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Research article

Enumeration of the Gutman and Schultz indices in the random polygonal chains

Wanlin Zhu, Minglei Fang*and Xianya Geng

School of mathematics and big data, Anhui University of Science and Technology, 232001 Huainan, China

* **Correspondence:** Email: fmlmath@sina.com.

Abstract: The Gutman index and Schultz index of a connected graph are degree-distance-based topological indices. In this paper, we devoted to establish the explicit analytical expressions for the simple formulae of the expected values of the Gutman and Schultz indices in a random polygonal. Based on these results above, we get the extremal values and average values of Gunman and Schultz indices of all polygonal chains.

Keywords: Gutman index; Schultz index; random polygonal chains; expected value; extremal value; average value

1. Introduction

In this paper, we only consider simple and finite connected graphs. Chemical graph theory is a branch of mathematical chemistry which deals with the nontrivial applications of graph theory to solve molecular problems. The basic method is to model the molecular structure of a compound [1–3]. Each atom is represented by a vertex, and the chemical bonds between atoms are represented by the edges between the vertices. Thus, the entire molecular structure is represented by a diagram, which is called a molecular diagram. For more detailed information, we can refer to [4,5] and the references cited therein.

In this paper, chemical diagrams are studied by topological indices [6–9]. According to the different parameters such as point degree, adjacent point degree and distance between two points, topological indices can be divided into many categories. A graph G is an ordered $(V(G), E(G))$ consisting of a nonempty set V(G) of vertices, a set $E(G)$, disjoint from $V(G)$, of edges. The degree $d_G(v)$ (or $d(v)$ for short) of a vertex v in G is the number of edges of G incident with v. The shortest distance between vertex u and vertex v is denoted by $d(u, v)$ [10–13].

Wiener index is defined as [14]

$$W(G) = \sum_{\{u,v\}\subseteq V_G} d_G(u,v). \tag{1.1}$$

The Wiener index is more and more widely used and studied, see [15–17]. Zhang, Li and so on [18,19] give the explicit analytical expressions for the expected values of the Schultz index, Gutman index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random polyphenylene chain. Now we will consider the random polygonal chains that are meaningful.

Gutman index is defined as

$$Gut(G) = \frac{1}{2}\sum_{u\in V_G}\sum_{v\in V_G}(d_G(u)d_G(v))d_G(u,v) = \sum_{u,v\subseteq V_G}(d_G(u)d_G(v))d_G(u,v). \tag{1.2}$$

Schultz index is defined as

$$S(G) = \frac{1}{2}\sum_{u\in V_G}\sum_{v\in V_G}(d_G(u)+d_G(v))d_G(u,v) = \sum_{u,v\subseteq V_G}(d_G(u)+d_G(v))d_G(u,v). \tag{1.3}$$

More articles on developing such a topology indices of the [20–23], such as mathematical properties, discrimination and applications refer to [24–27] .

A random polygonal chain G_n with n polygons is made up of a polygonal chain G_{n-1} with $n-1$ polygons to which a new terminal polygon H_n by a cut edge, see Figure 1. When $n \geq 3$, the terminal polygon H_n has k connection ways, these connections are recorded as G_n^1,G_n^2,G_n^3,...,G_n^k. see Figure 2. A random polygonal chain $G_n(p_1, p_2, p_3, \ldots, p_{k-1})$ has n polygons is a polygonal chain acquired by gradyally adding terminal polygons. Each step of adding can be randomly selected from k connection methods:

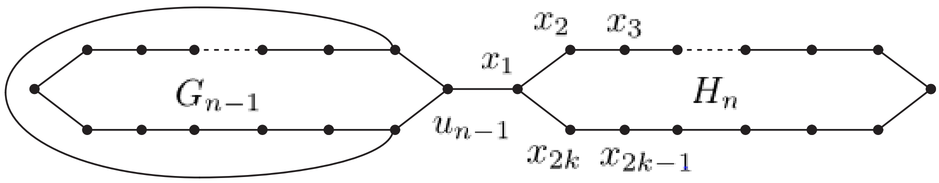

Figure 1. A polygonal chain G_n with n polygons.

