THE MODIFIED FORGOTTEN TOPOLOGICAL INDEX OF RANDOM $b$-ARY RECURSIVE TREES

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For any fixed integer $b \geq 2$, the $b$-ary recursive tree is a rooted, ordered, labeled tree where the out-degree is bounded by $b$, and the labels along each path beginning at the root increase. The modified forgotten topological index of a graph is defined as the sum of cubes of the vertex out-degrees of the graph. In this paper, we obtain the mean and variance of this index in random $b$-ary recursive trees.

Keywords: $b$-ary recursive tree, modified forgotten topological index, mean, variance

1. Introduction

Trees are defined as connected graphs without cycles, and their properties are basics of graph theory. A rooted tree is a tree with a countable number of nodes, in which a particular node is distinguished from the others and called the root node. Recursive trees are one of the most natural combinatorial tree models with applications in several fields, e.g., it has been introduced as a model for the spread of epidemics, for pyramid schemes, for the family trees of preserved copies of ancient texts and furthermore it is related to the Bolthausen-Sznitman coalescence model. A recursive tree with $n$ nodes is an unordered rooted tree, where the nodes are labelled by distinct integers from \{1, 2, 3, ..., $n$\} in such a way that the sequence of labels lying on the unique path from the root node to any node in the tree are always forming an increasing sequence [8].

For any fixed integer $b \geq 2$, the $b$-ary recursive tree is a rooted, ordered, labeled tree where the out-degree is bounded by $b$, and the labels along each path beginning at the root increase. There is a simple growth rule for the class of $d$-ary recursive trees. In this class, a random tree $T_n$, of order $n$, is obtained from $T_{n-1}$, a random tree of order $n-1$, by choosing a parent in $T_{n-1}$ and adjoining a node labeled $n$ to it. We explain the following evolution processes for random $b$-ary recursive trees of order $n$, which turns out to be appropriate when studying the forgotten topological index of these trees. The possible insertion positions to join a new node to a $b$-ary recursive tree, are called external nodes. In a $b$-ary recursive tree, the number of nodes can be attached to node $v$ of out-degree $\bar{d}_v$ is $b - \bar{d}_v$. Therefore the number of all external nodes in a $b$-ary recursive tree $T_n$ of order $n$ is $\sum_{v \in V(T_n)}(b - \bar{d}_v) = (b - 1)n + 1$. At step 1 the process starts with the root. At step $i$ the $i$-th node is attached to a previous node $v$ of the already grown $d$-ary recursive tree $T_{i-1}$ of order $i-1$ with probability $p_i(v) = \frac{b - \bar{d}_v}{(b - 1)(i - 1) + 1}$.

It is obvious that $\bar{d}_\text{root} = \bar{d}_\text{root}$ and for other vertices $\bar{d}_v = d_v - 1$. This fact specially implies that the higher outdegree vertices possess a lower attraction for new neighbors and there

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exists no vertex of outdegree greater than $b$. For more backgrounds for the random $b$-ary recursive trees, we refer the reader to [6] and [10].

2. Topological indices

A topological index for a (chemical) graph $G$ is a numerical quantity invariant under automorphisms of $G$. Topological indices and graph invariants based on the vertex degrees are widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activity of chemical compounds, and making their chemical applications.

The first variable Zagreb index of graph $G$ of order $n$ is defined by

$$M_n^\lambda = \sum_{i=1}^{n} d_{v_i}^{2\lambda},$$

where $\lambda$ is a real number and $d_{v_i}$ is the degree of vertex $v_i$ [1]. For different values of $\lambda$ there are the different names as follows:

1) The first Zagreb index,

$$Z_1^2(G) = M_1^1(G) = \sum_{i=1}^{n} d_{v_i}^{2}.$$  

2) The third Zagreb index or forgotten topological index,

$$Z_3^3(G) = M_3^{3/2}(G) = \sum_{i=1}^{n} d_{v_i}^{3}.$$  

3) The forth Zagreb index,

$$Z_4^4(G) = M_4^2(G) = \sum_{i=1}^{n} d_{v_i}^{4}.$$  

3) The fifth Zagreb index,

$$Z_5^5(G) = M_5^{5/2}(G) = \sum_{i=1}^{n} d_{v_i}^{5}.$$  

Furtula and Gutman [4] raised that the predictive ability of forgotten topological index is almost similar to that of first Zagreb index and for the acentric factor and entropy, and both of them obtain correlation coefficients larger than 0.95. This facts show some reasons that why forgotten topological index is useful for testing the chemical and pharmacological properties of drug molecular structures. Sun et al. [11] deduced some basic nature of forgotten topological index and reported that this index can reinforce the physico-chemical flexibility of Zagreb indices. Recently, Gao et al. [5] computed the forgotten topological index of some significant drug molecular structures.

