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Investigating several statistical parameters of topological indices for random caterpillars and related graphs

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Abstract

In the dynamic fields of mathematical chemistry and chemoinformatics, caterpillar trees are widely employed as a foundational tool for modeling the structures of unbranched benzenoid hydrocarbon molecules. They are a renowned topological index used to model QSPR and QSAR between molecules. This article explores into an intriguing class of caterpillar trees that integrates randomness, offering a fresh perspective on the Zagreb index and its generalizations. We meticulously compute the skewness and kurtosis associated with the Zagreb index, presenting analytical expressions for the expected value of its generalized form. Moreover, the asymptotic behavior of the generalized Zagreb index is characterized and analyzed for caterpillars generated randomly through the application of the Martingale Central Limit Theorem. Finally, we conduct thorough numerical experiments that analyze the behaviors of statistical parameters in this unique class.

Subject Classification (2020): *05C05, 05C09, 05C12, 05C80, 05C92.*

Keywords: *Caterpillar tree, Topological index, Random caterpillars, Moments, Martingale, Central limit theorem.*

1. Introduction

In the realm of chemical graph theory, mathematical chemistry, and chemoinformatics, the topological index stands as an indispensable tool for probing the physico-chemical properties and biological activities of the molecular structures. This index provides numerical value for molecular

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compounds, empowering researchers to effectively develop quantitative structure-property and structure-activity relationships (QSPR/QSAR) across different molecules [4, 9, 14, 17, 24, 35]. Over the past two decades, topological indices have surged in prominence within the field of random graphs, embracing a broad spectrum of applications such as connectivity, compactness, regularity, sparseness, and the small-world phenomenon. This flourishing interest among researchers underscores the utility of random graphs in elucidating evolving molecular networks, modeling discrete polymerization processes, and unraveling complexities in real-world networks [7, 9, 11, 14, 18, 25].

Specifically, a class of random graphs has emerged, featuring distinctive evolutionary steps that infuse randomness into *caterpillar graphs,* known as *random caterpillars.* Caterpillar graphs, or simply caterpillars, are acyclic graphs characterized by the presence of a path (referred to as the spine) where all the leaves have been pruned. In the domain of mathematical chemistry and chemoinformatics, caterpillar graphs play a pivotal role in characterizing the molecular structure of chemical compounds and unraveling the intrinsic properties of unbranched catacondensed benzenoid hydrocarbon molecules. For those seeking further insights, a wealth of resources awaits in [5, 6, 15, 29, 30, 31, 36, 39, 41].

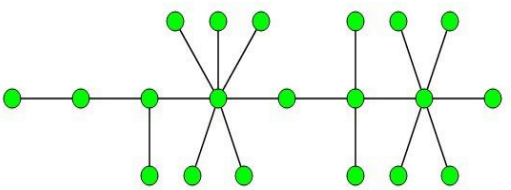

Figure 1
A representative caterpillar tree containing 8 spine nodes and 12 attached leaves

With the remarkable surge of interest and advancements in the realms of randomness and random tree models in modern science, we are inspired to delve into a captivating class of random caterpillars that evolves uniformly [12]. Recent years have seen the emergence and analysis of several intriguing indices such as the Zagreb, Randić, and Wiener indices considered on random graphs. Our motivation is to explore a fresh and insightful perspective on the Zagreb index and its generalizations, while also establishing the asymptotic distribution of these parameters through the elegant framework of the Martingale Central Limit Theorem (MCLT). At time 0, a spine is comprised of a fixed number of nodes ($m \geq 2$). During each subsequent time interval, each leaf attaches to a spine node, among the m spine nodes by means of an edge. Importantly, each spine node i has an equal chance of being selected, i.e. $\frac{1}{m}$, ensuring a balanced and engaging evolution of the model.

By time n, the topology of a random caterpillar is denoted by C_n. Initially, we will outline several important graph invariants of C_n, and introduce some

notations that will be consistently employed throughout the manuscript. The total number of nodes in C_n is denoted as $(n+m)$, while the total number of edges as $(n+m-1)$. The distinct numbers $\{1, 2, \dots, m\}$ (from left to right) are enumerated to the m spine nodes in order-preservance. Set $X_{i,n}$ to represent the leaf count linked with spine node i, and let $D_{i,n}$ correspond to its degree for $i = 1, 2, \dots, m$. There is an instantaneous relation between $X_{i,n}$ and $D_{i,n}$.

That is $D_{i,n} = X_{i,n} + 1$ for $i = 1, m$; $D_{i,n} = X_{i,n} + 2$ for $i = 2, 3, \dots, m-1$. A demonstrative model of the caterpillar tree is demonstrated in Figure 1. The evolution of random caterpillars reveals a fascinating joint distribution of $X_{i,n}'s$ that can be modeled using a multinomial approach with parameters n and $\mathbb{I}_{m\times 1/m}$, where $\mathbb{I}_{m\times 1}$ represents a column vector of all 1's.

This paper is structured in the following manner. From Sections 2 to 4, we delve into some statistical parameters of both the Zagreb index and the generalized Zagreb index of C_n. We will clearly define each index and provide insightful introductions to their applications, while also establishing the asymptotic distribution of the parameters, which aptly sets the stage for our analysis. In Section 5, we conduct rigorous numerical analyses to validate the theoretical insights derived in earlier sections, followed by some concluding observations and future scopes.

2. Zagreb Index

In 1972, Zagreb index was proposed by the well-known chemists Gutman and Trinajsti [11]. The Zagreb index and its variants play a crucial role in chemical graph theory and the exploration of quantitative structure-property/activity relationships (QSPR/QSAR). The Zagreb index is vital, as it represents the sum of the degree squares of all vertices comprising the graph. This not only enhances our comprehension of molecular structures but also aids in predicting their properties and activities effectively. Formally, it is expressed as

$$Zagreb(G) = \sum_{v\in V}(\deg(v))^2$$

where, $\deg(v)$ represents the degree of the vertex v.