- $G_{k-1} \to G_{2k}^1$ with probability p_1,
- $G_{k-1} \to G_{2k}^2$ with probability p_2,
- $\vdots$ $\vdots$ $\vdots$
- $G_{k-1} \to G_{2k}^3$ with probability p_3,
- $G_{k-1} \to G_{2k}^{k-1}$ with probability p_{k-1},
- $G_{k-1} \to G_{2k}^k$ with probability $p_k = 1 - p_1 - p_2 - p_3 - \cdots - p_{k-1}$,

where the probabilities p_1, p_2 ,p_3 , . . . , p_{k-1} are constants, there are independent of k.

Let G_n be a polygonal chain with n polygons H_1,H_2, . . . , H_n. $u_k\omega_k$ is connecting H_k and H_{k+1} with $u_k \in V_{H_k}$ in G_n, $\omega_k \in V_{H_{k+1}}$ $(k = 1, 2, \ldots, n-1)$. Obviously, both ω_k and u_{k+1} are thevertices in H_{k+1} and

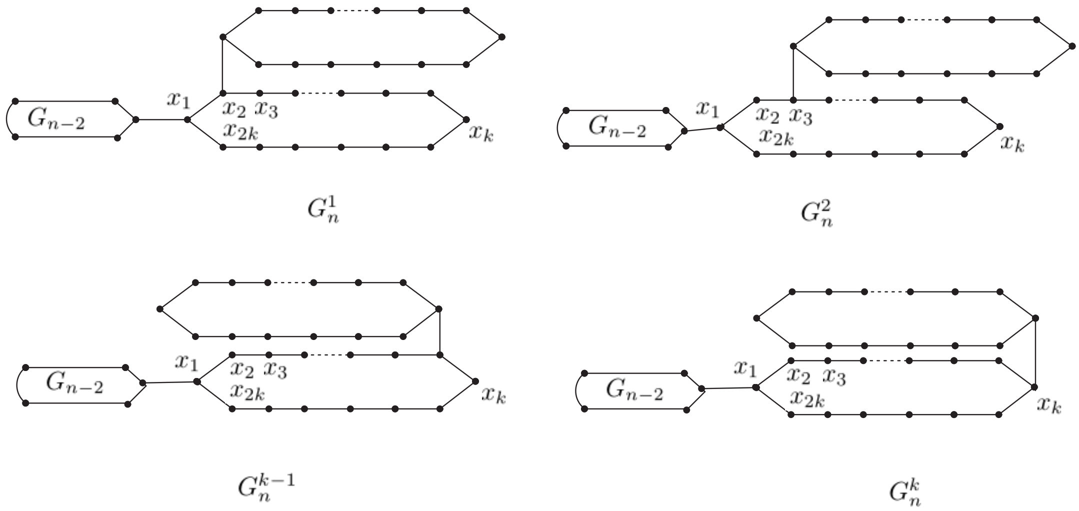

Figure 2. k types of local arrangements in a polygonal chain.

$d(\omega_k, u_{k+1}) \in \{1, 2, 3, \ldots, n\}$. Specially, G_n is the meta-chain M_n, the ortho-chain O_n^1,O_n^2, …,$O_n^{k-2}$and the para-chain Ln if $d(\omega_k, u_{k+1}) = 1$ (i.e.,$p_1 = 1$), $d(\omega_k, u_{k+1})$= 2 (i.e., $p_2 = 1$), $d(\omega_k, u_{k+1}) = 3$ (i.e., $p_3 = 1$) , …, $d(\omega_k, u_{k+1})$= k (i.e., $p_k = 1$) ($\forall\, k \in \{1, 2, \ldots, n-2\}$), respectively.

Zhang and Li et al.[18], obtained the random polyphenylene chain expected values of some topological indices. We calculate the explicit analytical expressions for the expected values of the Gutman index, Schultz index of a random polygonal chain. Based on above results, we get the extremal values and average values of Gunman and Schultz indices of random polygonal chains.

2. The Gutman index in a random polygonal chain

In this section, we will consider the expected values of Gutman index of the random polygonal chain. In fact, G_{n+1} is G_n linked to a new terminal polygonal H_{n+1} by an edge, H_{n+1} is made up with vertices x_1, x_2, x_3, …, x_{2k}, and the new edge is $u_n x_1$; see Figure 1. For $\forall v \in V_{G_n}$,

$$d(x_1, v) = d(u_n, v) + 1, \qquad d(x_2, v) = d(u_n, v) + 2, \qquad \ldots, \quad d(x_k, v) = d(u_n, v) + k, \tag{2.1}$$

$$d(x_{k+1}, v) = d(u_n, v) + k + 1,\ d(x_{k+2}, v) = d(u_n, v) + k,\ \ldots,\ d(x_{2k}, v) = d(u_n, v) + 2. \tag{2.2}$$

$$\sum_{v \in V_{G_n}} d_{G_{n+1}}(v) = [(2k-2) \cdot 2 + 2 \cdot 3]n - 1 = (4k+2)n - 1. \tag{2.3}$$

