&\leq 4^k b \frac{j-1-h(b)}{j-1} \mathbf{E}(Z_{1,i,b}^*) \\
&= 4^k b \frac{j-1-h(b)}{j-1} \mathbf{E}(\mathbf{E}(Z_{1,i,b}^* \mid \mathbf{M}_{i-1})) \\
&\leq \frac{(i-1-h(b))(j-1-h(b))}{(i-1)(j-1)} (4^k b)^2.
\end{aligned}$$

With the same manner, we can obtain the lower bound of $\mathbf{E}_{2,i,j,b,k}$.

We can study the ratio of the multiplicative Zagreb indices for different values of k as n and d are different with the above presented approach.

Corollary 2.7 For ordinary recursive trees,

$$\begin{aligned}
\mu_{k,n,1} &\leq 4^{k(n-2)}, & M(t) &\leq \exp(4^{n-2} t), \\
\gamma_{k,n,1} &\geq 4^{k(n-2)}, & N(t) &\geq \exp(4^{n-2} t)
\end{aligned}$$

Also, let $r, k \in [1, \infty]$ with $1/r + 1/k = 1$. By Holder's inequality,

$$\begin{aligned}
\mathbf{E}(Z_{1,n,b} Z_{1,m,b}) &\leq (\mu_{k,n,1})^{\frac{1}{k}} (\mu_{r,n,1})^{\frac{1}{r}} \\
&\leq 4^{m+n-4}.
\end{aligned}$$

Also

$$P_{1,2,n,1;k} \leq 4^{-k}, \quad P_{2,1,n,1;k} \geq 4^k$$

and

$$\mathbf{E}_{1,i,j,1,k} \leq 16^k, \quad \mathbf{E}_{2,i,j,1,k} \geq 16^k.$$

Then the bounds does not depend on i and j in ordinary recursive trees.

3. DISCUSSION AND CONCLUSION

So far, the multiplicative Zagreb indices have been studied vastly in literature from mathematical point of view. In this paper, we introduced the first probabilistic analysis of the multiplicative Zagreb indices in the random bucket recursive trees. Through the recurrence equations, an upper bound related to the first multiplicative Zagreb index and a lower bound related to the second multiplicative Zagreb index are obtained. As an interesting result it is shown that these bounds are the same in this model. It is difficult to

find a lower bound in Theorem 2.1 and an upper bound in Theorem 2.2, since the maximum degree of buckets of our model might not change for different values of n . However, we can study some probabilistic characteristics of these indices such as martingales, asymptotic normality and so on (see [4, 5, 6] for details). The lower and upper bounds for the moment generating function and moments are very important. For example, by Markov's inequality,

$$P(Z_{1,10,1} \geq 4^9) \leq \frac{1}{4}.$$

Eliasi *et al.* [2] considered a multiplicative version of the first Zagreb index defined as

$$\Pi_1^*(G) = \prod_{uv \in E(G)} (d(u) + d(v)).$$

With the same approach, we can obtain the lower and upper bounds related to this index. Generally, one can extend this approach to another indices and tree structures.

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