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The Limiting Behaviors of the Gutman and Schultz Indices in Random 2k-Sided Chains

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Abstract: The study of complex networks with topological indices has flourished in recent years. The aim of this paper is to study the limiting behaviors of Gutman and Schultz indices in random polygonal chains, whose graph-theoretic mathematical properties and their future applications have attracted the interest of scientists. By applying the concepts of symmetry and asymptotics as well as the knowledge of probability theory, we obtain explicit analytic expressions for the Gutman and Schultz indices of n random 2k-vertex chains and prove that they converge to a normal distribution, which contributes to a deeper understanding of the structural features of random polygonal chains and plays a crucial role in the study of the limiting behavior of topological indices and their applications.

Keywords: limiting behaviors; random polygonal chain; Gutman index; Schultz index

MSC: 2020; 62J10

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1. Introduction

In this paper, we only discuss finite, simple, and symmetrical connected graphs, which are mentioned in the work of Bondy and Murty [1] and the references they cite. Graph theory is closely intertwined with chemistry, and its applications within the field are extensive. The description of chemical compounds is based on chemical graph theory, with vertices representing atoms and edges representing the covalent bonds between atoms, whose fundamental technique involves creating a model of a compound's molecular structure [2,3].

The molecular formula of a compound can give an indication of different molecular structures and properties, but theoretical chemists are concerned with the physical and chemical properties of compounds and their relationship to their molecular formula [4,5].

We will use the following basic notations, as defined in [1]. Consider a graph G represented by the tuple $G = (V_G, E_G)$, where V_G is the set of vertices and E_G is the set of edges. Then, let $d_G(u, v)$ (simply $d(u, v)$) denote the distance between two vertices u and v in G, and the distance is defined as the length of the shortest path between u and v in G. The Wiener index (also known as the Wiener transmission) of a graph G with edge set E_G is defined as the sum of distances between all possible pairs of vertices in G. The index was introduced by H. Wiener in 1947 [6] and can be expressed mathematically as follows:

$$W(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V_G} d_G(u, v). \tag{1}$$

The Wiener index is a well-researched, comprehensively understood, and extensively employed molecular shape descriptor rooted in graph theory [7,8]. Furthermore, its usage and study have been progressively growing, as evidenced by [9,10].

A weighted graph (G, ω) is composed of a graph $G = (V_G, E_G)$ and a weight function ω: $V_G \to \mathbb{N}^+$. Suppose $\oplus$ represents one of the four arithmetic operations $+$, $-$, $\times$, and $\div$. Consequently, the weighted Wiener index $W(G, \omega)$ can be defined as follows:

$$W(G, \omega) = \frac{1}{2} \sum_{u \in V_G} \sum_{v \in V_G} (\omega(u) \oplus \omega(v)) d_G(u, v). \tag{2}$$

It is evident that when $\omega \equiv 1$ and $\oplus$ represent the operation $\times$, $W(G, \omega) = W(G)$.

Suppose $\oplus$ denotes the operation $\times$ and $\omega(\cdot) \equiv d_G(\cdot)$. In such a scenario, Equation (2) is identical to

$$Gut(G) = \frac{1}{2} \sum_{u \in V_G} \sum_{v \in V_G} (d_G(u) d_G(v)) d_G(u, v) = \sum_{\{u.v\} \subseteq V_G} (d_G(u) d_G(v)) d_G(u, v), \tag{3}$$

which is the Gutman index [11]. For more information on the prospective chemical uses of the Gutman index, alongside related metrics, as well as their theoretical analyses, wherein polycyclic molecules present more complex cases, please refer to [12].

Suppose $\oplus$ denotes the operation $+$ and $\omega(\cdot) \equiv d_G(\cdot)$. In such a scenario, Equation (2) is identical to

$$S(G) = \frac{1}{2} \sum_{u \in V_G} \sum_{v \in V_G} (d_G(u) + d_G(v)) d_G(u, v) = \sum_{\{u.v\} \subseteq V_G} (d_G(u) + d_G(v)) d_G(u, v), \tag{4}$$

which is the Schultz index. For further developments in topology indexes for [13–16], encompassing mathematical properties, discrimination, and applications, please refer to [17] for additional articles.

In this paper, we mainly talk about the polygonal chain G_n with n regular 2k-gon graphs, which are constructed in the following way. Firstly, G_1 is a 2k-sided polygon, and G_2 is the graph with two 2k-sided polygons connected by an edge, as shown in Figure 1. Secondly, to construct the random polygon chain G_{n+1}, a new terminal polygon with $2k$ sides, denoted as H_{n+1}, is attached to the existing polygon chain G_n which contains n 2k-gon polygons. This process is illustrated in Figure 2. As demonstrated in Figure 3, we can attach the terminal polygon with $2k$ sides H_{n+1} to G_n with k methods and denote the resulting figures with G_{n+1}^1, G_{n+1}^2, G_{n+1}^3, $\cdots$, G_{n+1}^k, respectively. At each step, one of the following possible constructions is randomly selected:

- $G_n \to G_{n+1}^1$ with probability p_1;
- $G_n \to G_{n+1}^2$ with probability p_2;
- $G_n \to G_{n+1}^3$ with probability p_3;

  $\vdots \quad \vdots \quad \vdots$
- $G_n \to G_{n+1}^{k-1}$ with probability p_{k-1};
- $G_n \to G_{n+1}^k$ with probability $p_k = 1 - p_1 - p_2 - p_3 - \cdots - p_{k-1}$.

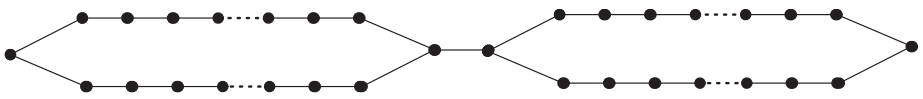


Figure 1. Graph G_2.