Che and Chen [3] provided new lower and upper bounds of the forgotten topological index in terms of graph irregularity, Zagreb indices, graph size, and maximum/minimum vertex degrees. They characterized all graphs that attain the new bounds of F-index and showed that the new bounds are better than the bounds given in [4] for all benzenoid systems with more than one hexagon. For more information on topological indices, see [2, 9] and references therein.
3. Preliminaries

Let $\mathcal{F}_n$ be the sigma-field generated by the procedure of the first \( n \) internal nodes in random \( b \)-ary recursive trees and \( U_n \) be a randomly chosen node belonging to these trees of order \( n \) [7].

We use the modified Zagreb indices of a random \( b \)-ary recursive tree of order \( n \) as

\[
\mathcal{Z}_n^m(G) = \sum_{i=1}^{n} \mathcal{Z}_i^m, \quad m \geq 2.
\]

Set \( s_n = n(b-1) + 1 \) and using the gamma function define

\[
\beta[n, i] = \frac{\Gamma \left( \frac{nb-n+1}{b-1} \right)}{\Gamma \left( \frac{nb-n+1+1}{b-1} \right)}, \quad i \geq 1, \quad n \geq 2, \quad b \geq 2.
\]

4. The Main Results

**Lemma 4.1.** For each integer \( k \geq 1 \),

\[
\frac{\beta[n-1, k]}{\beta[n, k]} = 1 - \frac{k}{s_{n-1}}
\]

and

\[
\frac{\beta[n-1, 2k]}{\beta[n, 2k]} = 2 \frac{\beta[n-1, k]}{\beta[n, k]} - 1.
\]

**Proof.** Let \( \Gamma(\cdot) \) be the gamma function. We have \( \Gamma(x) = (x-1)\Gamma(x-1) \). Then

\[
\frac{\beta[n-1, k]}{\beta[n, k]} = \frac{(n-2+\frac{k}{b-1})(n-3+\frac{k}{b-1}) \cdots (1+\frac{k}{b-1})\Gamma \left( \frac{k}{b-1} \right)}{(n-3+\frac{k}{b-1})(n-4+\frac{k}{b-1}) \cdots (1+\frac{k}{b-1})\Gamma \left( \frac{k}{b-1} \right)}
\]

\[
= \frac{n-2 + \frac{k}{b-1}}{n-1 + \frac{k}{b-1}}
\]

\[
= 1 - \frac{k}{s_{n-1}}.
\]

The second equality is obvious. \( \square \)

**Theorem 4.1.** Let \( \mathcal{Z}_n^m \) be the modified Zagreb index of a random \( b \)-ary recursive tree of order \( n \). Then

\[
\mathbb{E}(\mathcal{Z}_n^m) = \frac{1}{\beta[n, m]} \sum_{k=1}^{n-1} \beta[k+1, m] \alpha_m[k, b], \quad m = 2, 3, 4, 5, \quad n \geq 3,
\]

where

\[
\alpha_2[k, b] = \frac{2b(k-1)}{s_k} + 1,
\]

\[
\alpha_3[k, b] = \frac{3b(k-1)}{s_k} \mathbb{E}(\mathcal{Z}_k^2) + \frac{3b(k-1)}{s_k} + 1,
\]

\[
\alpha_4[k, b] = \frac{4b - 6}{s_k} \mathbb{E}(\mathcal{Z}_k^4) + \frac{6b - 4}{s_k} \mathbb{E}(\mathcal{Z}_k^2) + \frac{4b(nk-1)}{s_k} + 1,
\]

