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The limiting behaviors for the Gutman index and the Schultz index in a random $(2k+1)$-polygonal chain

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Abstract. The exact formulae for the variances of the Gutman index and the Schultz index of a random $(2k+1)$-polygonal chain is obtained in this paper. We also show that these two indices of a random $(2k+1)$-polygonal chain obey normal distributions asymptotically. We expanded on several previously published findings. We apply the unified formulae to get the limiting behaviors of the Gutman index and the Schultz index of a specific random polygonal chain, which have been extensively explored in statistical physics and organic chemistry.

1. Introduction

The topological index of the graph plays an important role in establishing the relationship between the molecular structure and features and characterizing the chemical molecular graph. It is widely used to predict the biological activities and physicochemical properties of compounds. The book[1] contains all notation not specified in this paper. Let $G = (V(G), E(G))$ be a simple finitely connected graph with $V(G)$ and $E(G)$ as the vertex and edge sets. The length of the shortest (u, v)-path in G is represented by the distance $d_G(u, v)$ between two vertices u and v of G. The degree of u is $d_G(u)$ for $u \in V(G)$.

H. Wiener developed the first topological index linked to molecular branching in 1947[2]. In 1971 H. Hosoya expanded it and presented the formal definition[3] of Wiener index of a graph G. Let $\omega : V(G) \to \mathbb{N}^+$ is a weight function and $\oplus$ is one of the four operations $+$, $-$, $\times$ and $\div$. Then the weighted Wiener index of a graph G is therefore defined as follows:

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

If $\oplus$ is the operation $\times$ and $\omega(\cdot) = d_G(\cdot)$, then the weighted Wiener index is commonly referred to as the Gutman index, which was introduced by Gutman in 1994 and denoted by $Gut(G)$. If $\oplus$ is the operation $+$

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and $\omega(\cdot) = d_G(\cdot)$, then the weighted Wiener index is known as the Schultz index and represented by $S(G)$. Many features of molecular structure are closely related to the Gutman index and the Schultz index([4]-[6]).

$$Gut(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u)d_G(v)d_G(u,v). \tag{1}$$

$$S(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u) + d_G(v))d_G(u,v). \tag{2}$$

Many academics have examined the computation of the Gutman index and the Schultz index of a range of special graphs and polygonal chains of some indices in recent years. See [7]-[8] for findings on the chemical applications of the Wiener index. Wei et al. achieved the expected value of Wiener index of a random polygonal chain[9]. The exact mathematical formulations of $\mathbb{E}(Gut(G_n))$, $\mathbb{E}(S(G_n))$, $\mathbb{E}(Kf^*(G_n))$ and $\mathbb{E}(Kf^+(G_n))$ in a random polyphenyl chain are developed by Zhang et al.[10]. The analytical formulations of $Var(Gut(G_n))$, $Var(S(G_n))$, $Var(Kf^*(G_n))$ and $Var(Kf^+(G_n))$ and their asymptotic behaviors in a random polyphenyl chain are constructed by Zhang et al.[11]. Li et al. studied the Kirchhoff indices of a random polygonal chain[12].

In this paper, we look into $Gut(G_n)$ and $S(G_n)$, where G_n is a set of n $(2k+1)$-polygons created in a recursive manner.

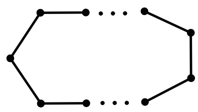

Figure 1: The specific form of a $(2k+1)$-polygonal chain G_1.

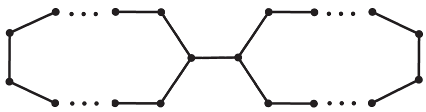

Figure 2: The specific form of a $(2k+1)$-polygonal chain G_2.

(1) The specific $(2k+1)$-polygonal chains for n=1 and n=2 are designated as G_1 and G_2, respectively(see Fig. 1 and Fig. 2).

(2) A new terminal $(2k+1)$-polygon O_{n+1} is attached to G_n to produce the $(2k+1)$-polygonal chain G_{n+1} with n+1 $(2k+1)$-polygons(see Fig. 3). We can connect the terminal $(2k+1)$-polygon O_{n+1} to G_n in k ways for any $n \geq 2$, and the resulting figures are denoted by $G^1_{n+1}, G^2_{n+1}, \cdots$, and G^k_{n+1}.

Inspired by [11], we perform a random selection in quick succession: the probability of receiving G^i_{n+1} from G_n is p_i for any $i = 1, 2, \cdots, k$. k random variables are represented by $Z^1_n, Z^2_n, \cdots, Z^k_n$. If we choice G^i_{n+1}, we set $Z^i_n = 1$; otherwise, we set $Z^i_n = 0$. Obviously,

$$\mathbb{P}(Z^i_n = 1) = p_i, \quad \mathbb{P}(Z^i_n = 0) = 1 - p_i, \quad \sum_{i=1}^{k} Z^i_n = 1, \quad i = 1, 2, \cdots, k. \tag{3}$$

For each i=1,2,$\cdots$,k, assume that the probability p_i is constant and independent on n. A zeroth-order Markov process is the mechanism outlined above. Then such a $(2k+1)$-polygonal chain is known as a random $(2k+1)$-polygonal chain and is indicated as $G_n(p_1, p_2, \cdots, p_k)$, abbreviated as G_n.

The following hypothesis is then put forward.