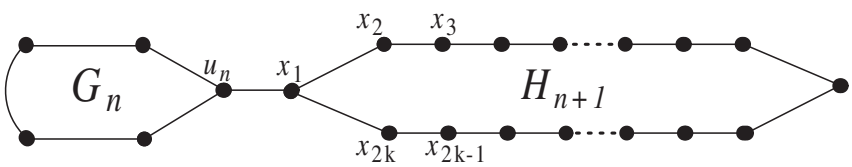


Figure 2. The formation of G_{n+1} by combining G_n and H_{n+1}.

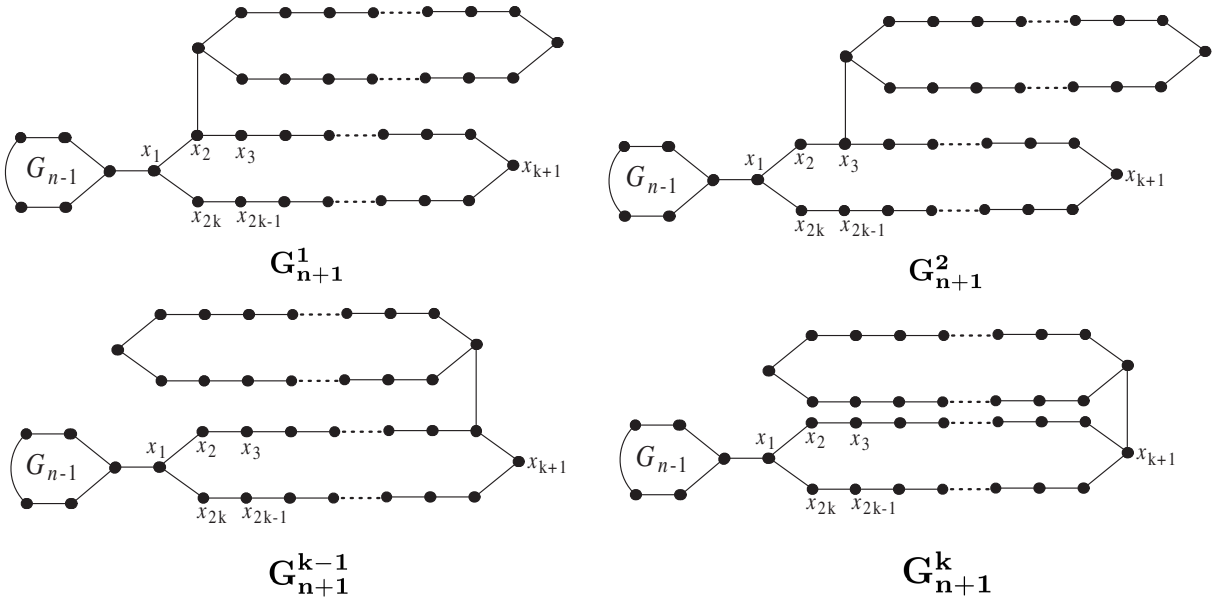


Figure 3. k methods for attaching the new terminal 2k-gon polygon H_{n+1} to G_n.

We define k random variables Z_n^1, Z_n^2, Z_n^3, $\cdots$, Z_n^k to represent our options. If we choose G_{n+1}^i, we set $Z_n^i = 1$; otherwise, $Z_n^i = 0$ for $i = 1, 2, 3, \cdots, k$. It is easy to see that

$$P(Z_n^i = 1) = p_i, P(Z_n^i = 0) = 1 - p_i, i = 1, 2, 3, \cdots, k \tag{5}$$

and $Z_n^1 + Z_n^2 + Z_n^3 + \cdots + Z_n^k = 1$.

Through the aforementioned procedures, we generate a random polygonal chain $G_n(p_1, p_2, p_3, \cdots, p_k)$ whose total number of sides is $2k$. That is to say, each cycle has $2k$ sides and it is called a chain of 2k cycles. We consistently abbreviate $G_n(p_1, p_2, p_3, \cdots, p_k)$ as G_n.

Noting that G_n is a random graph, both $Gut(G_n)$ and $S(G_n)$ are random variables in probability. In the view of probability, one problem appears naturally: when n is big enough, the distribution of $Gut(G_n)$ and $S(G_n)$ will either look or not look like Gaussian distribution.

In this paper, we quantify the distributions of values of $Gut(G_n)$ and $S(G_n)$.

Polyphenylenes, cyclooctatetraenes, and their derivatives have been the subject of considerable attention among chemists for many years, closely associated with certain classes of graphs. These graphs exhibit intriguing structures and properties, both of which have corresponding chains of chemical compounds, as detailed in [18–20]. We speculate whether the 2k cycle chains exhibit properties similar to those of polyphenylenes, cyclooctatetraenes, and their derivatives. The research methodologies in chemical graph theory assist in analyzing and describing the topological features, connectivity, and possible reaction pathways of these chains. By considering various indices and parameters, we can gain better insights into harnessing the role of 2k-gon chains in chemistry and materials science, paving the way for future innovations and advancements [21,22].

Researchers have investigated the mathematical properties of random polyphenylene chains and random cyclooctatetraene chains [23–26]. Zhu [27] conducted research on establishing explicit analytical expressions for the simple formulas of the expected values of Gutman and Schultz indices in a random polygon. By applying the concepts of symmetry and probability theory, we aim to derive the exact analytical expressions, as well as their asymptotic behaviors, for the variances of the Schultz index and Gutman index of a random chain composed of n 2k-gon polygons. This research plays a crucial role in the study and application of topological indices [28].

In this paper, we make the following hypothesis.

Hypothesis 1. *Our choice of attaching the new terminal 2k-gon polygon H_{n+1} to G_n, $n = 2, 3, \ldots$ is random and independent. In more accurate words, the series of random variables $Z_n^1, Z_n^2, Z_n^3, \cdots, Z_{nn=2}^{k\infty}$ is independent and has the same law (1.5). For $i \in 1, 2, 3, \cdots, k$, we have $0 < p_i < 1$.*

(a) Under Hypothesis 1, we give analytical expressions for the variances of $Gut(G_n)$ and $S(G_n)$.