Zagreb index has plethora of applications in mathematical chemistry and chemoinformatics, to analyze chirality [2], ZE-isomerism [1], molecular complexity [38]. The literature surveyed provides compelling insights on the Zagreb index associated with three random network models, which arise as extensions of well-known random graph models such as random recursive trees, random binary search trees, random m-ary trees, plain-oriented recursive trees and preferential attachment caterpillars, and critical Galton-Watson trees etc. [3, 8, 10, 21, 23, 32, 33]. In this section, we will delve into the calculation of the Zagreb index corresponding to a random caterpillar at time n, symbolized by $Z_n = Zagreb(C_n)$.

The Zagreb index of C_n is given by

$$Z_n = Zagreb(C_n) = \sum_{i=1}^{m} D_{i,n}^2 + \sum_{i=1}^{m} X_{i,n}.$$

Let $\mathbb{F}_n$ represent the $\sigma-$field created by the history of the first n stages of the growth of a caterpillar, and let $\mathbf{1}_n(i)$ represent the event describing the choice of the i^{th} spine node at time n. We now present the third and fourth moment of Z_n, following the skewness and kurtosis of Z_n.

Towards the third and fourth moment of Z_n, we require the mean of a new invariant constructed by summing the cubic degrees and quartic degrees of every nodes in C_n.

These index are denoted by Y_n and X_n and expressed as

$$Y_n = \sum_{i=1}^{m} D_{i,n}^3 + n \tag{1}$$

and

$$X_n = \sum_{i=1}^{m} D_{i,n}^4 + n \tag{2}$$

The mean of Y_n and X_n are reveal in the following lemma.

Lemma 1: *For $n \geq 0$, the mean of Y_n is given by*

$$\mathbb{E}[Y_n] = \frac{n^3}{m^2} + \frac{(9m-9)n^2}{m^2} + \frac{(20m^2-33m+8)n}{m^2} + (8m-14).$$

As $n \to \infty$, we have $\frac{Y_n}{n^3} \xrightarrow{L_1} \frac{1}{m^2}$. This convergence also occurs in probability.

Proof: An almost-sure (a.s.) relation between Y_n and Y_{n-1} is examined, under the condition on $\mathbf{1}_n(i)$ and $\mathbb{F}_{n-1}$:

$$Y_n = Y_{n-1} + (D_{i,n-1}+1)^3 - D_{i,n-1}^3 + 1 = Y_{n-1} + 3D_{i,n-1}^2 + 3D_{i,n-1} + 2. \tag{3}$$

By calculating the expectation relative to $\mathbf{1}_n(i)$, we get

$$\mathbb{E}[Y_n|\mathbb{F}_{n-1}] = Y_{n-1} + \frac{3}{m}\sum_{i=1}^{m} D_{i,n-1}^2 + \frac{3}{m}\sum_{i=1}^{m} D_{i,n-1} + 2$$

$$= Y_{n-1} + \frac{3}{m}\left(Z_{n-1} - (n-1)\right) + \frac{3}{m}(n+2m-3) + 2$$

By considering an additional expectation relative to $\mathbb{F}_{n-1}$, and then applying $\mathbb{E}[Z_{n-1}]$, we obtain the recurrence relation for $\mathbb{E}[Y_n]$ as

$$\mathbb{E}[Y_n] = \mathbb{E}[Y_{n-1}] + \frac{3}{m}\left(\frac{n^2+(6m-7)n+(6-6m)}{m}\right) + 20 - \frac{24}{m}.$$

By solving the recurrence for $\mathbb{E}[Y_n]$ with its initial condition $\mathbb{E}[Y_0] = Y_0 = 8m-14$, we have arrived at the desired result.

As $n \to \infty$, we have $\frac{Y_n}{n^3}$ converges to $\frac{1}{m^2}$ in L_1-space, suggesting that $\frac{Y_n}{n^3}$ converges to $\frac{1}{m^2}$ in probability as well.

Lemma 2; *For $n \geq 0$, the mean of X_n is given by*

$$\mathbb{E}[X_n] = \frac{n^4}{m^3} + \frac{(14m-14)n^3}{m^3} + \frac{(55m^2-102m+35)n^2}{m^3} + \frac{(66m^3-155m^2+88m-22)n}{m^3} + (16m-30).$$

As $n \to \infty$, we have $\frac{X_n}{n^4} \xrightarrow{L_1} \frac{1}{m^3}$. This convergence also occurs in probability as well.

Proof: An almost-sure relation between X_n and X_{n-1} is examined, under the condition on $\mathbf{1}_n(i)$ and $\mathbb{F}_{n-1}$:

$$X_n = X_{n-1} + (D_{i,n-1} + 1)^4 - D_{i,n-1}^4 + 1 = X_{n-1} + 4D_{i,n-1}^3 + 6D_{i,n-1}^2 + 4D_{i,n-1} + 2. \quad (4)$$

By calculating the expectation relative to $\mathbf{1}_n(i)$, we get

$$\mathbb{E}[X_n|\mathbb{F}_{n-1}] = X_{n-1} + \frac{4}{m}\sum_{i=1}^{m} D_{i,n-1}^3 + \frac{6}{m}\sum_{i=1}^{m} D_{i,n-1}^2 + \frac{4}{m}\sum_{i=1}^{m} D_{i,n-1} + 2$$

$$= X_{n-1} + \frac{4}{m}\big(Y_{n-1} - (n-1)\big) + \frac{6}{m}\big(Z_{n-1} - (n-1)\big) + \frac{4}{m}(n + 2m - 3) + 2$$

By considering an additional expectation relative to $\mathbb{F}_{n-1}$, and then applying $\mathbb{E}[Y_{n-1}]$ and $\mathbb{E}[Z_{n-1}]$, we obtain the recurrence relation for $\mathbb{E}[X_n]$ as

$$\mathbb{E}[X_n] = \mathbb{E}[X_{n-1}] + \frac{1}{m^3}(4n^3 + (42m - 48)n^2 + (110m^2 - 246m + 116)n + (66m^3 - 210m^2 + 204m - 72)).$$

Solving the recurrence for $\mathbb{E}[X_n]$ along with the condition $\mathbb{E}[X_0] = X_0 = 16m - 30$, we have arrived at the desired result.