Hypothesis 1.1. *(i) Our selection to link the new terminal* $(2k+1)$*-polygon* O_{n+1} *to* G_n, $n = 2, 3, \ldots$, *are random and independently. To put it another way, the series of random variables* $\{Z^1_n, Z^2_n \cdots, Z^k_n\}^\infty_{n=2}$ *are independently and share the same Eq. (3).*

(ii) we have $0 < p_i < 1$ *for some* $i \in 1, 2, \cdots, k$.

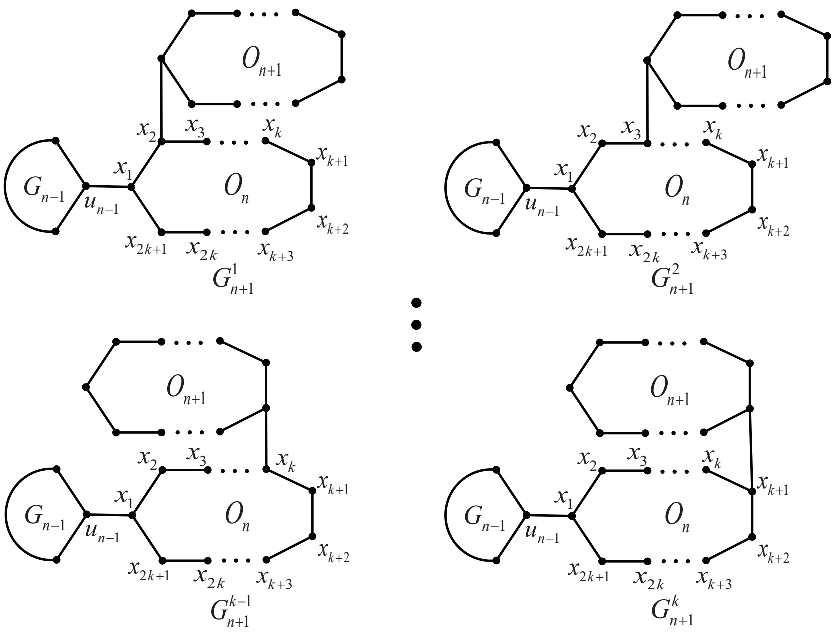

Figure 3: The k different forms of a $(2k+1)$-polygonal chain G_{n+1} with $n \geq 2$.

Under Hypothesis 1.1,

(a) We will construct analytical formulations for the variances of $Gut(G_n)$ and $S(G_n)$;

(b) We will show that the random variables $Gut(G_n)$ and $S(G_n)$ are asymptotic to normal distributions when n approaches infinity respectively. That is

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

To simplify the notations, we will use $d(u)$ and $d(u,v)$ instead of $d_G(u)$ and $d_G(u,v)$ respectively. Two functions of n are $f(n)$ and $g(n)$. We write $f(x) \asymp g(x)$ if $\lim_{x\to\infty} \frac{f(x)}{g(x)} = 1$, and $f(n) = O(g(n))$ if $\lim_{n\to\infty} \frac{f(n)}{g(n)} \leq C$ for some constant $C > 0$.

Zhang et al. researched the Gutman index and the Schultz index in a random polyphenyl chain (i.e. 6-polygonal chain) in 2021[11]. We will expand on the problem of the Gutman index and the Schultz index in a random polygonal chain, as inspired by [9]-[12]. Because G_n is a random graph, $Gut(G_n)$ and $S(G_n)$ are random variables in probability. In Section 2, we will provide the explicit formulae for the variances of the Gutman index and the Schultz index in a random $(2k+1)$-polygonal chain, as well as their asymptotic behaviors. In Section 3, we apply the unified formulae to get the limiting behaviors of the Gutman index and the Schultz index of a specific random polygonal chain.

2. The limiting behaviors for $Gut(G_n)$ and $S(G_n)$ in a random $(2k+1)$-polygonal chain

The limiting behaviors for $Gut(G_n)$ and $S(G_n)$ are determined in this section. According to Fig. 3, G_{n+1} is generated by connecting a new terminal $(2k+1)$-polygon O_{n+1} to G_n through an edge $u_n x_1$, with the vertices of O_{n+1} are recorded as $x_1, \cdots, x_{2k+1}$ in clockwise direction for $n \geq 2$. For any $v \in V(G_n)$ and $x_i \in O_{n+1}, i = 1, \cdots, 2k+1$,

$$d(x_i, v) = \begin{cases} d(u_n, v) + i, & i = 1, 2, \cdots, k+1, \\ d(u_n, v) + (2k+3-i), & i = k+2, k+3, \cdots, 2k+1, \end{cases} \tag{4}$$

and

$$\sum_{v\in V(G_n)} d_{G_{n+1}}(v) = (4k+4)n-1, \qquad \sum_{v\in V(G_{n-1})} d_{G_n}(v) = (4k+4)(n-1)-1. \tag{5}$$

Easy to see

$$\sum_{i=1}^{2k+1} d(x_i)d(x_j,x_i) = \begin{cases} 2k^2+2k+(j-1), & j=1,2,\cdots,k+1, \\ 2k^2+2k+(2k+2-j), & j=k+2,k+3,\cdots,2k+1, \end{cases} \tag{6}$$

and

$$\begin{aligned} &\sum_{i=1}^{2k+1} d(x_i)d(u_n,x_i) = 2k^2+6k+3, \\ &\sum_{i=1}^{2k+1} d(x_j,x_i) = k^2+k, \quad j=1,2,\cdots,2k+1. \end{aligned} \tag{7}$$