(b) We prove that the random variables $Gut(G_n)$ and $S(G_n)$ are asymptotic to normal distributions when $n \to \infty$. That is

$$\lim_{n\to\infty} \sup_{x\in\mathbb{R}} \left| \mathbb{P}\left(\left(\frac{Gut(G_n) - \mathbb{E}(Gut(G_n))}{\sqrt{Var(Gut(G_n))}}\right) \leq x\right) - \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}dt} \right| = 0$$

where $\mathbb{E}(X)$ and $Var(X)$ denote the expected value and variance of the random variable X, respectively.

2. The Limiting Behavior of the Gutman Index of a Random Polygon Chain

For a random chain G_n, which is composed of n 2k-gon polygons, both the Gutman index and the Schultz index are random variables. In this section, we will explore and compute the variances of $Gut(G_n)$ and $S(G_n)$. As depicted in Figure 1, G_{n+1} is obtained by connecting G_n to a new terminal hexagon H_{n+1} by the edge $u_n x_1$, with the vertices of H_{n+1} labeled $x_1, x_2, \cdots, x_{2k}$ in clockwise orientation, where $\forall n \geq 2$. On the one hand, for all $v \in V_{G_n} \subseteq V_{G_{n+1}}$, $\forall x_i \in H_{n+1}$, it holds that

$$d(x_1, v) = d(u_n, v) + 1, \ d(x_2, v) = d(u_n, v) + 2, \ \cdots, \ d(x_k, v) = d(u_n, v) + k, \tag{6}$$

$$d(x_{k+1}, v) = d(u_n, v) + k + 1, \ d(x_{k+2}, v) = d(u_n, v) + k, \ \cdots, \ d(x_{2k}, v) = d(u_n, v) + 2, \tag{7}$$

$$\sum_{v\in V_{G_n}} d_{G_{n+1}}(v) = (4k+2)n - 1. \tag{8}$$

On the other hand,

$$\sum_{i=1}^{2k} d(x_i)d(x_1, x_i) = 2k^2, \ \sum_{i=1}^{2k} d(x_i)d(x_2, x_i) = 2k^2 + 1, \ \cdots, \ \sum_{i=1}^{2k} d(x_i)d(x_{k+1}, x_i) = 2k^2 + k, \tag{9}$$

$$\sum_{i=1}^{2k} d(x_i)d(x_{k+2}, x_i) = 2k^2 + k + 1, \ \sum_{i=1}^{2k} d(x_i)d(x_{k+3}, x_i) = 2k^2 + k, \ \cdots, \ \sum_{i=1}^{2k} d(x_i)d(x_{2k}, x_i) = 2k^2 + 1. \tag{10}$$

In [27] Theorem 1, the author demonstrates that

$$\begin{aligned}\mathbb{E}(Gut(G_n)) =& \{(18k^3 + 16k^2 + 10k + 2) - (2k+1)\sum_{i=1}^{k-1}[4k^2 - (4i-2)k - 2i]p_i\}\frac{n^3}{3} \\ &- \{(4k^2 + 6k + 2) - (2k+1)\sum_{i=1}^{k-1}[4k^2 - (4i-2)k - 2i]p_i\}n^2 \\ &+ \{(4k^3 - 4k^2 + 8k + 7) - 2(2k+1)\sum_{i=1}^{k-1}[4k^2 - (4i-2)k - 2i]p_i\}\frac{n}{3} - 1.\end{aligned}$$

This section begins with the introduction of the first main result.

Theorem 1. *The following results obtained are dependent on whether the following Hypothesis 1 is true.*

(i) The Gutman index of G_n, which is a random 2k-sided chain, is $Gut(G_n)$, and the variance in it is determined by

$$Var(Gut(G_n)) = \frac{1}{30}(\sigma^2 n^5 - 5rn^4 + 10\tilde{\sigma}^2 n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2 + (-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)).$$

where

$$\sigma^2 = \sum_{i=1}^{k}(a_i^2 p_i) - (\sum_{i=1}^{k}(a_i p_i))^2$$
$$\tilde{\sigma}^2 = \sum_{i=1}^{k}(b_i^2 p_i) - (\sum_{i=1}^{k}(b_i p_i))^2$$
$$r = \sum_{i=1}^{k}(a_i b_i p_i) - \sum_{i=1}^{k}(a_i p_i)\sum_{i=1}^{k}(b_i p_i)$$

with

$$a_i = (i+1)(4k+2)^2$$
$$b_i = (4k+2)[(i+1)(4k+3) - (2k^2+i)]$$
$$i = 1, 2, 3, \cdots, k$$

(ii) As $n \to \infty$, the limiting behavior of $Gut(G_n)$ converges to a normal distribution. In other words,

$$\lim_{n\to\infty}\sup_{x\in\mathbb{R}}\left|\mathbb{P}\left(\frac{Gut(G_n) - \mathbb{E}(Gut(G_n))}{\sqrt{Var(Gut(G_n))}}\right) \le x) - \int_{-\infty}^{x}\frac{1}{\sqrt{2\pi}}e^{-\frac{t^2}{2}}du\right| = 0$$

Proof. (i) As concluded in [27], we can derive that

$$Gut(G_{n+1}) = Gut(G_n) + (4k+2)\sum_{v\in V_{G_n}} d(v)d(u_n, v) + (8k^3 + 20k^2 + 12k + 2)n + (4k^3 - 4k - 1). \quad (11)$$

Let

$$A_n := (4k+2)\sum_{v\in V_{G_n}} d(v)d(u_n, v).$$

and we can then obtain

$$Gut(G_{n+1}) = Gut(G_n) + A_n + (8k^3 + 20k^2 + 12k + 2)n + (4k^3 - 4k - 1). \quad (12)$$

□

With regard to the random variables $Z_n^1, Z_n^2, Z_n^3, \cdots, Z_n^k$ mentioned in the method of constructing G_{n+1} from G_n in Section 1, we can establish the following four equalities.

