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On the variable sum exdeg index of random tree structures

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Abstract. Through a recurrence equation, we determine the expectation and the variance of the variable sum exdeg index in random tree structures. Also, we show some convergence in probability based on this index. As the main result and through the martingale central limit theorem, the asymptotic normality of this index is given.

1. Introduction

Many topological indices have been introduced and studied on different graphs (see [1, 2, 7, 8, 13] and references therein). These studies have been done on deterministic structures and graphs with the lowest and highest values of these indices have been determined. On the other hand, the probabilistic study of these indices has received less attention due to the complexity of the calculations. Also, the probabilistic study is always accompanied by various restrictions during the investigation. One of these indices that has been studied less even in deterministic structures is the variable sum exdeg index. This index firstly introduced by Vukicević [11, 12] to predict some physicochemical properties of chemical compounds. Let G be a (finite, simple, and connected) graph with vertex set $V(G)$ and and edge set $E(G)$. The variable sum exdeg index of G is defined as

$$S_a(G) = \sum_{uv \in E(G)} (a^{d(u)} + a^{d(v)}) = \sum_{v \in V(G)} d(v) a^{d(v)},$$

where $a \in (0,1) \cup (1,\infty)$, and $d(v)$ is the degree of a vertex $v \in V(G)$. For more results on this index, refer to [3, 4, 9, 10] and references therein. The purpose of this article is to present the first probabilistic study of this index for domain $a \in (0,1)$. Lemma 2.1 specifies the reason for examining this index in this domain.

The paper is organized as follows. First, we show a recurrence for variable sum exdeg index of random tree, the expectation and variance are given. Then the asymptotic normality of this index, as the main result, is proved as the order of the tree grows to infinitely.

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2. Preliminaries

Using the gamma function, we define

$$\xi[n,k,a] = \frac{\Gamma(n)}{\Gamma(n+k(a-1))}, \qquad k \geq 0, \ \ n \geq 3, \ \ a \in (0,1).$$

The following lemma, despite its simplicity, plays a vital role throughout the paper.

Lemma 2.1. *For $k \geq 0$ and $a \in (0,1)$,*
1)

$$\frac{\xi[n-1,k,a]}{\xi[n,k,a]} = \frac{k(a-1)}{n-1} + 1.$$

2)

$$\frac{\xi[n-1,2k,a]}{\xi[n,2k,a]} = 2\frac{\xi[n-1,k,a]}{\xi[n,k,a]} - 1.$$

3) $\xi[n,k,a]$ is strictly increasing and $\xi[n,k,a] = n^{k(1-a)}(1+O(n^{-1}))$.

Proof. The proof is an immediate consequence of the definition of the gamma function and Stirling approximation. □

Examining the variable sum exdeg index requires examining another quantity. More precisely, determining the expectation and variance as well as the limiting behavior of the variable sum exdeg index are determined based on this quantity. In general, this quantity for a (finite, simple, and connected) graph G is defined as follows:

$$D_a(G) = \sum_{v \in V(G)} a^{d(v)}, \quad a \in (0,1).$$

Suppose that $D_{n,a} = \sum_{i=1}^{n} a^{d(v_i)}$, where $a \in (0,1)$, and $d(v_i)$ is the degree of a node v_i. Also, let $S_{n,a} = \sum_{i=1}^{n} d(v_i)a^{d(v_i)}$ be the variable sum exdeg index of random tree of order n. According to the rule of random tree growth, when the nth vertex is added to tree of order $n-1$, we have

$$\begin{aligned} D_{n,a} &= D_{n-1,a} + a^{d(V_{n-1})+1} - a^{d(V_{n-1})} + a \\ &= D_{n-1,a} + (a-1)a^{d(V_{n-1})} + a \end{aligned} \tag{1}$$

and

$$\begin{aligned} S_{n,a} &= S_{n-1,a} + (d(V_{n-1})+1))a^{d(V_{n-1})+1} - d(V_{n-1})a^{d(V_{n-1})} + a \\ &= S_{n-1,a} + (a-1)d(V_{n-1})a^{d(V_{n-1})} + a^{d(V_{n-1})+1} + a. \end{aligned} \tag{2}$$

See Figure 1 for the stochastic equations (1) and (2).