Theorem 2.1. *Assuming Hypothesis 1.1, the following results are obtained.*

(i) The expression of $Var(Gut(G_n))$ for a random $(2k+1)$-polygonal chain G_n is regarded as

$$\begin{aligned} Var(Gut(G_n)) = \frac{1}{30}(&\sigma^2n^5 - 5rn^4 + 10\tilde{\sigma}^2n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2 \\ &+ (-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)), \end{aligned} \tag{8}$$

where

$$\begin{aligned} \sigma^2 &= (4k+4)^4\{[\sum_{i=1}^{k}(i+1)^2p_i] - [\sum_{i=1}^{k}(i+1)p_i]^2\}, \\ \tilde{\sigma}^2 &= (4k+4)^2\{[\sum_{i=1}^{k}(-2k^2+2k+5+(4k+4)i)^2p_i] \\ &\quad - [\sum_{i=1}^{k}(-2k^2+2k+5+(4k+4)i)p_i]^2\}, \\ r &= (4k+4)^3\{[\sum_{i=1}^{k}(i+1)(-2k^2+2k+5+(4k+4)i)p_i] \\ &\quad - [\sum_{i=1}^{k}(i+1)p_i][\sum_{i=1}^{k}(-2k^2+2k+5+(4k+4)i)p_i]\}. \end{aligned}$$

(ii) when n approaches infinity, $Gut(G_n)$ is asymptotic to normal distribution, i.e.,

$$\lim_{n\to\infty}\sup_{x\in\mathbb{R}} |\mathbb{P}(\frac{Gut(G_n)-\mathbb{E}(Gut(G_n))}{\sqrt{Var(Gut(G_n))}} \le x) - \int_{-\infty}^{x}\frac{1}{\sqrt{2\pi}}e^{-\frac{t^2}{2}}dt| = 0. \tag{9}$$

Proof. Eq. (1) provides one

$$\begin{aligned}
Gut(G_{n+1}) &= \sum_{\{u,v\}\subseteq V(G_{n+1})} d(u)d(v)d(u,v)\\
&= \sum_{\{u,v\}\subseteq V(G_n)} d(u)d(v)d(u,v) + \sum_{v\in V(G_n)}\sum_{x_i\in V(O_{n+1})} d(v)d(x_i)d(v,x_i)\\
&\quad + \sum_{\{x_i,x_j\}\subseteq V(O_{n+1})} d(x_i)d(x_j)d(x_i,x_j)\\
&= \Delta_{11} + \Delta_{12} + \Delta_{13}.
\end{aligned}$$

Note that

$$\begin{aligned}
\Delta_{11} &= \sum_{\{u,v\}\subseteq V(G_n)} d(u)d(v)d(u,v)\\
&= \sum_{\{u,v\}\subseteq V(G_n)\setminus\{u_n\}} d(u)d(v)d(u,v) + \sum_{v\in V(G_n)\setminus\{u_n\}} d_{G_{n+1}}(u_n)d(v)d(u_n,v)\\
&= \sum_{\{u,v\}\subseteq V(G_n)\setminus\{u_n\}} d(u)d(v)d(u,v) + \sum_{v\in V(G_n)\setminus\{u_n\}} \Big(d_{G_n}(u_n)+1\Big)d(v)d(u_n,v)\\
&= \sum_{\{u,v\}\subseteq V(G_n)\setminus\{u_n\}} d(u)d(v)d(u,v) + \sum_{v\in V(G_n)} d_{G_n}(u_n)d(v)d(u_n,v) + \sum_{v\in V(G_n)} d(v)d(u_n,v)\\
&= Gut(G_n) + \sum_{v\in V(G_n)} d(v)d(u_n,v).
\end{aligned}$$

As Eq. (5) and Eq. (7), we have

$$\begin{aligned}
\Delta_{12} &= \sum_{v\in V(G_n)}\sum_{x_i\in V(O_{n+1})} d(v)d(x_i)d(v,x_i)\\
&= \sum_{v\in V(G_n)} d(v)\Big(\sum_{x_i\in V(O_{n+1})} d(x_i)d(v,x_i)\Big)\\
&= \sum_{v\in V(G_n)} d(v)\Big(\sum_{x_i\in V(O_{n+1})} d(x_i)(d(u_n,v)+d(u_n,x_i))\Big)\\
&= \sum_{v\in V(G_n)} d(v)\Big(\sum_{x_i\in V(O_{n+1})} d(x_i)d(u_n,v) + \sum_{x_i\in V(O_{n+1})} d(x_i)d(u_n,x_i)\Big)\\
&= \sum_{v\in V(G_n)} d(v)((4k+3)d(u_n,v) + (2k^2+6k+3))\\
&= (4k+3)\sum_{v\in V(G_n)} d(v)d(u_n,v) + (2k^2+6k+3)\sum_{v\in V(G_n)} d(v)\\
&= (4k+3)\sum_{v\in V(G_n)} d(v)d(u_n,v) + (2k^2+6k+3)((4k+4)n-1)\\
&= (4k+3)\sum_{v\in V(G_n)} d(v)d(u_n,v) + n(8k^3+32k^2+36k+12) - (2k^2+6k+3).
\end{aligned}$$