As $n \to \infty$, we have $\frac{X_n}{n^4}$ converges to $\frac{1}{m^3}$ in L_1 −space and probability as well.

We are prepared to calculate the third and fourth moments of Z_n in the forthcoming proposition.

Proposition 1: For $n \geq 0$, the third moment associated with the Zagreb index of random caterpillars is given by

$$\mathbb{E}[Z_n^3] = \frac{n^6 + (18m-15)n^5 + (120m^2 - 192m + 69)n^4 + O(n^3)}{m^3}$$

and

$$\mu[Z_n] = \frac{4n}{m^3}[(6m - 2)n^2 + (-36m^3 + 37m^2 + 3m - 16)n + (-108m^4 + 138m^3 - 113m^2 + 51m - 14)].$$

As $n \to \infty$, we have $\frac{\mu[Z_n]}{n^3} \xrightarrow{L_1} \frac{4(6m-2)}{m^3}$. This convergence occurs in probability as well.

Proof: We recall the a.s. recursion between Z_{n-1} and Z_n, conditional on $\mathbf{1}_n(i)$ and $\mathbb{F}_{n-1}$:

$$Z_n = Z_{n-1} + 2D_{i,n-1} + 2 \quad (5)$$

We cube it on both sides and get

$$Z_n^3 = (Z_{n-1} + 2D_{i,n-1} + 2)^3$$

$$= Z_{n-1}^3 + 8D_{i,n-1}^3 + 8 + 6Z_{n-1}^2 D_{i,n-1} + 24Z_{n-1}D_{i,n-1} + 6Z_{n-1}^2 + 12Z_{n-1} + 12Z_{n-1}\,D_{i,n-1}^2 + 24D_{i,n-1}^2 + 24D_{i,n-1}$$

Again, averaging it over i to obtain

$$\mathbb{E}[Z_n^3|\mathbb{F}_{n-1}] = Z_{n-1}^3 + \frac{8}{m}\sum_{i=1}^{m} D_{i,n-1}^3 + 8 + \frac{6Z_{n-1}^2}{m}\sum_{i=1}^{m} D_{i,n-1}$$
$$+\frac{24Z_{n-1}}{m}\sum_{i=1}^{m} D_{i,n-1} + 6Z_{n-1}^2 + 12Z_{n-1}$$
$$+\frac{12Z_{n-1}}{m}\sum_{i=1}^{m} D_{i,n-1}^2 + \frac{24}{m}\sum_{i=1}^{m} D_{i,n-1}^2 + \frac{24}{m}\sum_{i=1}^{m} D_{i,n-1}$$
$$= Z_{n-1}^3 + \frac{8}{m}\big(Y_{n-1} - (n-1)\big) + 8 + \frac{6(n+2m-3)}{m} Z_{n-1}^2 + \frac{24(n+2m-3)}{m} Z_{n-1}$$
$$+6Z_{n-1}^2 + 12Z_{n-1} + \frac{12Z_{n-1}}{m}\big(Z_{n-1} - (n-1)\big) + \frac{24}{m}\big(Z_{n-1} - (n-1)\big)$$
$$+ \frac{24(n+2m-3)}{m}$$

By calculating the expectation based on prior results, we can effectively derive the recurrence for $\mathbb{E}[Z_n^3]$ by first computing $\mathbb{E}[Z_n^3|\mathbb{F}_{n-1}]$ and then applying $\mathbb{E}[Y_{n-1}]$, $\mathbb{E}[Z_{n-1}^2]$ and $\mathbb{E}[Z_{n-1}]$.

$$\mathbb{E}[Z_n^3] = \mathbb{E}[Z_{n-1}^3] + \frac{6n+18m-6}{m}\ \mathbb{E}[Z_{n-1}^2] + \frac{12n+60m+12}{m}\ \mathbb{E}[Z_{n-1}]$$
$$+\frac{8}{m}\ \mathbb{E}[Y_{n-1}] + \frac{-8n+56m-40}{m}$$

Solving the recurrence along with the condition $\mathbb{E}[Z_0^3] = Z_0^3 = (4m-6)^3$, we derive the stated result in the proposition. Following, we obtained the exact expression of the skewness of Z_n.

By the expression of $\mathbb{E}[Z_n^3]$, we conclude that $\frac{Z_n^3}{n^6} \xrightarrow{L_1} \frac{1}{m^3}$, done in a similar manner as before.

As $n \to \infty$, we have $\frac{\mu[Z_n]}{n^3}$ converges to $\frac{4(6m-2)}{m^3}$ in L_1 −space and probability as well.

Proposition 2: For $n \geq 0$, the fourth moment associated with the Zagreb index of random caterpillars is given by

$$\mathbb{E}[Z_n^4] = \frac{n^8 + (24m-20)n^7 + O(n^6)}{m^4}$$

and

$$\kappa[Z_n] = \frac{n}{m^4}\Big[(-576m^3 + 8784m^2 - 1008m + 232)n^4 + (-2160m^4 + 5760m^3 - 5880m^2 + 2682m - 326)n^3 + \Big(4320m^4 - 12416m^3 + 18880m^2 + 31276m - \frac{940}{3}\Big)n^2 + (-6816m^4 + 17432m^3 - 8960m^2 + 3906m - 274)n + \Big(-2928m^5 + 8992m^4 - 6968m^3 + 7592m^2 - 568m - \frac{520}{6}\Big)\Big].$$

As $n \to \infty$, we have $\frac{\kappa[Z_n]}{n^5} \xrightarrow{L_1} \frac{-576m^3+8784m^2-1008m+232}{m^4}$. This convergence occurs in probability as well.