Equality 1.

$$A_n Z_n^1 = \{A_{n-1} + 2(4k+2)^2 n - (4k+2)[2(4k+3) - (2k^2+1)]\}Z_n^1$$

The above equality is trivial if $Z_n^1 = 0$, so our focus lies on the case in which $Z_n^1 = 1$, indicating the transition $G_n \longrightarrow G_{n+1}^1$. In this scenario, vertex u_n in G_n coincides with either vertex x_2 or x_{2k} in H_n. That is to say, $u_n = x_1$ would be replaced by $u_n = x_2$ or $u_n = x_{2k}$, as shown in Figure 4. As a result, A_n can be expressed as

$$
\begin{aligned}
(4k+2)\sum_{v\in V_{G_n}} d(v)d(x_2,v) &= (4k+2)\sum_{v\in V_{G_{n-1}}} d(v)d(x_2,v) + (4k+2)\sum_{v\in V_{H_n}} d(v)d(x_2,v)\\
&= (4k+2)\sum_{v\in V_{G_{n-1}}} d(v)(d(v,u_{n-1}) + d(x_2,u_{n-1})) + (4k+2)\sum_{v\in V_{H_n}} d(v)d(x_2,v)\\
&= (4k+2)\sum_{v\in V_{G_{n-1}}} d(v)(d(v,u_{n-1}) + 2) + (4k+2)(2k^2+1)\\
&= A_{n-1} + 2(4k+2)\sum_{v\in V_{G_{n-1}}} d(v) + (4k+2)(2k^2+1)\\
&= A_{n-1} + 2(4k+2)((4k+2)n - (4k+3)) + (4k+2)(2k^2+1),\\
&= A_{n-1} + 2(4k+2)^2 n - (4k+2)[2(4k+3) - (2k^2+1)]
\end{aligned}
$$

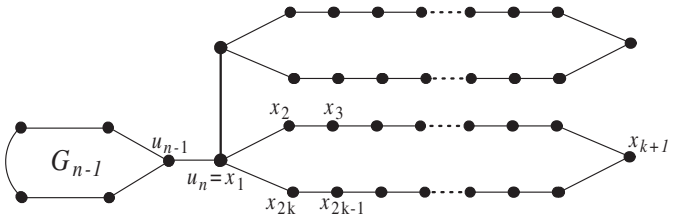


Figure 4. $G_n \to G^1_{n+1}$.

By employing Equations (6)–(8) mentioned above, we are able to establish the desired equality.

Equality 2.

$$A_n Z^2_n = \{A_{n-1} + 3(4k+2)^2 n - (4k+2)[3(4k+3) - (2k^2+2)]\}Z^2_n$$

Similar to the proof of Equality 1, we solely focus on the scenario where $Z^2_n = 1$, resulting in the transformation $G_n \longrightarrow G^2_{n+1}$. The proof follows a similar approach, and we have chosen to omit the specific details.

Similarly, when reaching the vertex labeled as x_{k+1} in H_n, we just only consider the case $Z^k_n = 1$, which corresponds to $G_n \longrightarrow G^k_{n+1}$. By doing so, we obtain the following result:

Equality 3.

$$A_n Z^k_n = \{A_{n-1} + (k+1)(4k+2)^2 n - (4k+2)[(k+1)(4k+3) - (2k^2+k)]\}Z^k_n$$

The proof follows the same steps as the previous equalities, and we will omit the details. Therefore, we can derive the general form of the analytic formula for $A_n Z^i_n$ as described below:

Equality 4.

$$A_n Z^i_n = \{A_{n-1} + (i+1)(4k+2)^2 n - (4k+2)[(i+1)(4k+3) - (2k^2+i)]\}Z^i_n$$

where $i \in 1, 2, \cdots, k$. We will restrict our analysis to the case where $Z^i_n = 1$, corresponding to $G_n \longrightarrow G^i_{n+1}$. The proof follows a similar approach as for the previously mentioned equalities and we will skip the details.

Taking into account the observation that $Z^1_n + Z^2_n + \cdots + Z^i_n + \cdots + Z^k_n = 1$, as mentioned earlier, we can conclude that

$$
\begin{aligned}
A_n &= A_n(Z_n^1 + Z_n^2 + \cdots + Z_n^i + \cdots + Z_n^k) \\
&= \{A_{n-1} + 2(4k+2)^2 n - (4k+2)[2(4k+3) - (2k^2+1)]\} Z_n^1 \\
&+ \{A_{n-1} + 3(4k+2)^2 n - (4k+2)[3(4k+3) - (2k^2+2)]\} Z_n^2 \\
&+ \cdots \\
&+ \{A_{n-1} + (i+1)(4k+2)^2 n - (4k+2)[(i+1)(4k+3) - (2k^2+i)]\} Z_n^i \\
&+ \cdots \\
&+ \{A_{n-1} + (k+1)(4k+2)^2 n - (4k+2)[(k+1)(4k+3) - (2k^2+k)]\} Z_n^k \\
&= A_{n-1}(Z_n^1 + Z_n^2 + \cdots + Z_n^i + \cdots + Z_n^k) \\
&+ [2(4k+2)^2 Z_n^1 + 3(4k+2)^2 Z_n^2 + \cdots + (i+1)(4k+2)^2 Z_n^i + \cdots + (k+1)(4k+2)^2 Z_n^k] n \\
&- \{(4k+2)[2(4k+3) - (2k^2+1)] Z_n^1 + (4k+2)[3(4k+3) - (2k^2+2)] Z_n^2 + \cdots \\
&+ (4k+2)[(i+1)(4k+3) - (2k^2+i)] Z_n^i + \cdots + (4k+2)[(k+1)(4k+3) - (2k^2+k)] Z_n^k\} \\
&= A_{n-1} + \sum_{i=1}^{k} (i+1)(4k+2)^2 Z_n^i - \sum_{i=1}^{k} (4k+2)[(i+1)(4k+3) - (2k^2+i)]\} Z_n^i \\
&= A_{n-1} + \sum_{i=1}^{k} a_i Z_n^i - \sum_{i=1}^{k} b_i Z_n^i \\
&= A_{n-1} + nU_n - V_n
\end{aligned}
$$