We obtain from Eq. (6)

$$\begin{aligned}\Delta_{13} &= \sum_{\{x_i,x_j\}\subseteq V(O_{n+1})} d(x_i)d(x_j)d(x_i,x_j)\\ &= \frac{1}{2}\sum_{i=1}^{2k+1}\sum_{j=1}^{2k+1} d(x_i)d(x_j)d(x_i,x_j)\\ &= \frac{1}{2}\sum_{i=1}^{2k+1} d(x_i)(\sum_{j=1}^{2k+1} d(x_j)d(x_i,x_j))\\ &= 4k^3+8k^2+4k.\end{aligned}$$

Then

$$\begin{aligned}Gut(G_{n+1}) = Gut(G_n) &+ (4k+4)\sum_{v\in V(G_n)} d(v)d(u_n,v)\\ &+ n(8k^3+32k^2+36k+12)+(4k^3+6k^2-2k-3).\end{aligned} \tag{10}$$

Let

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

Hence,

$$Gut(G_{n+1}) = Gut(G_n) + A_n + n(8k^3+32k^2+36k+12)+(4k^3+6k^2-2k-3). \tag{11}$$

For each i=1, 2, $\cdots$,k, we will address the i-th case.

$$A_nZ_n^i = \{A_{n-1} + n[m(4k+4)^2] - [(4k+4)(-2k^2-2k+1+2m(2k+2))]\}Z_n^i.$$

The aforementioned equality is clear if $Z_n^i = 0$. As a result, we only need to analyze $Z_n^i = 1$, which implies $G_n \to G_{n+1}^i$. In this case, the vertex marked x_m or x_{2k+3-m} coincides with u_n of G_n, as seen in Fig. 3. Due to Eq. (5) and Eq. (6), we get

$$\begin{aligned}A_n &= (4k+4)\sum_{v\in V(G_n)} d(v)d(x_m,v)\\ &= (4k+4)\sum_{v\in V(G_{n-1})} d(v)d(x_m,v) + (4k+4)\sum_{v\in V(O_n)} d(v)d(x_m,v)\\ &= (4k+4)\sum_{v\in V(G_{n-1})} d(v)(d(v,u_{n-1})+d(x_m,u_{n-1})) + (4k+4)\times(2k^2+2k+m-1)\\ &= (4k+4)\sum_{v\in V(G_{n-1})} d(v)(d(v,u_{n-1})+m) + (4k+4)\times(2k^2+2k+m-1)\\ &= (4k+4)\sum_{v\in V(G_{n-1})} d(v)d(v,u_{n-1}) + m(4k+4)\sum_{v\in V(G_{n-1})} d(v) + (4k+4)\times(2k^2+2k+m-1)\\ &= A_{n-1} + m(4k+4)\times((4k+4)(n-1)-1) + (4k+4)\times(2k^2+2k+m-1)\\ &= A_{n-1} + n(m(4k+4)^2) - (4k+4)(-2k^2-2k+1+2m(2k+2)).\end{aligned}$$

Due to the fact that $\sum_{i=1}^{k} Z_n^i = 1$, then

$$\begin{aligned} A_n &= A_n(\sum_{i=1}^{k} Z_n^i) \\ &= A_{n-1}(\sum_{i=1}^{k} Z_n^i) + n(\sum_{i=1}^{k} (4k+4)^2(i+1)Z_n^i) - (\sum_{i=1}^{k} (4k+4)(-2k^2-2k+1+(4k+4)(i+1))Z_n^i) \\ &= A_{n-1} + n(\sum_{i=1}^{k} (4k+4)^2(i+1)Z_n^i) - (\sum_{i=1}^{k} (4k+4)(-2k^2-2k+1+(4k+4)(i+1))Z_n^i), \end{aligned}$$

where

$$U_n = \sum_{i=1}^{k} (4k+4)^2(i+1)Z_n^i, \quad V_n = \sum_{i=1}^{k} (4k+4)(-2k^2-2k+1+(4k+4)(i+1))Z_n^i.$$

Eq. (11) gives us

$$\begin{aligned} Gut(G_n) &= Gut(G_{n-1}) + A_{n-1} + (n-1)(8k^3+32k^2+36k+12) + (4k^3+6k^2-2k-3) \\ &= Gut(G_1) + \sum_{i=1}^{n-1} A_i + \sum_{i=1}^{n-1} ((8k^3+32k^2+36k+12)i + (4k^3+6k^2-2k-3)) \\ &= Gut(G_1) + \sum_{i=1}^{n-1} (\sum_{j=1}^{i-1} (A_{j+1} - A_j) + A_1) \\ &\quad + \sum_{i=1}^{n-1} ((8k^3+32k^2+36k+12)i + (4k^3+6k^2-2k-3)) \\ &= Gut(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} (A_{j+1} - A_j) + (n-1)A_1 \\ &\quad + \sum_{i=1}^{n-1} ((8k^3+32k^2+36k+12)i + (4k^3+6k^2-2k-3)) \\ &= Gut(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((A_j + (j+1)U_{j+1} - V_{j+1}) - A_j) + (n-1)A_1 \\ &\quad + \sum_{i=1}^{n-1} ((8k^3+32k^2+36k+12)i + (4k^3+6k^2-2k-3)) \\ &= Gut(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + (n-1)A_1 \\ &\quad + \sum_{i=1}^{n-1} ((8k^3+32k^2+36k+12)i + (4k^3+6k^2-2k-3)) \\ &= Gut(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + O(n^2). \end{aligned} \tag{12}$$