Proof: We recall the a.s. recursive Z_{n-1} and Z_n, under the condition on $\mathbf{1}_n(i)$ and $\mathbb{F}_{n-1}$:

$$Z_n = Z_{n-1} + 2D_{i,n-1} + 2$$
$$Z_n^4 = (Z_{n-1} + 2D_{i,n-1} + 2)^4$$
$$= Z_{n-1}^4 + 8Z_{n-1}^3 D_{i,n-1} + 8Z_{n-1}^3 + 24Z_{n-1}^2 D_{i,n-1}^2 + 48Z_{n-1}^2 D_{i,n-1} + 24Z_{n-1}^2 + 32Z_{n-1}D_{i,n-1}^3 + 96Z_{n-1}D_{i,n-1}^2 + 96Z_{n-1}D_{i,n-1} + 32Z_{n-1} + 16D_{i,n-1}^4 + 64D_{i,n-1}^3 + 96D_{i,n-1}^2 + 64D_{i,n-1} + 16$$

Averaging it over i, we get

$$\mathbb{E}[Z_n^4|\mathbb{F}_{n-1}] = Z_{n-1}^4 + \frac{8Z_{n-1}^3}{m}\sum_{i=1}^m D_{i,n-1} + 8Z_{n-1}^3 + \frac{24Z_{n-1}^2}{m}\sum_{i=1}^m D_{i,n-1}^2 + \frac{48Z_{n-1}^2}{m}\sum_{i=1}^m D_{i,n-1} + 24Z_{n-1}^2 + \frac{32Z_{n-1}}{m}\sum_{i=1}^m D_{i,n-1}^3 + \frac{96Z_{n-1}}{m}\sum_{i=1}^m D_{i,n-1}^2 + \frac{96Z_{n-1}}{m}\sum_{i=1}^m D_{i,n-1} + 32Z_{n-1} + \frac{16}{m}\sum_{i=1}^m D_{i,n-1}^4 + \frac{64}{m}\sum_{i=1}^m D_{i,n-1}^3 + \frac{96}{m}\sum_{i=1}^m D_{i,n-1}^2 + \frac{64}{m}\sum_{i=1}^m D_{i,n-1} + 16$$
$$= Z_{n-1}^4 + \frac{8Z_{n-1}^3}{m}(n+3m) + \frac{24Z_{n-1}^2}{m}(n+5m-1) + \frac{32Z_{n-1}}{m}(-n+7m-2) + \frac{32}{m}Z_{n-1}Y_{n-1} + \frac{64}{m}Y_{n-1} + \frac{16}{m}X_{n-1} + \frac{16}{m}(-7n+9m-1)$$

The recurrence for $\mathbb{E}[Z_n^4]$ is obtained by first computing $\mathbb{E}[Z_n^4|\mathbb{F}_{n-1}]$ and then applying $\mathbb{E}[Z_{n-1}^3], \mathbb{E}[Z_{n-1}^2], \mathbb{E}[Z_{n-1}], \mathbb{E}[Z_{n-1}Y_{n-1}], \mathbb{E}[Y_{n-1}]$ and $\mathbb{E}[X_{n-1}]$. By solving the recurrence for $\mathbb{E}[Z_n^4]$ along with the condition $\mathbb{E}[Z_0^4] = Z_0^4 = (4m-6)^4$, we derive the stated result. Next, we obtained the exact expression of the kurtosis of Z_n.

By the expression of $\mathbb{E}[Z_n^4]$, we conclude that $\frac{Z_n^4}{n^8} \xrightarrow{L_1} \frac{1}{m^4}$.

As $n \to \infty$, we have $\frac{\kappa[Z_n]}{n^5}$ converges to $\frac{-576m^3+8784m^2-1008m+232}{m^4}$ in L_1 −space as well as in probability.

Theorem 1: *For* $k \geq 0$,

$$\mathbb{P}\left\{\left|Z_n - \left(\frac{n^2}{m} + \frac{(6m-5)n}{m} + (4m-6)\right)\right| \geq k\right\} \leq \frac{2n((m-1)n+3m-7)}{m^2k^2}$$

3. Generalized Zagreb index

In this section, we delve into the calculation of the generalized Zagreb index of a random caterpillar, denoted by $Z_n^g = Generalized\ Zagreb(C_n)$. This index represents a crucial measure in graph theory. Formally, it is the sum of the degrees of all graph vertices each raised to the power α. Researchers and enthusiasts in the field will find substantial value in examining the latest studies on this topic, often referred to as the general zeroth-order Randić index. We encourage readers to explore the referenced works [3, 8, 10, 13, 19, 22, 27, 28, 37] to enrich their understanding of the generalized Zagreb index with related applications in random graphs and algorithms. Mathematically, it is

$$Z_n^g(G) = \sum_{v\in V}(\deg(v))^\alpha\ ;\ \forall v \in V.$$

Specifically, if we consider $\alpha = 2$, Zagreb index is obtained and $\alpha = 3$, forgotten index is obtained.

According to the expression, the generalized Zagreb index of random caterpillars is expressed as

$$Z_n^g = \sum_{i=1}^{m} D_{i,n}^{\alpha} + n. \tag{6}$$

In the upcoming proposition, we will effectively present both the mean of Z_n^g and a relevant weak law to support our findings.