And,

$$\begin{aligned}
&\sum_{i=1}^{2k} d(x_i)d(x_1, x_i) = 2k^2, && \sum_{i=1}^{2k} d(x_i)d(x_2, x_i) = 2k^2 + 1,\\
&\sum_{i=1}^{2k} d(x_i)d(x_3, x_i) = 2k^2 + 2, \ \ldots, && \sum_{i=1}^{2k} d(x_i)d(x_k, x_i) = 2k^2 + k - 1,\\
&\sum_{i=1}^{2k} d(x_i)d(x_{k+1}, x_i) = 2k^2 + k, && \sum_{i=1}^{2k} d(x_i)d(x_{k+2}, x_i) = 2k^2 + k - 1,\\
&\qquad \ldots, && \qquad \ldots,\\
&\sum_{i=1}^{2k} d(x_i)d(x_{2k-1}, x_i) = 2k^2 + 2, && \sum_{i=1}^{2k} d(x_i)d(x_{2k}, x_i) = 2k^2 + 1.
\end{aligned} \tag{2.4}$$

Theorem 2.1 The $E(Gut(G_n))(n \geq 1)$ of the random polygonal chain G_n is

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

Proof. The random polygonal chain G_{n+1} is G_n linked a new terminal polygonal H_{n+1} by an edge, the H_{n+1} is made up with vertices x_1, x_2, x_3,…,x_{2k}, and the new edge is $u_n x_1$; see Figure 1. By(1.2), one has

$$Gut(G_{n+1}) = \sum_{\{u,v\}\subseteq V_{G_n}} d(u)d(v)d(u, v) + \sum_{v\in V_{G_n}}\sum_{x_i\in V_{H_{n+1}}} d(v)d(x_i)d(v, x_i) + \sum_{\{x_i x_j\}\subseteq V_{H_{n+1}}} d(x_i)d(x_j)d(x_i, x_j).$$

Note that

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

Recall that $d(x_1) = 3$ and $d(x_i) = 2$ ($i \in \{2, 3, 4, \ldots, 2k\}$). On the basis of (2.1)-(2.3), We get

$$\sum_{v\in V_{G_n}}\sum_{x_i\in V_{H_{n+1}}} d(v)d(x_i)d(v, x_i) = \sum_{v\in V_{G_n}} d(v)[3(d(u_n, v) + 1) + 2(d(u_n, v) + 2) + 2(d(u_n, v) + 3)$$

$$
\begin{aligned}
&+\cdots+2(d(u_n,v)+k+1)+2(d(u_n,v)+k)+2(d(u_n,v)+k-1)\\
&+\cdots+2(d(u_n,v)+2)]\\
=&\sum_{v\in V_{G_n}} d(v)[(4k+1)d(u_n,v)+(2k^2+4k+1)]\\
=&(4k+1)\sum_{v\in V_{G_n}} d(v)d(u_n,v)+(2k^2+4k+1)\sum_{v\in V_{G_n}} d(v)\\
=&(4k+1)\sum_{v\in V_{G_n}} d(v)d(u_n,v)+(2k^2+4k+1)[(4k+2)n-1].
\end{aligned}
$$

From (2.4), one has,

$$
\begin{aligned}
&\sum_{\{x_ix_j\}\subseteq V_{H_{n+1}}} d(x_i)d(x_j)d(x_i,x_j)\\
=&\frac{1}{2}\sum_{i=1}^{2k} d(x_i)(\sum_{j=1}^{2k} d(x_j)d(x_i,x_j))\\
=&\frac{1}{2}[3\times 2k^2+2\times(2k^2+1)+2\times(2k^2+2)+\cdots\\
&+2\times(2k^2+k-1)+2\times(2k^2+k)+2\times(2k^2+k-1)+\cdots+2\times(2k^2+1)]\\
=&4k^3+2k^2.
\end{aligned}
$$