Following routine computations,

$$Var(U_j) = \sigma^2, \;\; Var(V_j) = \tilde{\sigma}^2, \;\; Cov(U_j, V_j) = r. \tag{13}$$

According to the properties of the variance and switching the order of sums, we have

$$\begin{aligned}
&Var(Gut(G_n))\\
&= Var(Gut(G_1) + \sum_{i=1}^{n-1}\sum_{j=1}^{i-1}((j+1)U_{j+1} - V_{j+1}) + O(n^2))\\
&= Var(\sum_{i=1}^{n-1}\sum_{j=1}^{i-1}((j+1)U_{j+1} - V_{j+1}))\\
&= Var(\sum_{j=1}^{n-2}\sum_{i=j+1}^{n-1}((j+1)U_{j+1} - V_{j+1}))\\
&= Var(\sum_{j=1}^{n-2}((j+1)U_{j+1} - V_{j+1})(n-j-1))\\
&= \sum_{j=1}^{n-2}(n-j-1)^2 Var((j+1)U_{j+1} - V_{j+1})\\
&= \sum_{j=1}^{n-2}(n-j-1)^2 Cov((j+1)U_{j+1} - V_{j+1}, (j+1)U_{j+1} - V_{j+1})\\
&= \sum_{j=1}^{n-2}(n-j-1)^2((j+1)^2 Cov(U_{j+1}, U_{j+1}) - 2(j+1)Cov(U_{j+1}, V_{j+1}) + Cov(V_{j+1}, V_{j+1}))\\
&= \sum_{j=1}^{n-2}(n-j-1)^2((j+1)^2 Var(U_{j+1}) - 2(j+1)Cov(U_{j+1}, V_{j+1}) + Var(V_{j+1}))\\
&= \sum_{j=1}^{n-2}(n-j-1)^2((j+1)^2\sigma^2 - 2(j+1)r + \tilde{\sigma}^2).
\end{aligned}$$

The above equality suggests the desired result Eq. (8) with the aid of a computer.

Next we prove the second portion of this theorem. Set

$$u_n = \sum_{i=1}^{n-1}\sum_{j=1}^{i-1}(j+1)U_{j+1}, \quad v_n = \sum_{i=1}^{n-1}\sum_{j=1}^{i-1}V_{j+1}, \quad and \quad \mu = \mathbb{E}(U_j), \quad \phi(t) = \mathbb{E}e^{t(U_j-\mu)}.$$

Then

$$\begin{aligned}
&\mathbb{E}e^{t(u_n-\mathbb{E}(u_n))}\\
&= \mathbb{E}e^{t\sum_{i=1}^{n-1}\sum_{j=1}^{i-1}(j+1)(U_{j+1}-\mu)}\\
&= \mathbb{E}e^{t\sum_{j=1}^{n-2}\sum_{i=j+1}^{n-1}(j+1)(U_{j+1}-\mu)}\\
&= \mathbb{E}e^{t\sum_{j=1}^{n-2}(j+1)(n-j-1)(U_{j+1}-\mu)}\\
&= \prod_{j=1}^{n-2}\mathbb{E}e^{t(j+1)(n-j-1)(U_j-\mu)}\\
&= \prod_{j=1}^{n-2}\phi(t(j+1)(n-j-1))
\end{aligned} \tag{14}$$

and

$$v_n = \sum_{i=1}^{n-1}\sum_{j=1}^{i-1} V_{j+1} \le Cn^2 \tag{15}$$

for some constant $C > 0$.

Take note that $Var(Gut(G_n)) \asymp \frac{1}{30}\sigma^2 n^5$. By Taylar's formula and Eqs. (12), (14) and (15),

$$\begin{aligned}
&\lim_{n\to\infty}\mathbb{E}\exp\{t\frac{Gut(G_n)-\mathbb{E}(Gut(G_n))}{\sqrt{Var(Gut(G_n))}}\}\\
&=\lim_{n\to\infty}\mathbb{E}\exp\{t\frac{(Gut(G_1)+u_n-v_n+O(n^2))-\mathbb{E}(Gut(G_1)+u_n-v_n+O(n^2))}{\frac{\sigma n^{\frac{5}{2}}}{\sqrt{30}}}\}\\
&=\lim_{n\to\infty}\mathbb{E}\exp\{t\frac{\sqrt{30}(u_n-\mathbb{E}(u_n))}{\sigma n^{\frac{5}{2}}}\}\\
&=\lim_{n\to\infty}\prod_{j=1}^{n}\phi(\frac{\sqrt{30}t(j+1)(n-1-j)}{\sigma n^{\frac{5}{2}}})\\
&=\lim_{n\to\infty}\exp\{\sum_{j=1}^{n}\ln\phi(\frac{\sqrt{30}t(j+1)(n-1-j)}{\sigma n^{\frac{5}{2}}})\}\\
&=\lim_{n\to\infty}\exp\{\sum_{j=1}^{n}\ln(1+\frac{\sigma^2}{2}\frac{30t^2(j+1)^2(n-1-j)^2}{\sigma^2 n^5}+o(\frac{1}{n}))\}\\
&=\lim_{n\to\infty}\exp\{\sum_{j=1}^{n-2}(\frac{\sigma^2}{2}\frac{30t^2(j+1)^2(n-1-j)^2}{\sigma^2 n^5}+o(\frac{1}{n}))\}\\
&=e^{\frac{t^2}{2}},
\end{aligned}$$

where in the above equality we utilize $\phi(t) = 1 + \frac{\sigma^2}{2}t^2 + o(t^2)$ and $\sum_{j=1}^{n-2}(j+1)^2(n-1-j)^2 \asymp \frac{n^5}{30}$ which can be proved by a computer.