Proposition 3: For $n \geq 0$, we have

$$\mathbb{E}[Z_n^g] = 2^{\alpha}m + 2(1-2^{\alpha}) + 2n + \frac{1}{m}\sum_{i=1}^{m}\Big(\sum_{r=1}^{\alpha-1}\binom{\alpha}{r}\big(D_{i,0}^{\alpha-r} + D_{i,1}^{\alpha-r} + \cdots + D_{i,n-2}^{\alpha-r} + D_{i,n-1}^{\alpha-r}\big)\Big)$$

As $n \to \infty$, we have $\frac{Z_n^g}{n^{\alpha}} \xrightarrow{L_1} \frac{1}{m^{\alpha-1}}$. This convergence occurs in probability as well.

Proof: The following a.s. recursive relation between Z_{n-1}^g and Z_n^g is examined, under the condition on $\mathbf{1}_n(i)$ and $\mathbb{F}_{n-1}$:

$$\begin{aligned} Z_n^g &= Z_{n-1}^g + \big(D_{i,n-1} + 1\big)^{\alpha} - D_{i,n-1}^{\alpha} + 1 \\ &= Z_{n-1}^g + \binom{\alpha}{1}D_{i,n-1}^{\alpha-1} + \binom{\alpha}{2}D_{i,n-1}^{\alpha-2} + \cdots + \alpha D_{i,n-1} + 2. \end{aligned}$$

By averaging it over i, we get

$$\mathbb{E}[Z_n^g|\mathbb{F}_{n-1}] = \mathbb{E}[Z_{n-1}^g] + \frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-1} + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-2} + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m} D_{i,n-1} + 2 \tag{7}$$

Again,

$$\mathbb{E}[Z_{n-1}^g|\mathbb{F}_{n-2}] = \mathbb{E}[Z_{n-2}^g] + \frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m} D_{i,n-2}^{\alpha-1} + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m} D_{i,n-2}^{\alpha-2} + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m} D_{i,n-2} + 2 \tag{8}$$

Putting (8) in (7),

$$\mathbb{E}[Z_n^g] = \Big(\mathbb{E}[Z_{n-2}^g] + \frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m} D_{i,n-2}^{\alpha-1} + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m} D_{i,n-2}^{\alpha-2} + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m} D_{i,n-2} + 2\Big) + \Big(\frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-1} + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-2} + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m} D_{i,n-1} + 2\Big) \tag{9}$$

Continuing upto n^{th} steps,

$$\mathbb{E}[Z_n^g] = \Big(\mathbb{E}[Z_{n-n}^g] + \frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m} D_{i,n-n}^{\alpha-1} + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m} D_{i,n-n}^{\alpha-2} + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m} D_{i,n-n} + 2\Big) + \ldots + \Big(\frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-1} + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-2} + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m} D_{i,n-1} + 2\Big)$$

$$= \mathbb{E}\left[Z_0^g\right] + 2n + \frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m}\left(D_{i,0}^{\alpha-1} + D_{i,1}^{\alpha-1} + \cdots + D_{i,n-1}^{\alpha-1}\right) + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m}\left(D_{i,0}^{\alpha-2} + D_{i,1}^{\alpha-2} + \cdots + D_{i,n-1}^{\alpha-2}\right) + \cdots + \frac{\binom{\alpha}{\alpha-1}}{m}\sum_{i=1}^{m}\left(D_{i,0}^{\alpha-(\alpha-1)} + D_{i,1}^{\alpha-(\alpha-1)} + \cdots + D_{i,n-1}^{\alpha-(\alpha-1)}\right)$$

$$= \mathbb{E}\left[Z_0^g\right] + 2n + \frac{1}{m}\sum_{i=1}^{m}\left(\sum_{r=1}^{\alpha-1}\binom{\alpha}{r}\left(D_{i,0}^{\alpha-r} + D_{i,1}^{\alpha-r} + \cdots + D_{i,n-2}^{\alpha-r} + D_{i,n-1}^{\alpha-r}\right)\right)$$

$$\mathbb{E}\left[Z_n^g\right] = 2^\alpha m + 2(1-2^\alpha) + 2n + \frac{1}{m}\sum_{i=1}^{m}\left(\sum_{r=1}^{\alpha-1}\binom{\alpha}{r}\left(D_{i,0}^{\alpha-r} + D_{i,1}^{\alpha-r} + \cdots + D_{i,n-2}^{\alpha-r} + D_{i,n-1}^{\alpha-r}\right)\right).$$

As $n \to \infty$, we have $\frac{Z_n^g}{n^\alpha}$ converges to $\frac{1}{m^{\alpha-1}}$ in L_1 −space, suggesting that $\frac{Z_n^g}{n^\alpha}$ converges to $\frac{1}{m^{\alpha-1}}$ in probability as well.

Following our thorough investigation, we will develop a martingale array through a careful reformulation of Z_n^g and apply the Martingale Central Limit Theorem (MCLT). During the proof of Proposition (3), we demonstrate that the sequence $\left\{Z_n^g\right\}_n$

$$\mathbb{E}\left[Z_n^g \middle| \mathbb{F}_{n-1}\right] = Z_{n-1}^g + \frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-1} + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-2} + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m} D_{i,n-1} + 2,$$

does not form a martingale. The next lemma implements a transformation to Z_n^g, resulting in a new one that fulfills the criteria to be classified as a martingale.

Lemma 3: *The sequence* $\left\{M_n^g\right\}_n$ *such that*

$$M_n^g = Z_n^g - \left(\frac{1}{m}\sum_{i=1}^{m}\left\{\sum_{r=1}^{\alpha-1}\binom{\alpha}{r}\left(D_{i,0}^{\alpha-r} + D_{i,1}^{\alpha-r} + \cdots + D_{i,n-2}^{\alpha-r} + D_{i,n-1}^{\alpha-r}\right)\right\} + 2n\right)$$

is a martingale.