3. Expectations

To calculate the expectation of $\mathbb{E}(S_{n,a})$, we must first calculate the expectation of $\mathbb{E}(D_{n,a})$. Therefore, we prove the following lemma.

Lemma 3.1. *For $n \geq 3$,*

$$\mathbb{E}(D_{n,a}) = \frac{a}{\xi[n,1,a]} \sum_{j=1}^{n-1} \xi[j+1,1,a], \ \ a \in (0,1).$$

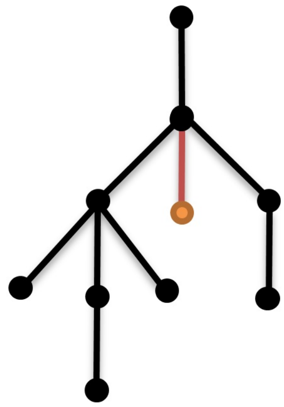

Figure 1: Random tree growth process. In this figure, the new vertex is shown with a different color.

Proof. Let $\mathcal{S}_n$ be the sigma-field generated by the first n stages of the tree structure and V_n be a randomly chosen vertex in the tree of order n with the conditional law [5]:

$$P(V_n = k|\mathcal{S}_{n-1}) = \frac{1}{n-1}, \quad k = 1, ..., n-1.$$

From relation (1), Lemma 2.1 (part 1) and law of iterated expectation,

$$\begin{aligned}
\mathbb{E}(D_{n,a}) &= \mathbb{E}(\mathbb{E}(D_{n,a}|\mathcal{S}_{n-1})) \\
&= \mathbb{E}\Big(\mathbb{E}\Big(\big(D_{n-1,a} + (a-1)a^{d(V_{n-1})} + a\big)|\mathcal{S}_{n-1}\Big)\Big) \\
&= \mathbb{E}\Big(D_{n-1,a} + (a-1)\sum_{k=1}^{n-1} a^{d(v_k)} P(V_n = k|\mathcal{S}_{n-1}) + a\Big) \\
&= \mathbb{E}(D_{n-1,a}) + \frac{a-1}{n-1}\mathbb{E}(D_{n-1,a}) + a \\
&= \Big(\frac{a-1}{n-1} + 1\Big)\mathbb{E}(D_{n-1,a}) + a \\
&= \frac{\xi[n-1,1,a]}{\xi[n,1,a]}\mathbb{E}(D_{n-1,a}) + a.
\end{aligned}$$

By iteration,

$$\mathbb{E}(D_{n,a}) = \frac{a}{\xi[n,1,a]}\sum_{j=1}^{n-1} \xi[j+1,1,a],$$

and $D_{2,a} = 2a$. □

Theorem 3.2. *We have*

$$\mathbb{E}(S_{n,a}) = \frac{1}{\xi[n,1,a]}\sum_{j=1}^{n-1} \xi[j+1,1,a]\alpha_1[j,a], \quad a \in (0,1), n \geq 3$$

where

$$\alpha_1[j,a] = \frac{a}{j}\mathbb{E}(D_{j,a}) + a, \quad j \geq 1.$$

Proof. From equality (2) and Lemma 3.1,

$$\begin{aligned}
\mathbb{E}(S_{n,a}) &= \mathbb{E}(\mathbb{E}(S_{n,a}|\mathcal{S}_{n-1})) \\
&= \mathbb{E}\Big(\mathbb{E}\Big(\Big(S_{n-1,a} + (a-1)d(V_{n-1})a^{d(V_{n-1})} + a^{d(V_{n-1})+1} + a\Big)|\mathcal{S}_{n-1}\Big)\Big) \\
&= \mathbb{E}\Big(S_{n-1,a} + (a-1)\sum_{k=1}^{n-1} d(V_{n-1})a^{d(V_{n-1})}P(V_n = k|\mathcal{S}_{n-1}) + a\sum_{k=1}^{n-1} a^{d(V_{n-1})}P(V_n = k|\mathcal{S}_{n-1}) + a\Big) \\
&= \mathbb{E}(S_{n-1,a}) + \frac{a-1}{n-1}\mathbb{E}(S_{n-1,a}) + \frac{a}{n-1}\mathbb{E}(D_{n-1,a}) + a \\
&= \Big(\frac{a-1}{n-1} + 1\Big)\mathbb{E}(S_{n-1,a}) + \frac{a}{n-1}\mathbb{E}(D_{n-1,a}) + a \\
&= \frac{\xi[n-1,1,a]}{\xi[n,1,a]}\mathbb{E}(S_{n-1,a}) + \alpha_1[n-1,a].
\end{aligned}$$