\[
\alpha_5[k, b] = \frac{5b - 10}{s_k} \mathbb{E}(\mathcal{Z}_k^5) + \frac{10b - 10}{s_k} \mathbb{E}(\mathcal{Z}_k^3) + \frac{10b - 5}{s_k} \mathbb{E}(\mathcal{Z}_k^2) + \frac{5b(k-1)}{s_k} + 1.
\]
Proof. By stochastic growth role of the $b$-ary recursive tree,
\[ Z_n^2 = Z_{n-1}^2 + 2d_{U_{n-1}} + 1 \]
and
\[ Z_n^3 = Z_{n-1}^3 + 3d_{U_{n-1}}^2 + 3d_{U_{n-1}} + 1. \]
From Lemma 4.1,
\[ E(Z_n^2) = E(E(Z_n^2|F_{n-1})) = E(E(Z_{n-1}^2 + 2d_{U_{n-1}} + 1|F_{n-1})) = \frac{\beta[n - 1, 2]}{\beta[n, 2]} E(Z_{n-1}^2) + \alpha_2[n - 1, b]. \]
By iteration,
\[ E(Z_n^2) = \frac{1}{\beta[n, 2]} \sum_{k=1}^{n-1} \beta[k + 1, 2] \alpha_2[k, b], \]
since $Z_1^2 = 0$. Also,
\[ E(Z_n^3) = E(E(Z_n^3|F_{n-1})) = E(Z_{n-1}^3 + 3E(d_{U_{n-1}}^2|F_{n-1}) + 3E(d_{U_{n-1}}|F_{n-1}) + 1) = \frac{\beta[n - 1, 3]}{\beta[n, 3]} E(Z_{n-1}^3) + \alpha_3[n - 1, b]. \]
By iteration,
\[ E(Z_n^3) = \frac{1}{\beta[n, 3]} \sum_{k=1}^{n-1} \beta[k + 1, 3] \alpha_3[k, b]. \]
We have
\[ Z_n^4 = Z_{n-1}^4 + 4d_{U_{n-1}}^3 + 6d_{U_{n-1}}^2 + 4d_{U_{n-1}} + 1 \]
and
\[ Z_n^5 = Z_{n-1}^5 + 5d_{U_{n-1}}^4 + 10d_{U_{n-1}}^3 + 10d_{U_{n-1}}^2 + 5d_{U_{n-1}} + 1. \]
By the same manner, proof is completed. \(\square\)

Corollary 4.1. Let $Z_n^m$ for $m \geq 2$ be the modified Zagreb index of a random $b$-ary recursive tree of order $n$. Then
\[ E(Z_n^m) = \frac{1}{\beta[n, m]} \sum_{k=1}^{n-1} \beta[k + 1, m] \alpha_m[k, b], \quad n \geq 3, \]
where $\alpha_m[k, b]$ is a specific function of $n, b$ and $E(Z_n^t)$ for $t < m$.

Theorem 4.2. Let $Z_n^m$ be the modified Zagreb index of a random $b$-ary recursive tree of order $n$. Then
\[ E(Z_n^m) = f_m[b]n + O(1), \]
where

\[ f_2[b] = \frac{3b - 1}{b - 1}, \]
\[ f_3[b] = \frac{13b^2 - 9b + 2}{(b + 1)(b + 2)}, \]
\[ f_4[b] = \frac{75b^3 - 82b^2 + 37b - 6}{(b + 1)(b + 2)(b + 3)}, \]
\[ f_5[b] = \frac{541b^4 - 830b^3 + 575b^2 - 190b + 24}{(b + 1)(b + 2)(b + 3)(b + 4)}. \]

Proof. By definition of gamma function,

\[ \beta[n, b] = n^{\frac{1}{b - 1}}(1 + \mathcal{O}(n^{-1})). \]

It is not difficult to show that

\[ a_2[k, b] = \frac{3b - 1}{b - 1} + \mathcal{O}(n^{-1}), \]
\[ a_3[k, b] = \frac{13b^2 - 9b + 2}{(b + 1)(b + 1)} + \mathcal{O}(n^{-1}), \]
\[ a_4[k, b] = \frac{75b^3 - 82b^2 + 37b - 6}{(b + 1)(b + 2)(b + 1)} + \mathcal{O}(n^{-1}), \]
\[ a_5[k, b] = \frac{541b^4 - 830b^3 + 575b^2 - 190b + 24}{(b + 1)(b + 2)(b + 3)(b + 1)} + \mathcal{O}(n^{-1}). \]

Now, the proof is completed by Theorem 4.1.

Theorem 4.3. Let Cov\((\mathbb{Z}_n^2, \mathbb{Z}_n^3)\) be the covariance between \(\mathbb{Z}_n^2\) and \(\mathbb{Z}_n^3\). Then

\[
\text{Cov}(\mathbb{Z}_n^2, \mathbb{Z}_n^3) = \frac{1}{\beta[n, 3]} \sum_{k=1}^{n-1} \beta[k + 1, 3] \eta[k, b]
\]
\[
+ \left( \frac{2}{\beta[n - 1, 1]} \sum_{k=1}^{n-2} \beta[k + 1, 1] \frac{b}{s_k} + 1 - \mathbb{E}(Z_n^2) \right) \mathbb{E}(Z_n^3),
\]

where

\[ \eta[k, b] = \frac{3b(k - 1)}{s_k} \mathbb{E}(Z_k^2) + \left( \frac{3b(k - 1)}{s_k} + 1 \right) \mathbb{E}(Z_k^2). \]