Then

$$
Gut(G_{n+1})=Gut(G_n)+(4k+2)\sum_{v\in V_{G_n}} d(v)d(u_n,v)+(2k^2+4k+1)[(4k+2)n-1]+4k^3+2k^2. \quad (2.5)
$$

For a random polygonal chain G_n, the number $\sum_{v\in V_{G_n}} d(v)d(u_n,v)$ is a random variable. We let

$$
A_n := E(\sum_{v\in V_{G_n}} d(v)d(u_n,v)).
$$

Substituting A_n into (2.5), we obtain the recurrence formula of $E(Gut(G_n))$

$$
E(Gut(G_{n+1})) =E(Gut(G_n))+(4k+2)A_n+(8k^3+20k^2+12k+2)n+(4k^3-4k-1). \quad (2.6)
$$

We continue to consider the following k possible ways.

Way 1. $G_n \longrightarrow G^1_{n+1}$. In this way, u_n same as the vertex x_2 or x_{2k}. Then, $\sum_{v\in V_{G_n}} d(v)d(u_n,v)$ is described as $\sum_{v\in V_{G_n}} d(v)d(x_2,v)$ or $\sum_{v\in V_{G_n}} d(v)d(x_{2k},v)$ with probability p_1.

Way 2. $G_n \longrightarrow G^2_{n+1}$. In this way, u_n same as the vertex x_3 or x_{2k-1}. Then, $\sum_{v\in V_{G_n}} d(v)d(u_n,v)$ is described as $\sum_{v\in V_{G_n}} d(v)d(x_3,v)$ or $\sum_{v\in V_{G_n}} d(v)d(x_{2k-1},v)$ with probability p_2.

Way 3. $G_n \longrightarrow G^3_{n+1}$. In this way, u_n same as the vertex x_4 or x_{2k-2}. Then, $\sum_{v\in V_{G_n}} d(v)d(u_n,v)$ is described as $\sum_{v\in V_{G_n}} d(v)d(x_4,v)$ or $\sum_{v\in V_{G_n}} d(v)d(x_{2k-2},v)$ with probability p_3.

$\vdots \quad \vdots \quad \vdots$

Way k-3. $G_n \longrightarrow G_{n+1}^{k-3}$. In this way, u_n same as the vertex x_{k-2} or x_{k+4}. Then, $\sum_{v\in V_{G_n}} d(v) d(u_n, v)$ is described as $\sum_{v\in V_{G_n}} d(v)d(x_{k-2}, v)$ or $\sum_{v\in V_{G_n}} d(v)d(x_{k+4}, v)$ with probability p_{k-3}.
Way k-2. $G_n \longrightarrow G_{n+1}^{k-2}$. In this way, u_n same as the vertex x_{k-1} or x_{k+3}. Then, $\sum_{v\in V_{G_n}} d(v) d(u_n, v)$ is described as $\sum_{v\in V_{G_n}} d(v)d(x_{k-1}, v)$ or $\sum_{v\in V_{G_n}} d(v)d(x_{k+3}, v)$ with probability p_{k-2}.
Way k-1. $G_n \longrightarrow G_{n+1}^{k-1}$. In this way, u_n same as the vertex x_k or x_{k+2}. Then, $\sum_{v\in V_{G_n}} d(v)d(u_n, v)$ is described as $\sum_{v\in V_{G_n}} d(v)d(x_k, v)$ or $\sum_{v\in V_{G_n}} d(v)d(x_{k+2}, v)$ with probability p_{k-1}.
Way k. $G_n \longrightarrow G_{n+1}^{k}$, then u_n is the vertex x_{k+1}. Then, $\sum_{v\in V_{G_n}} d(v)d(u_n, v)$ is described as $\sum_{v\in V_{G_n}} d(v)d(x_{k+1}, v)$ with probability $1 - p_1 - p_2 - p_3 - \cdots - p_{k-3} - p_{k-2} - p_{k-1}$.