where for each n,$i \in \{1, 2, 3, \cdots, k\}$,

$$U_n = \sum_{i=1}^{k} a_i Z_n^i, \;\; V_n = \sum_{i=1}^{k} b_i Z_n^i.$$

From Equation (12), we can deduce

$$
\begin{aligned}
Gut(G_n) &= Gut(G_1) + \sum_{i=1}^{n-1} A_i + \sum_{i=1}^{n-1} [(8k^3 + 20k^2 + 12k + 2)n + (4k^3 - 4k - 1)] \\
&= Gut(G_1) + \sum_{i=1}^{n-1} (\sum_{j=1}^{i-1} (A_{j+1} - A_j) + A_1) + \sum_{i=1}^{n-1} [(8k^3 + 20k^2 + 12k + 2)n + (4k^3 - 4k - 1)] \\
&= Gut(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} (A_{j+1} - A_j) + (n-1)A_1 + \sum_{i=1}^{n-1} [(8k^3 + 20k^2 + 12k + 2)n + (4k^3 - 4k - 1)] \\
&= Gut(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + (n-1)A_1 + \sum_{i=1}^{n-1} [(8k^3 + 20k^2 + 12k + 2)n + (4k^3 - 4k - 1)]
\end{aligned}
$$

Since both A_1 and $\sum_{i=1}^{n-1} [(8k^3 + 20k^2 + 12k + 2)n + (4k^3 - 4k - 1)]$ are constant terms and both are independent of i, $Gut(G_n)$ can be written as

$$Gut(G_n) = Gut(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + O(n^2)$$

Directly calculating shows that $Var(U_j) = \sigma^2$, $Var(V_j) = \tilde{\sigma}^2$, and $Cov(U_j, V_j) = r$, and $Cov(X, Y) := \mathbb{E}(XY) - \mathbb{E}(X)\mathbb{E}(Y)$ denotes the covariance of any two random variables X and Y. Applying the properties of variance and the rule of interchanging the order of sums yields the following

$$
\begin{aligned}
Var(Gut(G_n)) &= Var(\sum_{i=1}^{n-1}\sum_{j=1}^{i-1}((j+1)U_{j+1}-V_{j+1})) \\
&= Var(\sum_{j=1}^{n-2}\sum_{i=j+1}^{n-1}((j+1)U_{j+1}-V_{j+1})) \\
&= Var(\sum_{j=1}^{n-2}((j+1)U_{j+1}-V_{j+1})(n-j-1)) \\
&= \sum_{j=1}^{n-2}(n-j-1)^2 Var((j+1)U_{j+1}-V_{j+1}) \\
&= \sum_{j=1}^{n-2}(n-j-1)^2 Cov((j+1)U_{j+1}-V_{j+1},(j+1)U_{j+1}-V_{j+1}) \\
&= \sum_{j=1}^{n-2}(n-j-1)^2((j+1)^2 Cov(U_{j+1},U_{j+1})-2(j+1)Cov(U_{j+1},V_{j+1})+Cov(V_{j+1},V_{j+1})) \\
&= \sum_{j=1}^{n-2}(n-j-1)^2((j+1)^2\sigma^2-2(j+1)r+\tilde{\sigma}^2)
\end{aligned}
$$

By utilizing computational, ad hoc tools (see Appendix A for details), the aforementioned equality suggests the intended outcome of $Var(Gut(G_n))$.

(ii) We are now ready to demonstrate the second part of this theorem. First, for any $n \in \mathbb{N}$, we set

$$\mathcal{U}_n = \sum_{i=1}^{n-1}\sum_{j=1}^{i-1}(j+1)U_{j+1}, \mathcal{V}_n = \sum_{i=1}^{n-1}\sum_{j=1}^{i-1}V_{j+1}$$

and $\mu = \mathbb{E}(U_j)$, $\phi(t) = \mathbb{E}\exp\{t(U_j-\mu)\}$. With these notations, we can explicitly obtain that

$$
\begin{aligned}
\mathbb{E}\exp\{t(\mathcal{U}_n-\mathbb{E}(\mathcal{U}_n))\} &= \mathbb{E}\exp\left\{t(\sum_{i=1}^{n-1}\sum_{j=1}^{i-1}(j+1)(U_{j+1}-\mu))\right\} \\
&= \mathbb{E}\exp\left\{t(\sum_{j=1}^{n-2}\sum_{i=j+1}^{n-1}(j+1)(U_{j+1}-\mu))\right\} \\
&= \mathbb{E}\exp\left\{t(\sum_{j=1}^{n-2}(n-j-1)(j+1)(U_{j+1}-\mu))\right\} \\
&= \Pi_{j=1}^{n-2}\mathbb{E}\exp\{t(n-j-1)(j+1)(U_{j+1}-\mu)\} \\
&= \Pi_{j=1}^{n-2}\phi(t(n-j-1)(j+1))
\end{aligned}
$$