Also,

\[ \text{Cov}(\mathbb{Z}_n^2, \mathbb{Z}_n^3) = \mathcal{O}(\mathbb{E}(Z_n^2)^4)). \]

Proof. Kazemi and Behtoei [7] showed that

\[ \mathbb{E}(\mathcal{U}_n) = \frac{1}{\beta[n, 1]} \sum_{i=1}^{n-1} \beta[i + 1, 1] \frac{b}{s_i}. \]

We have

\[ \mathbb{E}(\mathbb{Z}_n^2 \mathbb{Z}_n^3) = \mathbb{E}(\mathbb{Z}_{n-1}^2 \mathbb{Z}_n^3) + 2 \mathbb{E}(\mathcal{U}_{n-1} \mathbb{Z}_n^3) + \mathbb{E}(\mathbb{Z}_n^3). \]
Theorem 4.4. Let \( \text{Cov}(Z_n^3, Z_{n-1}^3) \) be the covariance between \( Z_n^3 \) and \( Z_{n-1}^3 \). Then

\[
\text{Cov}(Z_n^3, Z_{n-1}^3) = \frac{3(b-1)}{s_{n-1}} \text{Cov}(Z_{n-1}^3, Z_{n-1}^3) + \frac{\beta[n-1, 3]}{\beta[n, 3]} \text{Var}(Z_{n-1}^3).
\]

Proof. We have

\[
\text{Cov}(Z_n^3, Z_{n-1}^3) = \mathbb{E} \left[ (Z_n^3 - \mathbb{E}[Z_n^3]) (Z_{n-1}^3 - \mathbb{E}[Z_{n-1}^3]) \right]
= \mathbb{E} \left[ (Z_{n-1}^3 + \mathbb{E}[Z_{n-1}^3]) \mathbb{E} \left[ (Z_n^3 - \mathbb{E}[Z_n^3]) | \mathcal{F}_{n-1} \right] \right] \tag{1}
\]

Furthermore,

\[
\mathbb{E} \left[ (Z_n^3 - \mathbb{E}[Z_n^3]) | \mathcal{F}_{n-1} \right] = \frac{\beta[n-1, 3]}{\beta[n, 3]} (Z_{n-1}^3 - \mathbb{E}[Z_{n-1}^3])
+ \frac{3(b-1)}{s_{n-1}} (Z_{n-1}^3 - \mathbb{E}[Z_{n-1}^3]) \tag{2}
\]

Using the relations (1) and (2),

\[
\text{Cov}(Z_n^3, Z_{n-1}^3) = \mathbb{E} \left[ (Z_{n-1}^3 - \mathbb{E}[Z_{n-1}^3]) \left( \frac{\beta[n-1, 3]}{\beta[n, 3]} (Z_{n-1}^3 - \mathbb{E}[Z_{n-1}^3]) + \frac{3(b-1)}{s_{n-1}} (Z_{n-1}^3 - \mathbb{E}[Z_{n-1}^3]) \right) \right]
= \frac{3(b-1)}{s_{n-1}} \text{Cov}(Z_{n-1}^3, Z_{n-1}^3) + \frac{\beta[n-1, 3]}{\beta[n, 3]} \text{Var}(Z_{n-1}^3).
\]

Set

\[
A[k, b] = \frac{9b}{s_k} \mathbb{E}[Z_k^1] - \frac{9}{s_k} \mathbb{E}[Z_k^5] + \frac{9b}{s_k} \mathbb{E}[Z_k^2] \]

\[
- \frac{9}{s_k} \mathbb{E}[Z_k^5] + \frac{18b}{s_k} \mathbb{E}[Z_k^2] - \frac{18}{s_k} \mathbb{E}[Z_k^1]
\]
The modified forgotten topological index of random $b$-ary recursive trees

and

$$B[k, b] = \left[ \frac{3}{s_k} \left( (b - 1)E[Z_k^2] - E[Z_k^3] + b(k - 1) \right) \right]^2$$

$$- \frac{6(b - 1)Cov(Z_k^2, Z_k^3)}{s_k}, \quad k \geq 1.$$

**Theorem 4.5.** Let $\mathcal{Z}_n^3$ be the modified forgotten topological index of a random $b$-ary recursive tree of order $n$. Then

$$\text{Var}(\mathcal{Z}_n^3) = \frac{1}{\beta[n, 6]} \sum_{k=1}^{n-1} \beta[k + 1, 6] \gamma_3[k, b],$$

where

$$\gamma_3[k, b] = A[k, b] - B[k, b].$$

**Proof.** To computation variance of $\mathcal{Z}_n^3$, we have

$$(\mathcal{Z}_n^3 - \mathcal{Z}_{n-1}^3 - 1)^2 = 9(\mathcal{d}_{V_{n-1}} + \mathcal{d}_{V_{n-1}}^2)^2.$$