By iteration, proof is completed. □

Corollary 3.3. *From Lemma 2.1, Part (3), we have*

$$\mathbb{E}(S_{n,a}) = \frac{2a}{(2-a)^2}n + O(1), \qquad a \in (0,1),$$

since

$$\begin{aligned}
\mathbb{E}(D_{n,a}) &= \frac{a}{n^{1-a}}\int_0^n x^{1-a}dx + O(1) = \frac{a}{2-a}n + O(1), \\
\alpha_1[j,a] &= \frac{2a}{2-a} + O(1).
\end{aligned}$$

4. Variance

The main definition and direct method cannot be used to calculate the variance of $S_{n,a}$ because it is not possible to calculate the second order moment $\mathbb{E}(S_{n,a}^2)$. In the following method, there is no need to calculate the variance of $D_{n,a}$. Formally, a stochastic process is a martingale if $\mathbb{E}(X_n|\sigma(X_0,...,X_{n-1})) = X_{n-1}$ where $X_0, X_1, X_2, ...$ is a sequence of random variables. Therefore, first the following lemma is proved.

Lemma 4.1. *Assume $D_{n,a} = \mathbb{E}(D_{n,a})$. The sequence $\{\xi[n,1,a](S_{n,a} - \mathbb{E}(S_{n,a}))\}_{n\geq 1}$ is a martingale relative to the sigma-field $\mathcal{S}_{n-1}$ where $a \in (0,1)$.*

Proof. From Theorem 3.2,

$$\mathbb{E}(\xi[n,1,a](S_{n,a} - \mathbb{E}(S_{n,a}))|\mathcal{S}_{n-1}) = \xi[n-1,1,a](S_{n-1,a} - \mathbb{E}(S_{n-1,a})),$$

and by definition of a martingale proof is completed [5]. □

Set

$$\Phi_{n,a} := S_{n,a} - S_{n-1,a} - (a-1)d(V_{n-1})a^{d(V_{n-1})} - a, \qquad n \geq 3,\ a \in (0,1).$$

Then, with the approach used in the proof of Theorem 3.2,

$$\mathbb{E}(\Phi_{n,a}) = \mathbb{E}(\mathbb{E}(\Phi_{n,a}|\mathcal{S}_{n-1})) = \alpha_1[n-1,a] - a = \frac{a}{n-1}\mathbb{E}(D_{n-1,a}).$$

From relation (2),

$$\begin{aligned}\mathbb{E}(\Phi^2_{n,a}|\mathcal{S}_{n-1}) &= a^2\mathbb{E}(a^{2d(V_{n-1})}|\mathcal{S}_{n-1}) \\ &= a^2\sum_{k=1}^{n-1} a^{2d(v_k)}P(V_n = k|\mathcal{S}_{n-1}) \\ &= \frac{a^2}{n-1}D_{n-1,a^2}. \end{aligned} \tag{3}$$