There exists $C > 0$ such that

$$\mathcal{V}_n = \sum_{i=1}^{n-1}\sum_{j=1}^{i-1}V_{j+1} \leq Cn^2. \tag{13}$$

If without confusion, we consider $f(n)$, $g(n)$ two functions of n, we can define $f(n) \asymp g(n)$ if $\lim_{n\to\infty}\frac{f(n)}{g(n)} = 1$, and for some $C > 0$, we denote $f(n) = O(g(n))$ if $\overline{\lim_{n\to\infty}}\frac{f(n)}{g(n)} \leq C$. Considering the relationship $Var(Gut(G_n)) \asymp \frac{1}{30}\sigma^2 n^5$ and the above equations, by using Taylor's formula, one can deduce that

$$\lim_{n\to\infty}\mathbb{E}\exp\left\{t\frac{Gut(G_n)-\mathbb{E}(Gut(G_n))}{\sqrt{Var(Gut(G_n))}}\right\}$$
$$=\lim_{n\to\infty}\mathbb{E}\exp\left\{t\frac{(Gut(G_1)+\mathcal{U}_n-\mathcal{V}_n+O(n^2))-\mathbb{E}(Gut(G_1)+\mathcal{U}_n-\mathcal{V}_n+O(n^2))}{\frac{\sigma n^{\frac{5}{2}}}{\sqrt{30}}}\right\}$$
$$=\lim_{n\to\infty}\mathbb{E}\exp\left\{t\frac{\sqrt{30}(\mathcal{U}_n-\mathbb{E}(\mathcal{U}_n))}{\sigma n^{\frac{5}{2}}}\right\}$$
$$=\lim_{n\to\infty}\Pi_{j=1}^{n}\phi\left(\frac{\sqrt{30}t(n-j-1)(j+1)}{\sigma n^{\frac{5}{2}}}\right)$$
$$=\lim_{n\to\infty}\mathbb{E}\exp\left\{\sum_{j=1}^{n}\ln\phi\left(\frac{\sqrt{30}t(n-j-1)(j+1)}{\sigma n^{\frac{5}{2}}}\right)\right\}$$

where we employ $\phi(t)=1+\frac{\sigma^2}{2}t^2+o(t^2)$ such that

$$\lim_{n\to\infty}\mathbb{E}\exp\left\{t\frac{Gut(G_n)-\mathbb{E}(Gut(G_n))}{\sqrt{Var(Gut(G_n))}}\right\}$$
$$=\lim_{n\to\infty}\mathbb{E}\exp\left\{\sum_{j=1}^{n}\ln\left(1+\frac{\sigma^2}{2}\frac{30t^2(n-j-1)^2(j+1)^2}{\sigma^2n^5}+o(\frac{1}{n})\right)\right\}$$
$$=\lim_{n\to\infty}\mathbb{E}\exp\left\{\sum_{j=1}^{n-2}\left(\frac{\sigma^2}{2}\frac{30t^2(n-j-1)^2(j+1)^2}{\sigma^2n^5}+o(\frac{1}{n})\right)\right\}$$
$$=e^{\frac{t^2}{2}}$$

where we applied $\sum_{j=1}^{n-2}(n-j-1)^2(j+1)^2\asymp\frac{n^5-30n^2+59n-30}{30}\asymp\frac{1}{30}n^5$, which can be confirmed by computational methods. When i is in the complex field and satisfies the condition $i^2=-1$, by substituting t with it in the above equation, we obtain

$$\lim_{n\to\infty}\mathbb{E}\exp\left\{ti\frac{Gut(G_n)-\mathbb{E}(Gut(G_n))}{\sqrt{Var(Gut(G_n))}}\right\}=e^{-\frac{t^2}{2}}$$

Based on the aforementioned equality in Chapter 1 of [29] and the continuity theory in Chapter 15 of [30] for characteristic functions in probability, we have successfully provided proof of Theorem 1 (ii).

3. The Limiting Behavior of the Schultz Index of a Random Polygon Chain

We will now delve into the variance of the Schultz index for a random polygonal chain. In [27], Theorem 2.3 states that:

$$\begin{aligned}\mathbb{E}(S(G_n))=&\{(8k^3+12k^2+4k)-2\sum_{i=1}^{k-1}[4k^3-(4i-2)k^2-2ik]p_i\}\frac{n^3}{3}\\&-\{(2k^2+2k)-2\sum_{i=1}^{k-1}[4k^3-(4i-2)k^2-2ik]p_i\}n^2\\&+\{(4k^3-6k^2+2k)-2\cdot2\sum_{i=1}^{k-1}[4k^3-(4i-2)k^2-2ik]p_i\}\frac{n}{3}.\end{aligned}$$

Next, we present our findings.

Theorem 2. *Given Hypothesis 1, the following results are valid:*
(i) The Schultz index of G_n, which is a random $2k-$sided chain, is $S(G_n)$, and the variance in it is determined by

$$\begin{aligned} Var(S(G_n)) =& \frac{1}{30}(\sigma^2 n^5 - 5rn^4 + 10\tilde{\sigma}^2 n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2 \\ &+ (-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)). \end{aligned}$$

where

$$\begin{aligned} \sigma^2 &= \sum_{i=1}^{k}(c_i^2 p_i) - (\sum_{i=1}^{k}(c_i p_i))^2 \\ \tilde{\sigma}^2 &= \sum_{i=1}^{k}(d_i^2 p_i) - (\sum_{i=1}^{k}(d_i p_i))^2 \\ r &= \sum_{i=1}^{k}(c_i d_i p_i) - \sum_{i=1}^{k}(c_i p_i)\sum_{i=1}^{k}(d_i p_i) \end{aligned}$$

with

$$\begin{aligned} c_i =& (i+1)(16k^2 + 8k) \\ d_i =& i(16k^2 + 8k) - 8k^3 + 14k^2 + 10k \\ i =& 1, 2, 3, \cdots, k \end{aligned}$$

(ii) As $n \to \infty$, the limiting behavior of $S(G_n)$ converges to a normal distribution. In other words,

$$\lim_{n\to\infty} \sup_{x\in\mathbb{R}} \left| \mathbb{P}\left(\frac{S(G_n) - \mathbb{E}(S(G_n))}{\sqrt{Var(S(G_n))}}\right) \leq x) - \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}du} \right| = 0$$