On the basis of the above k ways, we get

$$\begin{aligned}
A_n =& p_1 \sum_{v\in V_{G_n}} d(v)d(x_2, v) + p_2 \sum_{v\in V_{G_n}} d(v)d(x_3, v) + p_3 \sum_{v\in V_{G_n}} d(v)d(x_4, v) \\
&+ \cdots + p_{k-3} \sum_{v\in V_{G_n}} d(v)d(x_{k-2}, v) + p_{k-2} \sum_{v\in V_{G_n}} d(v)d(x_{k-1}, v) + p_{k-1} \sum_{v\in V_{G_n}} d(v)d(x_k, v) \\
&+ (1 - p_1 - p_2 - p_3 - \cdots - P_{k-3} - P_{k-2} - p_{k-1}) \sum_{v\in V_{G_n}} d(v)d(x_{k+1}, v) \\
=& p_1[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1}, v) + 2 \sum_{v\in V_{G_{n-1}}} d(v) + 2k^2 + 1] \\
&+ p_2[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1}, v) + 3 \sum_{v\in V_{G_{n-1}}} d(v) + 2k^2 + 2] \\
&+ p_3[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1}, v) + 4 \sum_{v\in V_{G_{n-1}}} d(v) + 2k^2 + 3] \\
&+ \cdots \\
&+ p_{k-3}[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1}, v) + (k-2) \sum_{v\in V_{G_{n-1}}} d(v) + 2k^2 + k - 3] \\
&+ p_{k-2}[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1}, v) + (k-1) \sum_{v\in V_{G_{n-1}}} d(v) + 2k^2 + k - 2] \\
&+ p_{k-1}[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1}, v) + k \sum_{v\in V_{G_{n-1}}} d(v) + 2k^2 + k - 1] \\
&+ (1 - p_1 - p_2 - p_3 - \cdots - p_{k-3} - p_{k-2} - p_{k-1})[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1}, v) + (k+1) \sum_{v\in V_{G_{n-1}}} d(v) + 2k^2 + k].
\end{aligned}$$

Substitute the expectation for the above equation, let $E(A_n) = A_n$, we obtain

$$\begin{aligned}
A_n =& A_{n-1} + \{(4k^2 + 6k + 2) - \sum_{i=1}^{k-1}[4k^2 - (4i-2)k - 2i]p_i\}n \\
&+ \sum_{i=1}^{k-1}[4k^2 - (4i-2)k - 2i]p_i - (2k^2 + 6k + 3).
\end{aligned}$$

Let

$$M = \sum_{i=1}^{k-1}[4k^2 - (4i-2)k - 2i]p_i.$$

$$N_i = (2k+1)[4k^2 - (4i-2)k - 2i]p_i.$$

Hence,

$$A_n = A_{n-1} + [(4k^2 + 6k + 2) - M]n + M - (2k^2 + 6k + 3).$$

By the calculation

$$A_1 = E(\sum_{v \in V_{G_n}} d(v)d(u_1, v)) = 2k^2.$$

Based on the above results, we have

$$\begin{aligned} A_n =& \{(2k \cdot k + 3k + 1) - \sum_{i=1}^{k-1}[2k^2 - (2i-1)k - i]p_i\}n^2 \\ &+ \{\sum_{i=1}^{k-1}[2k^2 - (2i-1)k - i]p_i - (3k+2)\}n + 1. \end{aligned}$$

Thus,

$$A_n =[(2k \cdot k + 3k + 1) - \frac{1}{2}M]n^2 + [\frac{1}{2}M - (3k+2)]n + 1.$$

Substitute A_n into (2.6), we have,

$$\begin{aligned} E(Gut(G_{n+1})) =& E(Gut(G_n)) + (4k+2)A_n + (8k^3 + 20k^2 + 12k + 2)n + (4k^3 - 4k - 1) \\ =& E(Gut(G_n)) + (4k+2)\{[(2k \cdot k + 3k + 1) - \frac{1}{2}M]n^2 + [\frac{1}{2}M - (3k+2)]n + 1\} \\ &+ (8k^3 + 20k^2 + 12k + 2)n + (4k^3 - 4k - 1). \end{aligned}$$

By the calculation $E(Gut(G_1)) = 4k^3$.
Finally, we get the expected expression

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

as desired. □

Specially, if $p_1 = 1$, which implies $p_2 = p_3 = \cdots = p_k = 0$, then $G_n \cong M_n$. Similarly, if $p_2 = 1$ (resp. $p_3 = 1, \ldots, p_{k-2} = 1, p_{k-1} = 1$,), which implies $p_1 = p_3 = \cdots = p_k = 0$ (resp. $p_1 = p_2 = p_4 = \cdots = p_k = 0, p_1 = \cdots = p_{k-3} = p_{k-1} = p_k = 0, p_1 = p_2 \cdots = p_{k-2} = p_k = 0$), then