Then

$$\mathbb{E}(\Phi^2_{n,a}) = \frac{a^2}{n-1}\mathbb{E}(D_{n-1,a^2}). \tag{4}$$

On the other hand, with simple but relatively long calculations,

$$\begin{aligned}\mathbb{E}(\Phi^2_{n,a}) &= \mathbb{E}\Big(\Big(\Phi_{n,a} - \mathbb{E}(S_{n,a}) + \mathbb{E}(S_{n,a}) - \mathbb{E}(S_{n-1,a}) + \mathbb{E}(S_{n-1,a})\Big)^2\Big) \\ &= \mathbb{V}ar(S_{n,a}) - 2\mathbb{E}((S_{n,a} - \mathbb{E}(S_{n,a}))(S_{n-1,a} - \mathbb{E}(S_{n-1,a}))) \\ &+ \mathbb{V}ar(S_{n-1,a}) + (\alpha_1[n-1,a] - a)^2. \end{aligned} \tag{5}$$

From Lemma 4.1,

$$\mathbb{E}((S_{n,a} - \mathbb{E}(S_{n,a}))(S_{n-1,a} - \mathbb{E}(S_{n-1,a}))) = \frac{\xi[n-1,1,a]}{\xi[n,1,a]}\mathbb{V}ar(S_{n-1,a}).$$

Hence, from part (2) in Lemma 2.1, the relation (5) leads to

$$\begin{aligned}\mathbb{E}(\Phi^2_{n,a}) &= \mathbb{V}ar(S_{n,a}) + \mathbb{V}ar(S_{n-1,a}) - 2\frac{\xi[n-1,1,a]}{\xi[n,1,a]}\mathbb{V}ar(S_{n-1,a}) + (\alpha_1[n-1,a] - a)^2 \\ &= \mathbb{V}ar(S_{n,a}) + \Big(1 - 2\frac{\xi[n-1,1,a]}{\xi[n,1,a]}\Big)\mathbb{V}ar(S_{n-1,a}) + \Big(\frac{a}{n-1}\mathbb{E}(D_{n-1,a})\Big)^2. \end{aligned} \tag{6}$$

Theorem 4.2. *Let $S_{n,a}$ be the variable sum exdeg index of random tree of order $n \geq 3$. Then*

$$\mathbb{V}ar(S_{n,a}) = \frac{1}{\xi[n,2,a]}\sum_{k=1}^{n-1}\xi[j+1,2,a]\alpha_2[j,a], \quad a \in (0,1)$$

where

$$\alpha_2[j,a] = \frac{a^2}{j}\mathbb{E}(D_{j,a^2}) - \Big(\frac{a}{j}\mathbb{E}(D_{j,a})\Big)^2, \quad j \geq 1.$$

Proof. From (4) and (6),

$$\mathbb{V}ar(S_{n,a}) = \Big(2\frac{\xi[n-1,1,a]}{\xi[n,1,a]} - 1\Big)\mathbb{V}ar(S_{n-1,a}) + \frac{a^2}{n-1}\mathbb{E}(D_{n-1,a^2}) - \Big(\frac{a}{n-1}\mathbb{E}(D_{n-1,a})\Big)^2.$$

Now, from part (2) in Lemma 2.1,

$$\mathbb{V}ar(S_{n,a}) = \frac{\xi[n-1,2,a]}{\xi[n,2,a]}\mathbb{V}ar(S_{n-1,a}) + \alpha_2[n-1,a].$$

By iteration and just similar to proof of Theorem 3.2, proof is completed . □

Corollary 4.3. *From Lemma 2.1, Part (3), and similar to Corollary 3.3, we have*

$$\mathbb{V}ar(S_{n,a}) = \sigma_2^2(a)n + O(1),$$

where $\sigma_2^2(a) = \frac{2a^4(a-1)^2}{(2a-3)(a-2)^2(a^2-2)}$ *and* $a \in (0,1)$.

Figure 2 shows the behavior $\sigma_2^2(a)$ for domain $a \in (0,1)$.

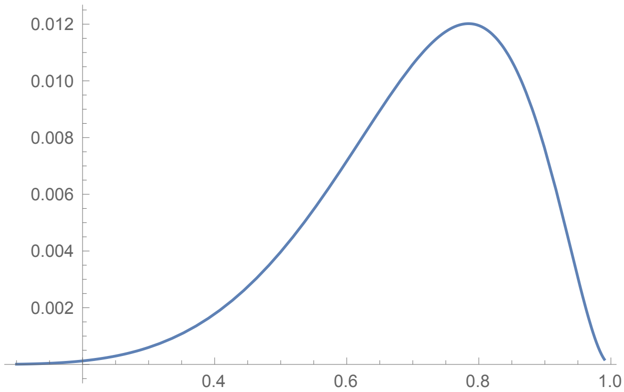

Figure 2: Behavior $\sigma_2^2(a)$ for domain $a \in (0,1)$.