Proof. (i) As concluded in [27], we can derive that

$$S(G_{n+1}) = S(G_n) + (4k+2)\sum_{v\in V_{G_n}} d(u_n, v) + 2k\sum_{v\in V_{G_n}} d(v)d(u_n, v) + (8k^3 + 18k^2 + 6k)n + (4k^3 - 2k). \tag{14}$$

Let

$$B_n := \sum_{v\in V_{G_n}} [(4k+2) + 2kd(v)]d(u_n, v).$$

and we can then obtain

$$S(G_{n+1}) = S(G_n) + B_n + (8k^3 + 18k^2 + 6k)n + (4k^3 - 2k).$$

□

With regard to the random variables $Z_n^1, Z_n^2, Z_n^3, \cdots, Z_n^k$ mentioned in Section 1, this signifies the approach we have taken in constructing G_{n+1} from G_n. Consequently, we can establish the following four equalities:

Equality 1.

$$B_n Z_n^1 = \{B_{n-1} + 2(16k^2 + 8k)n - [2(16k^2 + 8k) - 8k^3 + 14k^2 + 10k]\}Z_n^1$$

The above equality is trivial if $Z_n^1 = 0$, so our focus lies on the case where $Z_n^1 = 1$, indicating the transition $G_n \longrightarrow G_{n+1}^1$. In this scenario, vertex u_n in G_n coincides with either vertex x_2 or x_{2k} in H_n, as shown in Figure 4. As a result, B_n can be expressed as

$$
\begin{aligned}
B_n &= \sum_{v\in V_{G_n}} [(4k+2)+2kd(v)]d(x_2,v) \\
&= \sum_{v\in V_{G_{n-1}}} [(4k+2)+2kd(v)]d(x_2,v) + \sum_{v\in V_{Hn}} [(4k+2)+2kd(v)]d(x_2,v) \\
&= \sum_{v\in V_{G_{n-1}}} [(4k+2)+2kd(v)](d(u_{n-1},v)+2) + (4k+2)k^2 + 2k(2k^2+1) \\
&= \sum_{v\in V_{G_{n-1}}} [(4k+2)+2kd(v)]d(u_{n-1},v) + 2\sum_{v\in V_{G_{n-1}}} [(4k+2)+2kd(v)] + (4k+2)k^2 + 2k(2k^2+1) \\
&= \sum_{v\in V_{G_{n-1}}} [(4k+2)+2kd(v)]d(u_{n-1},v) + 2\{(4k+2)2k(n-1) + 2k[(4k+2)(n-1)-1]\} + (4k+2)k^2 + 2k(2k^2+1) \\
&= B_{n-1} + 2(16k^2+8k)n - 2(16k^2+8k) + 8k^3 + 2k^2 + 2k \\
&= B_{n-1} + 2(16k^2+8k)n - [2(16k^2+8k) - 8k^3 + 14k^2 + 10k]
\end{aligned}
$$

By employing Equations (6)–(8) mentioned above, we are able to establish the desired equality.

Equality 2.

$$B_n Z_n^2 = \{B_{n-1} + 3(16k^2+8k)n - [3(16k^2+8k) - 8k^3 + 14k^2 + 10k]\}Z_n^2$$

Similar to the proof of Equality 1, we solely focus on the scenario where $Z_n^2 = 1$, resulting in the transformation $G_n \longrightarrow G_{n+1}^2$. The proof follows a similar approach, and we have chosen to omit the specific details.

Similarly, when reaching the vertex labeled as x_{k+1} in H_n, we just only consider the case $Z_n^k = 1$, which corresponds to $G_n \longrightarrow G_{n+1}^k$. In doing so, we obtain the following result:

Equality 3.

$$B_n Z_n^k = \{B_{n-1} + (k+1)(16k^2+8k)n - [k(16k^2+8k) - 8k^3 + 14k^2 + 10k]\}Z_n^k$$

The proof follows the same steps as the previous equalities, and we will omit the details. Therefore, we can derive the general form of the analytic formula for $A_n Z_n^i$ as described below:

Equality 4.

$$B_n Z_n^i = \{B_{n-1} + (i+1)(16k^2+8k)n - [i(16k^2+8k) - 8k^3 + 14k^2 + 10k]\}Z_n^i$$

where $i \in 1, 2, \cdots, k$. We will restrict our analysis to the case where $Z_n^i = 1$, corresponding to $G_n \longrightarrow G_{n+1}^i$. The proof follows a similar approach as for the previously mentioned equalities, and we will skip the details.

Taking into account the observation that $Z_n^1 + Z_n^2 + \cdots + Z_n^i + \cdots + Z_n^k = 1$, as mentioned earlier, we can conclude that

$$
\begin{aligned}
B_n &= B_n(Z_n^1 + Z_n^2 + \cdots + Z_n^i + \cdots + Z_n^k) \\
&= \{B_{n-1} + 2(16k^2+8k)n - [1(16k^2+8k) - 8k^3 + 14k^2 + 10k]\}Z_n^1 \\
&+ \{B_{n-1} + 3(16k^2+8k)n - [2(16k^2+8k) - 8k^3 + 14k^2 + 10k]\}Z_n^2 \\
&+ \cdots \\
&+ \{B_{n-1} + (i+1)(16k^2+8k)n - [i(16k^2+8k) - 8k^3 + 14k^2 + 10k]\}Z_n^i \\
&+ \cdots \\
&+ \{B_{n-1} + (k+1)(16k^2+8k)n - [k(16k^2+8k) - 8k^3 + 14k^2 + 10k]\}Z_n^k \\
&= B_{n-1}(Z_n^1 + Z_n^2 + \cdots + Z_n^i + \cdots + Z_n^k) \\
&+ [2(16k^2+8k)Z_n^1 + 3(16k^2+8k)Z_n^2 + \cdots + (i+1)(16k^2+8k)Z_n^i + \cdots + (k+1)(16k^2+8k)Z_n^k]n \\
&- \{[1(16k^2+8k) - 8k^3 + 14k^2 + 10k]Z_n^1 + [2(16k^2+8k) - 8k^3 + 14k^2 + 10k]Z_n^2 + \cdots \\
&+ [i(16k^2+8k) - 8k^3 + 14k^2 + 10k]Z_n^i + \cdots + [k(16k^2+8k) - 8k^3 + 14k^2 + 10k]Z_n^k\} \\
&= B_{n-1} + \sum_{i=1}^{k}(i+1)(16k^2+8k)Z_n^i - \sum_{i=1}^{k}[i(16k^2+8k) - 8k^3 + 14k^2 + 10k]Z_n^i \\
&= B_{n-1} + \sum_{i=1}^{k} c_i Z_n^i - \sum_{i=1}^{k} d_i Z_n^i \\
&= B_{n-1} + nU_n - V_n
\end{aligned}
$$