$G_n \cong O_n^1$ (resp. $G_n \cong O_n^2, \ldots, G_n \cong O_n^{k-2}$). If $p_k = 1$, which implies $p_1 = p_2 = \cdots = p_{k-1} = 0$, then $G_n \cong L_n$. According to Theorem 2.1 we can receive the Gutman index of the polygonal meta-chain M_n, the polygonal ortho-chain $O_n^1, O_n^2, O_n^3, \ldots, O_n^{k-2}$, the polygonal para-chain L_n, as

$$\begin{aligned}
Gut(M_n) &= (16k^2+16k+4)\frac{n^3}{3} + (8k^3-4k^2-12k-4)n^2 - (12k^3+4k^2-20k-11)\frac{n}{3} - 1\\
Gut(O_n^1) &= (24k^2+24k+6)\frac{n^3}{3} + (8k^3-12k^2-20k-6)n^2 - (12k^3-12k^2-36k-15)\frac{n}{3} - 1,\\
Gut(O_n^2) &= (32k^2+32k+8)\frac{n^3}{3} + (8k^3-20k^2-28k-8)n^2 - (12k^3-28k^2-52k-19)\frac{n}{3} - 1,\\
&\vdots \qquad \vdots \qquad \vdots\\
Gut(O_n^{k-3}) &= (8k^3-6k-2)\frac{n^3}{3} + (12k^2+10k+2)n^2 - (4k^3-36k^2-24k-1)\frac{n}{3} - 1,\\
Gut(O_n^{k-2}) &= (8k^3+8k^2+2k)\frac{n^3}{3} + (4k^2+2k)n^2 - (4k^3-20k^2-8k+3)\frac{n}{3} - 1,\\
Gut(L_n) &= (8k^3+16k^2+10k+2)\frac{n^3}{3} - (4k^2+6k+2)n^2 + (4k^3-4k^2+8k+7)\frac{n}{3} - 1.\\
Gut(o_n^i) &= [(8k^3+16k^2+10k+2)-N_{i+1}]\frac{n^3}{3} - [N_{i+1}-(4k^2+6k+2)]n^2 + [(4k^3-4k^2+8k+7)-2N_{i+1}]\frac{n}{3} - 1.
\end{aligned}$$

Obviously

$$Gut(M_n) + Gut(L_n) = Gut(O_n^1) + Gut(O_n^2) + \ldots + Gut(O_n^{k-2}).$$

Corollary 2.2 For a random polygonal chain G_n ($n \geq 3$), the para-chain L_n gets to the maximum and the meta-chain M_n gets to the minimum of $E(Gut(G_n))$.

Proof. By Theorem 2.1

$$E(Gut(G_n)) = \sum_{i=1}^{k-1}(-N_i\frac{n^3}{3}+N_in^2-2N_i\frac{n}{3})p_i+(8k^3+16k^2+10k+2)\frac{n^3}{3}-(4k^2+6k+2)n^2+(4k^3-4k^2+8k+7)\frac{n}{3}-1.$$

When $n \geq 3$, take the partial derivative of $E(Gut(G_n)$

$$\begin{aligned}
\frac{\partial E(Gut(G_n))}{\partial p_i} &= -N_i\frac{n^3}{3} + N_in^2 - \frac{2}{3}N_in < 0,\\
\frac{\partial E(Gut(G_n))}{\partial p_1} &= (8k^3-6k-2)\frac{n^3}{3} + (8k^3-6k-2)n^2 - 2(8k^3-6k-2)\frac{n}{3} < 0,\\
\frac{\partial E(Gut(G_n))}{\partial p_2} &= (8k^3-8k^2-14k-4)\frac{n^3}{3} + (8k^3-8k^2-14k-4)n^2 - 2(8k^3-8k^2-14k-4)\frac{n}{3} < 0,\\
\frac{\partial E(Gut(G_n))}{\partial p_3} &= (8k^3-16k^2-22k-6)\frac{n^3}{3} + (8k^3-16k^2-22k-6)n^2 - 2(8k^3-16k^2-22k-6)\frac{n}{3} < 0,\\
&\vdots \qquad \vdots \qquad \vdots\\
\frac{\partial E(Gut(G_n))}{\partial p_{k-1}} &= -(8k^2+8k+2)\frac{n^3}{3} + (8k^2+8k+2)n^2 - 2(8k^2+8k+2)\frac{n}{3} < 0.
\end{aligned}$$