5. Limiting rules

Suppose that $\xrightarrow{P}$ represents convergence in probability [5].

Theorem 5.1. *As $n \to \infty$,*

$$\frac{S_{n,a}}{n} \xrightarrow{P} \frac{2a}{(2-a)^2}, \qquad a \in (0,1).$$

Proof. The claim is a consequence of Corollary 4.3 and Chebyshev's inequality. □

Lemma 5.2. *As $n \to \infty$,*

$$n^{3-2a} \sum_{k=2}^{n} \frac{\xi[k,1,a]^2}{k-1}\Big(S_{k-1,a} - \mathbb{E}(S_{k-1,a})\Big) \xrightarrow{P} 0, \qquad a \in (0,1).$$

Proof. We have

$$\sum_{k=2}^{n} \frac{\xi[k,1,a]^2}{\xi[k-1,1,a](k-1)} = O(n^{1-a}),$$

and

$$\begin{aligned}\mathbb{E}\Big(\max_{2\le k\le n}\Big(\xi[k-1,1,a]\big(S_{k-1,a} - \mathbb{E}(S_{k-1,a})\big)\Big)^2\Big) &\le \xi[n,1,a]^2 \mathbb{V}ar(S_{n,a}) \\ &= O(n^{3-2a}).\end{aligned}$$

For any $\varepsilon > 0$, by Chebyshev's inequality,

$$\begin{aligned}&P\Big(\sum_{k=2}^{n} \frac{\xi[k,1,a]^2}{k-1}\big(S_{k-1,a} - \mathbb{E}(S_{k-1,a})\big) > \varepsilon n^{2a-3}\Big) \\ &\le \frac{1}{\varepsilon^2 n^{2(2a-3)}} \mathbb{E}\Big(\sum_{k=2}^{n} \frac{\xi[k,1,a]^2}{k-1}\big(S_{k-1,a} - \mathbb{E}(S_{k-1,a})\big)\Big)^2 \\ &\le \frac{1}{\varepsilon^2 n^{2(2a-3)}} \Big(\sum_{k=2}^{n} \frac{\xi[k,1,a]^2}{\xi[k-1,1,a](k-1)}\Big)^2 \mathbb{E}\Big(\max_{2\le k\le n}(\xi[k-1,1,a](S_{k-1,a} - \mathbb{E}(S_{k-1,a}))\Big)^2 \\ &= O(n^{-1}),\end{aligned}$$

and the proof is completed. □

Now the conditions are ready to prove the main result. Suppose that $\xrightarrow{D}$ represents convergence in distribution and $N(\mu, \sigma^2)$ is the normal random variable with mean μ and variance σ^2 [5].

Theorem 5.3. *As $n \to \infty$,*

$$S^*_{n,a} = \frac{S_{n,a} - \frac{2a}{(2-a)^2}n}{\sqrt{\frac{2a^4(a-1)^2}{(2a-3)(a-2)^2(a^2-2)}n}} \xrightarrow{D} N(0,1), \quad a \in (0,1).$$

Proof. To show the asymptotic normailty of the variable sum exdeg index, we introduce an appropriate martingale difference sequence. We define

$$W_{k,a} = \xi[k,1,a](S_{k,a} - \mathbb{E}(S_{k,a})) - \xi[k-1,1,a](S_{k-1,a} - \mathbb{E}(S_{k-1,a})),$$

with $W_{1,a} = 0$. It is abvious that the process $\{W_{k,a}\}_{k\geq 1}$ is a martingale difference sequence. By expression of the $\mathbb{V}ar(S_{n,a})$, we should prove that, for any $\varepsilon > 0$ [5]:

$$\frac{1}{\xi[n,1,a]^2\sigma_2^2(a)n}\sum_{k=2}^{n}\mathbb{E}(W_{k,a}^2|\mathcal{S}_{k-1})) \xrightarrow{P} 1$$

and

$$\frac{1}{\xi[n,1,a]^2 n}\sum_{k=2}^{n}\mathbb{E}\Big(W_{k,a}^2 I\Big(\Big|\frac{W_{k,a}}{\xi[n,1,a]\sqrt{n}}\Big| > \varepsilon\Big)\Big|\mathcal{S}_{k-1}\Big) \xrightarrow{P} 0. \tag{7}$$