where for each n,$i \in \{1, 2, 3, \cdots, k\}$,

$$U_n = \sum_{i=1}^{k} c_i Z_n^i, \;\; V_n = \sum_{i=1}^{k} d_i Z_n^i.$$

From Equation (12), we can deduce

$$
\begin{aligned}
S(G_n) &= S(G_1) + \sum_{i=1}^{n-1} B_i + \sum_{i=1}^{n-1}[(8k^3 + 18k^2 + 6k)n + (4k^3 - 2k)] \\
&= S(G_1) + \sum_{i=1}^{n-1}(\sum_{j=1}^{i-1}(B_{j+1} - B_j) + B_1) + \sum_{i=1}^{n-1}[(8k^3 + 18k^2 + 6k)n + (4k^3 - 2k)] \\
&= S(G_1) + \sum_{i=1}^{n-1}\sum_{j=1}^{i-1}(B_{j+1} - B_j) + (n-1)B_1 + \sum_{i=1}^{n-1}[(8k^3 + 18k^2 + 6k)n + (4k^3 - 2k)] \\
&= S(G_1) + \sum_{i=1}^{n-1}\sum_{j=1}^{i-1}((j+1)U_{j+1} - V_{j+1}) + (n-1)B_1 + \sum_{i=1}^{n-1}[(8k^3 + 18k^2 + 6k)n + (4k^3 - 2k)] \\
&= S(G_1) + \sum_{i=1}^{n-1}\sum_{j=1}^{i-1}((j+1)U_{j+1} - V_{j+1}) + O(n^2)
\end{aligned}
$$

Directly calculating shows that $Var(U_j) = \sigma^2$, $Var(V_j) = \tilde{\sigma}^2$, and $Cov(U_j, V_j) = r$, and $Cov(X, Y) := \mathbb{E}(XY) - \mathbb{E}(X)\mathbb{E}(Y)$ denote the covariance of any two random variables X and Y. Applying the properties of variance and the rule of interchanging the order of sums yields the result that

$$
\begin{aligned}
Var(S(G_n)) &= Var(\sum_{i=1}^{n-1}\sum_{j=1}^{i-1}((j+1)U_{j+1}-V_{j+1})) \\
&= Var(\sum_{j=1}^{n-2}\sum_{i=j+1}^{n-1}((j+1)U_{j+1}-V_{j+1})) \\
&= Var(\sum_{j=1}^{n-2}((j+1)U_{j+1}-V_{j+1})(n-j-1)) \\
&= \sum_{j=1}^{n-2}(n-j-1)^2 Var((j+1)U_{j+1}-V_{j+1}) \\
&= \sum_{j=1}^{n-2}(n-j-1)^2 Cov((j+1)U_{j+1}-V_{j+1},(j+1)U_{j+1}-V_{j+1}) \\
&= \sum_{j=1}^{n-2}(n-j-1)^2((j+1)^2 Cov(U_{j+1},U_{j+1})-2(j+1)Cov(U_{j+1},V_{j+1})+Cov(V_{j+1},V_{j+1})) \\
&= \sum_{j=1}^{n-2}(n-j-1)^2((j+1)^2\sigma^2-2(j+1)r+\tilde{\sigma}^2)
\end{aligned}
$$

Using the same procedure as used in Gutman index, we obtain $Var(S(G_n))$.

(ii) Similarly to the aforementioned derivation process of the Gutman index, we can obtain that

$$\lim_{n\to\infty}\mathbb{E}\exp\left\{ti\frac{S(G_n)-\mathbb{E}(S(G_n))}{\sqrt{Var(S(G_n))}}\right\}=e^{-\frac{t^2}{2}}$$

4. Concluding Remarks

In this paper, we obtain explicit analytical expressions for the variances of the Gutman index and the Schultz index of a random polygonal chain composed of n 2k-sided polygons. Furthermore, we proved that the random variables $Gut(G_n)$ and $(S(G_n)$ approach normal distributions asymptotically as $n \to \infty$. These findings will significantly contribute to our comprehension of the inherent patterns and trends exhibited by the Gutman and Schultz indices in random-sided graphs. By further elucidating the limiting behaviors, we can gain deeper insights into the structural characteristics and properties of these graphs. Furthermore, the continuous advancement and progress of science are driving forces behind the continuous discovery and creation of new molecules, leading to advancements in various fields and applications. Researchers are extensively studying polygonal chains in chemical graph theory. Establishing exact formulas for the variances of certain indices in a random polygonal chain composed of n regular polygons is within the realm of possibility. Furthermore, we can anticipate obtaining the additional behaviors of the random-sided chain graph and its physicochemical properties in the near future through these studies. We are able not only to obtain precise expressions for the variance of random-sided graph chains but also to study their asymptotic behavior. As a result of these discoveries, future research in this field will undergo remarkable growth and expansion.

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Appendix A

matlab codes; syms n k d1 r d2; $f = (n-k-1)^2 * ((k+1)^2 * d1^2 - 2 * (k+1) * r + d2^2)$; $f2 = simplify(symsum(f, k, 1, n-2)); collect(f2, n)$.

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