Proof: Let us consider $M_n^g = Z_n^g + \beta_n^g$ such that the following martingale property to hold; namely,

$$\mathbb{E}\left[Z_n^g + \beta_n^g \middle| \mathbb{F}_{n-1}\right] = Z_{n-1}^g + \frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-1} + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-2} + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m} D_{i,n-1} + 2 + \beta_n^g$$

$$= Z_{n-1}^g + \beta_{n-1}^g$$

where

$$\beta_{n-1}^g = \frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-1} + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-2} + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m} D_{i,n-1} + 2 + \beta_n^g$$

This produces a recurrence for β_n^g, namely,

$$\beta_n^g = \beta_{n-1}^g - \left(\frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-1} + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m} D_{i,n-1}^{\alpha-2} + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m} D_{i,n-1} + 2\right) \tag{10}$$

Applying recurrence on (10),

$$\beta_{n-1}^{g} = \beta_{n-2}^{g} - \left(\frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m} D_{i,n-2}^{\alpha-1} + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m} D_{i,n-2}^{\alpha-2} + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m} D_{i,n-2} + 2\right) \tag{11}$$

Putting (11) in (10) and continuing upto n^{th} steps, we get

$$\beta_{n}^{g} = \beta_{0}^{g} - \left(\frac{\binom{\alpha}{1}}{m}\sum_{i=1}^{m}\left(D_{i,n-1}^{\alpha-1} + D_{i,n-2}^{\alpha-1} + \cdots + D_{i,0}^{\alpha-1}\right) + \frac{\binom{\alpha}{2}}{m}\sum_{i=1}^{m}\left(D_{i,n-1}^{\alpha-2} + D_{i,n-2}^{\alpha-2} + \ldots + D_{i,0}^{\alpha-2}\right) + \cdots + \frac{\alpha}{m}\sum_{i=1}^{m}\left(D_{i,n-1} + D_{i,n-2} + \cdots + D_{i,0}\right) + 2n\right)$$

$$= \beta_{0}^{g} - \frac{1}{m}\sum_{i=1}^{m}\left(\sum_{r=1}^{\alpha-1}\binom{\alpha}{r}\left(D_{i,0}^{\alpha-r} + D_{i,1}^{\alpha-r} + D_{i,2}^{\alpha-r} \ldots + D_{i,n-2}^{\alpha-r} + D_{i,n-1}^{\alpha-r}\right)\right) - 2n$$

The solution is $\beta_{n}^{g} = -\left(\frac{1}{m}\sum_{i=1}^{m}\left\{\sum_{r=1}^{\alpha-1}\binom{\alpha}{r}\left(D_{i,0}^{\alpha-r} + D_{i,1}^{\alpha-r} + \cdots + D_{i,n-2}^{\alpha-r} + D_{i,n-1}^{\alpha-r}\right)\right\} + 2n\right)$, revealed by choosing the initial condition $\beta_{0}^{g} = 0$.

The Martingale Central Limit Theorem (MCLT) we leverage to establish asymptotic normality is fundamentally rooted in martingale differences, articulated through a difference operator, i.e., $\nabla M_{j}^{g} := M_{j}^{g} - M_{j-1}^{g}$. Indeed, there are various forms of MCLTs detailed in reference [26], each with specific requirements. The MCLT pertinent to our analysis is outlined in [26] (Corollary 3.2), and necessitates two essential conditions:

the conditional Lindeberg's and variance conditions. In the following lemma, we will convincingly demonstrate that the first condition is satisfied.

Lemma 4: *The conditional Lindeberg's condition is given by*

$$U_{n} := \sum_{j=1}^{n} E\left[\left(\frac{\nabla M_{j}}{\sqrt{n^{\alpha}}}\right)^{2} \mathbf{1}_{\left\{\left|\frac{\nabla M_{j}}{\sqrt{n^{\alpha}}}\right| > \epsilon\right\}} | \mathbb{F}_{j-1}\right] \xrightarrow{P} 0$$

for arbitrary $\epsilon > 0$.

Proof: We prove an absolutely uniform bound valid for all $j \leq n$.

Constructing the martingale, we have

$$\left|\nabla M_{j}^{g}\right| = \left|M_{j}^{g} - M_{j-1}^{g}\right|$$

$$\leq \left|Z_{j}^{g} - Z_{j-1}^{g}\right| + \left|\frac{1}{m}\sum_{i=1}^{m}\left\{\sum_{r=1}^{\alpha-1}\binom{\alpha}{r} D_{i,j-1}^{\alpha-r}\right\} + 2\right|$$

$$\leq \binom{\alpha}{1}\max_{i} D_{i,j-1}^{\alpha-1} + \binom{\alpha}{2}\max_{i} D_{i,j-1}^{\alpha-2} + \cdots + \alpha \max_{i} D_{i,j-1} + 2 + \frac{1}{m}\sum_{i=1}^{m}\left\{\sum_{r=1}^{\alpha-1}\binom{\alpha}{r} D_{i,j-1}^{\alpha-r}\right\} + 2$$

$$\leq \binom{\alpha}{1}(2 + j - 1)^{\alpha-1} + \binom{\alpha}{2}(2 + j - 1)^{\alpha-2} + \cdots + \alpha(2 + j - 1) + 2 + \frac{1}{m}\sum_{i=1}^{m}\left\{\sum_{r=1}^{\alpha-1}\binom{\alpha}{r} D_{i,j-1}^{\alpha-r}\right\} + 2$$

$$= \binom{\alpha}{1}(j + 1)^{\alpha-1} + \binom{\alpha}{2}(j + 1)^{\alpha-2} + \cdots + \alpha(j + 1) + 2 + \frac{1}{m}\sum_{i=1}^{m}\left\{\sum_{r=1}^{\alpha-1}\binom{\alpha}{r} D_{i,j-1}^{\alpha-r}\right\} + 2$$