Let i be a complex number with $i^2 = -1$, we replace t by it in the above equality, Then

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

Using the aforementioned equality and the continuity theory for characteristic function in probability([13]-[14]), we complete the proof of Eq. (9). It is required in the proof of Theorem 2.1 that $\sigma^2 \neq 0$, which is equal to Hypothesis 1.1 (ii) . ∎

Theorem 2.2. *Assuming Hypothesis 1.1, the following results are obtained.*

(i) The expression of $Var(S(G_n))$ for a random $(2k+1)$-polygonal chain G_n is regarded as

$$\begin{aligned}
Var(S(G_n)) = \frac{1}{30}(&\sigma^2 n^5 - 5rn^4 + 10\tilde{\sigma}^2 n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2\\
&+ (-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)),
\end{aligned} \tag{16}$$

where

$$\sigma^2 = (16k^2+24k+8)^2\{[\sum_{i=1}^{k}(i+1)^2 p_i] - [\sum_{i=1}^{k}(i+1)p_i]^2\},$$

$$\tilde{\sigma}^2 = [\sum_{i=1}^{k}((16k^2+24k+8)i - 8k^3+2k^2+20k+9)^2 p_i]$$
$$- [\sum_{i=1}^{k}((16k^2+24k+8)i - 8k^3+2k^2+20k+9)p_i]^2,$$

$$r = (16k^2+24k+8)\{[\sum_{i=1}^{k}(i+1)((16k^2+24k+8)i - 8k^3+2k^2+20k+9)p_i]$$
$$- [\sum_{i=1}^{k}(i+1)p_i][\sum_{i=1}^{k}((16k^2+24k+8)i - 8k^3+2k^2+20k+9)p_i]\}.$$

(ii) when n approaches infinity, $S(G_n)$ is asymptotic to normal distribution, i.e.,

$$\lim_{n\to\infty}\sup_{x\in\mathbb{R}}|\mathbb{P}(\frac{S(G_n)-\mathbb{E}(S(G_n))}{\sqrt{Var(S(G_n))}} \le x) - \int_{-\infty}^{x}\frac{1}{\sqrt{2\pi}}e^{-\frac{t^2}{2}}dt| = 0. \tag{17}$$

Proof. Eq. (2) provides one

$$\begin{aligned}
S(G_{n+1}) &= \sum_{\{u,v\}\subseteq V(G_{n+1})}(d(u)+d(v))d(u,v)\\
&= \sum_{\{u,v\}\subseteq V(G_n)}(d(u)+d(v))d(u,v) + \sum_{v\in V(G_n)}\sum_{x_i\in V(O_{n+1})}(d(v)+d(x_i))d(v,x_i)\\
&\quad + \sum_{\{x_i,x_j\}\subseteq V(O_{n+1})}(d(x_i)+d(x_j))d(x_i,x_j)\\
&= \Delta_{21}+\Delta_{22}+\Delta_{23}.
\end{aligned}$$

Note that

$$\begin{aligned}
\Delta_{21} &= \sum_{\{u,v\}\subseteq V(G_n)}(d(u)+d(v))d(u,v)\\
&= \sum_{\{u,v\}\subseteq V(G_n)\backslash\{u_n\}}(d(u)+d(v))d(u,v) + \sum_{v\in V(G_n)\backslash\{u_n\}}(d_{G_{n+1}}(u_n)+d(v))d(u_n,v)\\
&= \sum_{\{u,v\}\subseteq V(G_n)\backslash\{u_n\}}(d(u)+d(v))d(u,v) + \sum_{v\in V(G_n)\backslash\{u_n\}}(d_{G_n}(u_n)+1+d(v))d(u_n,v)\\
&= \sum_{\{u,v\}\subseteq V(G_n)\backslash\{u_n\}}(d(u)+d(v))d(u,v) + \sum_{v\in V(G_n)}(d_{G_n}(u_n)+d(v))d(u_n,v) + \sum_{v\in V(G_n)}d(u_n,v)\\
&= S(G_n) + \sum_{v\in V(G_n)}d(u_n,v).
\end{aligned}$$