Then

$$E\left[ (\mathcal{Z}_n^3 - \mathcal{Z}_{n-1}^3 - 1)^2 | \mathcal{F}_{n-1} \right] = E\left[ 9 \left( \mathcal{d}_{V_{n-1}} + \mathcal{d}_{V_{n-1}}^2 \right)^2 | \mathcal{F}_{n-1} \right]$$

$$= 9 \sum_{k=1}^{n-1} \left( \mathcal{d}_k + 2\mathcal{d}_k^2 \right) \frac{b - \mathcal{d}_k}{s_{n-1}}$$

$$= \frac{9b}{s_{n-1}} Z_n^4 - \frac{9}{s_{n-1}} Z_n^5 + \frac{9b}{s_{n-1}} Z_n^6 - \frac{9}{s_{n-1}} Z_n^4 + \frac{9b}{s_{n-1}} Z_n^5 - \frac{18b}{s_{n-1}} Z_n^7 - \frac{18}{s_{n-1}} Z_n^7$$

Taking the expectation of both sides relation (3),

$$E\left[ (\mathcal{Z}_n^3 - \mathcal{Z}_{n-1}^3 - 1)^2 \right] = \frac{9b}{s_{n-1}} E[Z_n^4] - \frac{9}{s_{n-1}} E[Z_n^5] + \frac{9b}{s_{n-1}} E[Z_n^6]$$

$$- \frac{9}{s_{n-1}} E[Z_n^4] + \frac{18b}{s_{n-1}} E[Z_n^5] - \frac{18}{s_{n-1}} E[Z_n^7]$$

$$= A[n - 1, b].$$

It is not difficult to prove that

$$E[Z_n^2] - E[Z_{n-1}^2] - 1 = \frac{3}{s_{n-1}} \left[ (b - 1)E[Z_{n-1}^2] - E[Z_{n-1}^3] + b(n - 2) \right].$$

(5)

From (5) and Theorem 4.4,

$$E\left( Z_{3,n} - Z_{3,n-1} - 1 \right)^2 = E\left( Z_{3,n} - E[Z_{3,n}] - Z_{3,n-1} + E[Z_{3,n-1}] \right)^2$$

$$+ \left[ E[Z_{3,n}] - E[Z_{3,n-1}] - 1 \right]^2$$

$$= E\left( Z_{3,n} - E[Z_{3,n}] \right)^2 + E\left( Z_{3,n-1} - E[Z_{3,n-1}] \right)^2.$$
\[ - \left[ \mathbb{E}[Z_{3,n}] - \mathbb{E}[Z_{3,n-1}] - 1 \right]^2 - 2\text{Cov}(Z_{3,n}^3, Z_{3,n-1}^3) \]
\[ = \text{Var}(Z_{3,n}^3) + \text{Var}(Z_{3,n-1}^3) \left( 1 - 2 \frac{\beta[n-1,3]}{\beta[n,3]} \right) + B[n-1, b]. \]
\[ (6) \]

From Lemma 4.1, relations (4) and (6),
\[ \text{Var}(Z_{3,n}^3) = \frac{\beta[n-1,6]}{\beta[n,6]} \text{Var}(Z_{3,n-1}^3) + \gamma_3[k, b] \]
\[ (7) \]
By iteration, proof is completed.

**Corollary 4.2.** Let \( Z_n^m \) for \( m \geq 2 \) be the modified Zagreb index of a random \( b \)-ary recursive tree of order \( n \). Then
\[ \text{Var}(Z_n^m) = \frac{1}{\beta[n,2m]} \sum_{k=1}^{n-1} \beta[k+1,2m] \gamma_m[k, b], \quad n \geq 3, \]
where \( \gamma_m[k, b] \) is a specific function of \( n, b \).

**Corollary 4.3.** Let \( Z_n^3 \) be the modified forgotten topological index of a random \( b \)-ary recursive tree of order \( n \).
\[ \text{Var}(Z_n^3) = \sigma^2[b]n + O(1), \]
where \( \sigma^2[b] \) is a constant independent of \( n \).

**5. Conclusion**

In this paper, we obtained the mean and variance of the modified forgotten topological index of random \( b \)-ary recursive trees. As an open problem, it would be interesting to consider the asymptotic normality of this index via the martingale central limit theorem.

**REFERENCES**