We have (considering the conditional expectation in relation (6)):

$$\begin{aligned}\mathbb{E}(\Phi_{k,a}^2|\mathcal{S}_{n-1}) &= \mathbb{E}\Big((S_{k,a} - \mathbb{E}(S_{k,a}))^2|\mathcal{S}_{n-1}\Big)\\ &+ \Big(1 - 2\frac{\xi[k-1,1,a]}{\xi[k,1,a]}\Big)(S_{k-1,a} - \mathbb{E}(S_{k-1,a}))^2 + \Big(\frac{a}{k-1}D_{k-1,a}\Big)^2.\end{aligned} \tag{8}$$

Thus, from (3),

$$\mathbb{E}\Big((S_{k,a} - \mathbb{E}(S_{k,a}))^2|\mathcal{S}_{n-1}\Big) = \frac{a^2}{k-1}D_{k-1,a^2} - \Big(1 - 2\frac{\xi[k-1,1,a]}{\xi[k,1,a]}\Big)(S_{k-1,a} - \mathbb{E}(S_{k-1,a}))^2 - \Big(\frac{a}{k-1}D_{k-1,a}\Big)^2.$$

Now, from Lemma 2.1, part (1),

$$\begin{aligned}\sum_{k=2}^{n}\mathbb{E}(W_{k,a}^2|\mathcal{S}_{n-1}) &= \sum_{k=2}^{n}\Big(\xi[k,1,a]^2\mathbb{E}\Big((S_{k,a} - \mathbb{E}(S_{k,a}))^2|\mathcal{S}_{n-1}) - \xi[k-1,1,a]^2(S_{k-1,a} - \mathbb{E}(S_{k-1,a}))^2\Big)\\ &= \sum_{k=2}^{n}\frac{a^2\xi[k,1,a]^2}{k-1}D_{k-1,a^2} - (a-1)^2\sum_{k=2}^{n}\frac{\xi[k,1,a]^2}{(k-1)^2}(S_{k-1,a} - \mathbb{E}(S_{k-1,a}))^2\\ &- \sum_{k=2}^{n}\frac{a^2\xi[k,1,a]^2}{(k-1)^2}D_{k-1,a}^2.\end{aligned}$$

Hence, by Lemmas 2.1 and 5.2,

$$\frac{1}{\xi[n,1,a]^2\sigma_2^2(a)n}\sum_{k=2}^{n}\mathbb{E}(W_{k,a}^2|\mathcal{S}_{k-1}) \xrightarrow{P} 1 - 0 - 0 = 1.$$

Also, from relation (2) and the expectation of $S_{n,a}$, we can rewrite $W_{k,a}$ as

$$W_{k,a} = \xi[k,1,a]\Big((a-1)d(V_{k-1})a^{d(V_{k-1})} + a^{d(V_{k-1})+1} + a - \frac{a-1}{k-1}S_{k-1,a} - \alpha_1[k-1,a]\Big).$$

Also, there exist a positive constant c_a (only depends on a) such that

$$\max_{2\leq k\leq n} |W_{k,a}| \leq c_a \xi[n,1,a] = o(\xi[n,1,a]\sqrt{n}),$$

which implies that convergence in (7) is holds (see [5] for more details). □

6. Conclusion

In this article, the probabilistic properties of the variable sum exdeg index of random tree structures were investigated. Due to the dependence of these random variables (dependency on the order of the tree structure) through Martingale's central limit theorem, the asymptotic normality of this index was shown.

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