As Eqs. (4), (5) and (7), we have

$$
\begin{aligned}
\Delta_{22} &= \sum_{v\in V(G_n)} \sum_{x_i\in V(O_{n+1})} (d(v)+d(x_i))d(v,x_i) \\
&= \sum_{v\in V(G_n)} \sum_{x_i\in V(O_{n+1})} d(v)d(v,x_i) + \sum_{v\in V(G_n)} \sum_{x_i\in V(O_{n+1})} d(x_i)d(v,x_i) \\
&= \sum_{v\in V(G_n)} d(v) \sum_{x_i\in V(O_{n+1})} d(v,x_i) + \sum_{v\in V(G_n)} \sum_{x_i\in V(O_{n+1})} d(x_i)(d(u_n,v)+d(u_n,x_i)) \\
&= \sum_{v\in V(G_n)} d(v) \sum_{x_i\in V(O_{n+1})} (d(u_n,v)+d(u_n,x_i)) + \sum_{v\in V(G_n)} \sum_{x_i\in V(O_{n+1})} d(x_i)d(u_n,v) \\
&\quad + \sum_{v\in V(G_n)} \sum_{x_i\in V(O_{n+1})} d(x_i)d(u_n,x_i) \\
&= \sum_{v\in V(G_n)} d(v) \sum_{x_i\in V(O_{n+1})} d(u_n,v) + \sum_{v\in V(G_n)} d(v) \sum_{x_i\in V(O_{n+1})} d(u_n,x_i) \\
&\quad + \sum_{v\in V(G_n)} d(u_n,v) \sum_{x_i\in V(O_{n+1})} d(x_i) + \sum_{v\in V(G_n)} \sum_{x_i\in V(O_{n+1})} d(x_i)d(u_n,x_i) \\
&= \sum_{v\in V(G_n)} d(v)d(u_n,v) \sum_{x_i\in V(O_{n+1})} 1 + \sum_{v\in V(G_n)} d(v) \sum_{x_i\in V(O_{n+1})} (d(x_1,x_i)+1) \\
&\quad + (4k+3) \sum_{v\in V(G_n)} d(u_n,v) + (2k^2+6k+3) \sum_{v\in V(G_n)} 1 \\
&= (2k+1) \sum_{v\in V(G_n)} d(v)d(u_n,v) + \sum_{v\in V(G_n)} d(v)\Big(\sum_{x_i\in V(O_{n+1})} d(x_1,x_i) + \sum_{x_i\in V(O_{n+1})} 1\Big) \\
&\quad + (4k+3) \sum_{v\in V(G_n)} d(u_n,v) + (2k^2+6k+3)\times(2k+1)n \\
&= (2k+1) \sum_{v\in V(G_n)} d(v)d(u_n,v) + ((4k+4)n-1)((k^2+k)+(2k+1)) \\
&\quad + (4k+3) \sum_{v\in V(G_n)} d(u_n,v) + (2k^2+6k+3)\times(2k+1)n \\
&= (2k+1) \sum_{v\in V(G_n)} d(v)d(u_n,v) + (4k+3) \sum_{v\in V(G_n)} d(u_n,v) \\
&\quad + n(8k^3+30k^2+28k+7) - (k^2+3k+1).
\end{aligned}
$$

We obtain from Eq. (6)

$$
\begin{aligned}
\Delta_{23} &= \sum_{\{x_i,x_j\}\subseteq V(O_{n+1})} (d(x_i)+d(x_j))d(x_i,x_j) \\
&= \frac{1}{2} \sum_{i=1}^{2k+1} \sum_{j=1}^{2k+1} (d(x_i)+d(x_j))d(x_i,x_j) \\
&= \sum_{i=1}^{2k+1} \sum_{j=1}^{2k+1} d(x_j)d(x_i,x_j) \\
&= 4k^3+7k^2+3k.
\end{aligned}
$$

Then

$$S(G_{n+1}) = S(G_n) + (2k+1)\sum_{v\in V(G_n)} d(v)d(u_n,v) + (4k+4)\sum_{v\in V(G_n)} d(u_n,v) \\ + n(8k^3+30k^2+28k+7) + (4k^3+6k^2-1). \tag{18}$$

Let

$$B_n = \sum_{v\in V(G_n)} (4k+4+(2k+1)d(v))d(u_n,v).$$

Hence,

$$S(G_{n+1}) = S(G_n) + B_n + n(8k^3+30k^2+28k+7) + (4k^3+6k^2-1). \tag{19}$$

For each i=1, 2, $\cdots$,k, we will address the i-th case.

$$B_n Z_n^i = \{B_{n-1} + n[m(16k^2+24k+8)] - [m(16k^2+24k+8) - 8k^3 - 14k^2 - 4k + 1]\}Z_n^i.$$

The aforementioned equality is clear if $Z_n^i = 0$. As a result, we only need to analyze $Z_n^i = 1$, which implies $G_n \to G_{n+1}^i$. In this case, the vertex marked x_m or x_{2k+3-m} coincides with u_n of G_n, as seen in Fig. 3. Due to Eqs. (5)-(7), we get

$$\begin{aligned}
B_n &= \sum_{v\in V(G_n)} (4k+4+(2k+1)d(v))d(x_m,v) \\
&= \sum_{v\in V(G_{n-1})} (4k+4+(2k+1)d(v))d(x_m,v) + \sum_{v\in V(O_n)} (4k+4+(2k+1)d(v))d(x_m,v) \\
&= \sum_{v\in V(G_{n-1})} (4k+4+(2k+1)d(v))(d(v,u_{n-1}) + d(x_m,u_{n-1})) \\
&\quad + ((4k+4)\sum_{v\in V(O_n)} d(x_m,v) + (2k+1)\sum_{v\in V(O_n)} d(v)d(x_m,v)) \\
&= \sum_{v\in V(G_{n-1})} (4k+4+(2k+1)d(v))(d(v,u_{n-1}) + m) \\
&\quad + ((4k+4)(k^2+k) + (2k+1)(2k^2+2k+m-1)) \\
&= \sum_{v\in V(G_{n-1})} (4k+4+(2k+1)d(v))d(v,u_{n-1}) + m\sum_{v\in V(G_{n-1})} (4k+4+(2k+1)d(v)) \\
&\quad + (8k^3+14k^2+4k-1+m(2k+1)) \\
&= B_{n-1} + m\times((4k+4)\times(2k+1)(n-1) + (2k+1)\times((4k+4)(n-1)-1)) \\
&\quad + (8k^3+14k^2+4k-1+m(2k+1)) \\
&= B_{n-1} + n(m(16k^2+24k+8)) - (m(16k^2+24k+8) - 8k^3 - 14k^2 - 4k + 1).
\end{aligned}$$