$$= \sum_{s=1}^{\alpha-1}\binom{\alpha}{s}(j+1)^{\alpha-s} + \frac{1}{m}\sum_{i=1}^{m}\left\{\sum_{r=1}^{\alpha-1}\binom{\alpha}{r}D_{i,j-1}^{\alpha-r}\right\} + 4$$

$$= \sum_{r=1}^{\alpha-1}\binom{\alpha}{r}\left[\frac{1}{m}\sum_{i=1}^{m}D_{i,j-1}^{\alpha-r} + (j+1)^{\alpha-s}\right] + 4,$$

which is an increasing function of j for any given integer $m \geq 2$. Thus, the quantity $\left|\frac{\nabla M_j}{\sqrt{n^{\alpha}}}\right|$ is uniformly bounded by n. In simpler terms, for any $\in > 0$, we can identify an $n_0(\in) > 0$ such that the relevant sets $\left\{\left|\frac{\nabla M_j}{\sqrt{n^{\alpha}}}\right| > \in\right\}$ remain empty for all $n > n_0(\in)$.

Moreover, it is evident that the sequence U_n converges to 0 almost surely, a condition that surpasses the convergence in probability stipulated by Lindeberg's condition.

Theorem 2: *As* $n \to \infty, \frac{Z_n^g}{n^{\alpha-1}}$ *follows a Gaussian law, namely,*

$$\frac{Z_n^g - \frac{n^{\alpha}}{m^{\alpha-1}}}{n^{\alpha-1}} \xrightarrow{D} \mathcal{N}\left(0, \frac{\alpha(m-1)}{m^{2(\alpha-1)}}\right).$$

The proof follows directly by referencing the MCLT [26], outlined in Corollary 3.2.

4. Applications

This section brings to light two prominent topological indices, the *Gordon − Scantlebury index* [20] and the *Platt index* [16, 34]. These indices are intrinsically connected to the Zagreb index and play a vital role in progressing the random functional polycondensation theory, as well as in analyzing the additive bond properties of paraffin.

Gordon-Scantlebury index

The Gordon-Scantlebury index S_n, at time $n \geq 1$, confirms that $Z_n = 2(S_n + E_n)$, where E_n represents the total number of edges at time n. The random caterpillar produced at time n comprises $n + m$ nodes and $n + m - 1$ edges, thus $S_n = \frac{Z_n}{2} - n - m + 1$. For $n \geq 1$, we have following proposition:

Proposition 4: For $n \geq 1$, it is verified that

$$\mathbb{E}[S_n] = \frac{n^2}{2m} + \frac{(4m-5)n}{2m} + m - 2.$$

$$\mathbb{V}[S_n] = \frac{(m-1)n^2}{2m^2} + \frac{(3m-7)n}{2m^2} + 6m.$$

$$\mu[S_n] = \frac{1}{8m^3}[(24m-8)n^3 + (-72m^3 + 148m^2 - 132m - 64)n^2 + (72m^5 - 504m^4 + 714m^3 - 452m^2 + 204m - 56)n + (-48m^5 + 192m^4)].$$

$$\text{As } n \to \infty, \frac{S_n - \frac{n^2}{2m}}{n} \xrightarrow{D} \mathcal{N}\left(0, \frac{(m-1)}{2m^2}\right).$$

For $k > 0$,

$$\mathbb{P}\left\{\left|S_n - \left(\frac{n^2}{2m} + \frac{(4m-5)n}{2m} + (m-2)\right)\right| \geq k\right\} \leq \frac{(m-1)n^2+(3m-7)n+12m^3}{2m^2k^2}.$$

Platt index

Let P_n represent the Platt index at time $n \geq 1$, confirmimg that $P_n = 2S_n$. Thus, we have following proposition:

Proposition 5: For $n \geq 1$, it is verified that

$$\mathbb{E}[P_n] = \frac{n^2}{m} + \frac{(4m-5)n}{m} + 2(m-2).$$

$$2.\ \mathbb{V}[P_n] = \frac{(2m-2)n^2}{m^2} + \frac{(6m-14)n}{m^2} + 24m.$$

$$3.\ \mu[P_n] = 8\mu[S_n].$$

$$4.\ \text{As } n \to \infty, \frac{P_n - \frac{n^2}{m}}{n} \xrightarrow{D} \mathcal{N}\left(0, \frac{2m-2}{m^2}\right).$$

5. For $k > 0$,

$$\mathbb{P}\left\{\left|P_n - \left(\frac{n^2}{m} + \frac{(4m-5)n}{m} + 2(m-2)\right)\right| \geq k\right\} \leq \frac{(2m-2)n^2+(6m-14)n+24m^3}{m^2k^2}.$$

Forgotten index

Recently, a wave of researchers has been drawn to the extension of the Zagreb index, often called the *forgotten topological index*, owing to its profound applications in mathematical chemistry, environmental chemistry, and bioinformatics. Some applications of forgotten index are referred in [40, 42] for interested readers to survey. The forgotten index, denoted by Y_n, captures the essence of summing cubic degrees of each nodes in a graph, to arrive into new possibilities and discoveries. Thus, we have following proposition:

Proposition 6: For $n \geq 1$, it is verified that

$$\mathbb{E}[Y_n] = \frac{n^3}{m^2} + \frac{(9m-9)n^2}{m^2} + \frac{(20m^2-33m+8)n}{m^2} + (8m-14).$$

$$\mathbb{V}[Y_n] = \frac{(9m-9)n^4}{m^4} + \frac{(113m^2-282m+80)n^3}{m^4} + \frac{(849m^3-3870m^2+3582m-882)n^2}{2m^4} + \frac{(840m^4-6813m^3+7732m^2-3996m+740)n}{2m^4}.$$

$$\text{As } n \to \infty, \frac{Y_n - \frac{n^3}{m^2}}{n^2} \xrightarrow{D} \mathcal{N}\left(0, \frac{9m-9}{m^4}\right).$$

5. Numerical Experiments

Initially, we analyze the skewness of the Zagreb index pertaining to random caterpillar structures over time n, denoted as $\mu[Z_n]$. The computational evaluation of skewness is carried out using *Phython* for various time n increments up to an upper limit of 10, 000. We select 5 distinct values of m: 100, 500, 1000, 5000 and 10,000.