Due to the fact that $\sum_{i=1}^{k} Z_n^i = 1$, then

$$
\begin{aligned}
B_n &= B_n(\sum_{i=1}^{k} Z_n^i) \\
&= B_{n-1}(\sum_{i=1}^{k} Z_n^i) + n(\sum_{i=1}^{k} (i+1)(16k^2+24k+8)Z_n^i) \\
&\quad - (\sum_{i=1}^{k} ((i+1)(16k^2+24k+8) - 8k^3 - 14k^2 - 4k + 1)Z_n^i) \\
&= B_{n-1} + n(\sum_{i=1}^{k} (i+1)(16k^2+24k+8)Z_n^i) \\
&\quad - (\sum_{i=1}^{k} ((i+1)(16k^2+24k+8) - 8k^3 - 14k^2 - 4k + 1)Z_n^i).
\end{aligned}
$$

where

$$
U_n = \sum_{i=1}^{k} (i+1)(16k^2+24k+8)Z_n^i, \quad V_n = \sum_{i=1}^{k} ((i+1)(16k^2+24k+8) - 8k^3 - 14k^2 - 4k + 1)Z_n^i.
$$

Eq. (19) gives us

$$
\begin{aligned}
S(G_n) &= S(G_{n-1}) + B_{n-1} + (n-1)(8k^3+30k^2+28k+7) + (4k^3+6k^2-1) \\
&= S(G_1) + \sum_{i=1}^{n-1} B_i + \sum_{i=1}^{n-1} ((8k^3+30k^2+28k+7)i + (4k^3+6k^2-1)) \\
&= S(G_1) + \sum_{i=1}^{n-1} (\sum_{j=1}^{i-1} (B_{j+1} - B_j) + B_1) \\
&\quad + \sum_{i=1}^{n-1} ((8k^3+30k^2+28k+7)i + (4k^3+6k^2-1)) \\
&= S(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} (B_{j+1} - B_j) + (n-1)B_1 \\
&\quad + \sum_{i=1}^{n-1} ((8k^3+30k^2+28k+7)i + (4k^3+6k^2-1)) \\
&= S(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((B_j + (j+1)U_{j+1} - V_{j+1}) - B_j) + (n-1)B_1 \\
&\quad + \sum_{i=1}^{n-1} ((8k^3+30k^2+28k+7)i + (4k^3+6k^2-1)) \\
&= S(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + (n-1)B_1 \\
&\quad + \sum_{i=1}^{n-1} ((8k^3+30k^2+28k+7)i + (4k^3+6k^2-1))
\end{aligned}
$$

$$= S(G_1) + \sum_{i=1}^{n-1}\sum_{j=1}^{i-1}((j+1)U_{j+1} - V_{j+1}) + O(n^2). \tag{20}$$

Following similar computations with Eq. (13), we obtain

$$Var(U_j) = \sigma^2, \;\; Var(V_j) = \tilde{\sigma}^2, \;\; Cov(U_j, V_j) = r.$$

The rest of the proof of this theorem is the same as that of Theorem 2.1 if $Gut(G_n)$ is replaced with $S(G_n)$ in the proof of Theorem 2.1. We leave out the specifics. ■

3. Applications of Theorems 2.1 and 2.2

Remember that Theorems 2.1 and 2.2 give two accurate formulae for the limiting behaviors of the Gutman index and the Schultz index of a random $(2k+1)$-polygonal chain. In this section, we use them to find the limiting behaviors for the Gutman index and the Schultz index of some class of a random $(2k+1)$-polygonal chain, such as the random 5-polygonal chain, which have been extensively addressed in organic chemistry or statistical physics.

Theorem 3.1. *Assuming Hypothesis 1.1, the following results are obtained.*
(i) The expression of $Var(Gut(G_n))$ for a random 5-polygonal chain G_n is regarded as

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

where

$$\sigma^2 = 288^2 p_1 + 432^2 p_2 - (288p_1 + 432p_2)^2,$$
$$\tilde{\sigma}^2 = 156^2 p_1 + 300^2 p_2 - (156p_1 + 300p_2)^2,$$
$$r = (288 \times 156p_1 + 432 \times 300p_2) - (288p_1 + 432p_2)(156p_1 + 300p_2).$$

(ii) when n approaches infinity, $Gut(G_n)$ is asymptotic to normal distribution, i.e.,

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

Theorem 3.2. *Assuming Hypothesis 1.1, the following results are obtained.*
(i) The expression of $Var(S(G_n))$ for a random 5-polygonal chain G_n is regarded as

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

where

$$\sigma^2 = 240^2 p_1 + 360^2 p_2 - (240p_1 + 360p_2)^2,$$
$$\tilde{\sigma}^2 = 113^2 p_1 + 233^2 p_2 - (113p_1 + 233p_2)^2,$$
$$r = (240 \times 113p_1 + 360 \times 233p_2) - (240p_1 + 360p_2)(113p_1 + 233p_2).$$

(ii) when n approaches infinity, $S(G_n)$ is asymptotic to normal distribution, i.e.,

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

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