For each selected m, we rigorously conduct 10,000 experiments (i.e. the replication number is 10,000) to thoroughly examine the skewness of the Zagreb index in random caterpillars over time. The results are presented in Figure 2. In addition, we notice that $\mu[Z_n]$ decreases as m increases in Figure 2, we are eager to investigate the asymptotic property of $\mu[Z_n]$, as well as the rate at which $\mu[Z_n]$ decreases with respect to m. This exploration is crucial for understanding the behavior of the function in various applications.

We conduct another experiment of the expected mean of Gordon-Scantlebury index by setting $n = 10{,}000$ in simulated 26 various values of m. The parameter m was varied over the interval 500 to 13,000 with common difference of 500. Figure 3 presents a scattered graph of the results from which we conjecture that $\mathbb{E}[S_n]$ appears to be decreasing for

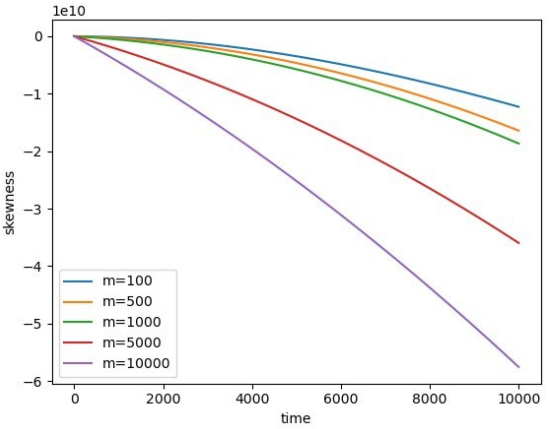

Figure 2
Skewness behavior of the Zagreb index across time *n* for five selected *m*

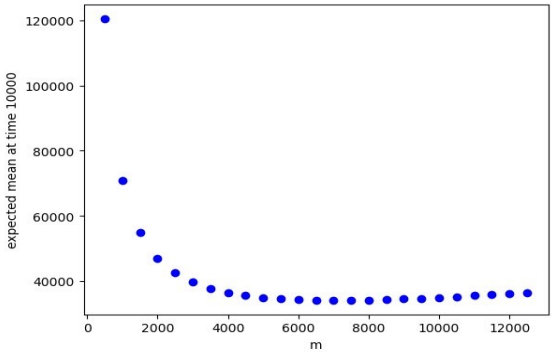

Figure 3
The expected mean of the Gordon-Scantlebury index at $n = 10,000$ for 26 choices of m

$m < 7500$ and an overall increasing for $m \geq 7500$. In addition, we look into the $\mathbb{V}[S_n]$ via boxplot. We have discussed about the median of data of the variance for 4 different values of n and 20 various values of m, beginning at $m = 500$ and culminating at 10,000 with common difference of 500. Figure 4 concludes that the median of the data increases as n increases.

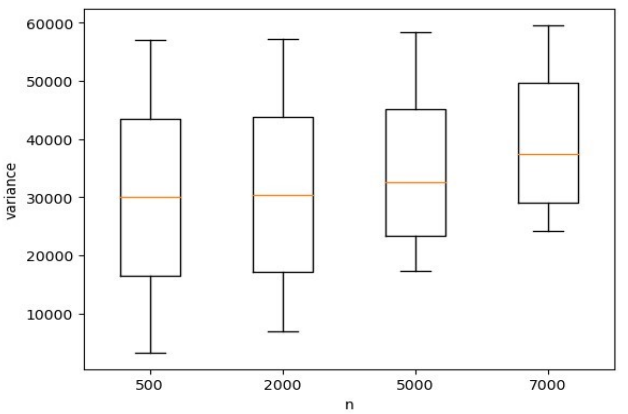

Figure 4
Box plot of the data of the variance of the Gordon-Scantlebury index at $n = 500, 2000, 5000, 7000$ for 20 different values of m

6. Conclusion

In today's era, the topological index is a powerful tool with diverse applications in structural graph studies, computational chemistry, and chemical data informatics, enabling accurate modeling of QSPR and QSAR relationships between molecules. In this work, we offer insightful concluding remarks and propose exciting avenues for future exploration. Our investigation embarks on a profound exploration of the statistical parameters of the Zagreb index and its generalizations within a unique class of random caterpillars. The study focuses on analyzing both symmetry and the distribution behavior in relative to a normal distribution. Furthermore, our analysis encompasses the mean of the generalized Zagreb index, and we introduce a martingale to illustrate the asymptotic behavior of the topological indices through the Martingale Central Limit Theorem. Moreover, this paper presents a range of applications of the Zagreb index in different domains, demonstrating its potential to enhance deterministic models in capturing key characteristics effectively. The study culminates with numerical experiments aimed at exploring the statistical parameters of the aforesaid index, thereby highlighting its significant implications in the field. Looking forward, our focus will be on exploring other statistical indices of the generalized Zagreb index that have yet to be explored, including variance, skewness, and kurtosis, which hold the key to numerous related applications. Noteworthy possibilities include analyzing the generalized Randić index for the same random structure with parameter α, and investigating complex random

networks or random trees, enriching our methods to compute the moments. Moreover, we are enthusiastic about delving into the combinatorial and physical properties of benzenoid hydrocarbons via random caterpillars. As we embark on this journey, we are committed to thorough investigation and will eagerly share our findings.

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