When $p_1 = p_2 = \cdots = p_{k-1} = 0$ (i.e. $p_k = 1$), the para-chain L_n gets to the maximum of $E(Gut(G_n))$, that is $G_n \cong L_n$. If $p_1 + p_2 + p_3 + \cdots + p_{k-1} = 1$, let $p_{k-1} = 1 - p_1 - p_2 - \cdots - p_{k-2}$ $(0 \le p_1 \le 1,\ 0 \le p_2 \le 1, \ldots, 0 \le p_{k-1} \le 1)$, we have

$$\begin{aligned} E(Gut(G_n)) = &\sum_{i=1}^{k-2}(-N_i\frac{n^3}{3} + N_i n^2 - 2N_i\frac{n}{3})p_i + (-N_{k-1}\frac{n^3}{3} + N_{k-1}n^2 - 2N_{k-1}\frac{n}{3})(1 - p_1 - p_2 - \cdots p_{k-2}) \\ &+(8k^3 + 16k^2 + 10k + 2)\frac{n^3}{3} - (4k^2 + 6k + 2)n^2 + (4k^3 - 4k^2 + 8k + 7)\frac{n}{3} - 1. \end{aligned}$$

Therefore,

$$\begin{aligned} \frac{\partial E(Gut(G_n))}{\partial p_i} &= -(N_i - N_{k-1})\frac{n^3}{3} + (N_i - N_{k-1})n^2 - 2(N_i - N_{k-1})\frac{n}{3} < 0, \\ \frac{\partial E(Gut(G_n))}{\partial p_1} &= -(8k^3 - 8k^2 - 14k - 4)\frac{n^3}{3} + (8k^3 - 8k^2 - 14k - 4)n^2 - 2(8k^3 - 8k^2 - 14k - 4)\frac{n}{3} < 0, \\ \frac{\partial E(Gut(G_n))}{\partial p_2} &= -(8k^3 - 16k^2 - 22k - 6)\frac{n^3}{3} + (8k^3 - 16k^2 - 22k - 6)n^2 - 2(8k^3 - 16k^2 - 22k - 6)\frac{n}{3} < 0, \\ \vdots \qquad & \qquad \vdots \qquad \qquad \vdots \\ \frac{\partial E(Gut(G_n))}{\partial p_{k-2}} &= -(8k^2 + 8k + 2)\frac{n^3}{3} + (8k^2 + 8k + 2)n^2 - 2(8k^2 + 8k + 2)\frac{n}{3} < 0. \end{aligned}$$

So $p_1 = p_2 = \cdots = p_{k-2} = 0$ (i.e. $p_{k-1} = 1$), $E(Gut(G_n))$ can't attain the minimum value [28]. With the same calculations as the same above, If $p_1 + p_2 + p_3 + \ldots + p_i = 1$, let $p_i = 1 - p_1 - p_2 - \ldots - p_{i-1}$ $(0 \le p_1 \le 1,\ 0 \le p_2 \le 1, \ldots, 0 \le p_{i-1} \le 1)$, $(i \ge 3)$, we have

$$\begin{aligned} E(G(Gut_n)) = &\sum_{i=1}^{k-3}(-N_i\frac{n^3}{3} + N_i n^2 - 2N_i\frac{n}{3})p_i + (-N_{k-2}\frac{n^3}{3} + N_{k-2}n^2 - 2N_{k-2}\frac{n}{3})(1 - p_1 - p_2 - \cdots - p_{k-3}) \\ &+(8k^3 + 16k^2 + 10k + 2)\frac{n^3}{3} - (4k^2 + 6k + 2)n^2 + (4k^3 - 4k^2 + 8k + 7)\frac{n}{3} - 1. \end{aligned}$$

Therefore,

$$\frac{\partial E(G(Gut_n))}{\partial p_i} = -(N_i - N_{k-2})\frac{n^3}{3} + (N_i - N_{k-2})n^2 - 2(N_i - N_{k-2})\frac{n}{3} < 0, (k - 3 \ge 3).$$

only when $p_1 + p_2 = 1$, they may get to the minimum value [29,30]. Then let $p_1 = 1 - p_2$ $(0 \le p_2 \le 1)$

$$\begin{aligned} E(G(Gut_n)) = &(-N_1\frac{n^3}{3} + N_1 n^2 - 2N_1\frac{n}{3})(1 - p_2) + (-N_2\frac{n^3}{3} + N_2 n^2 - 2N_2\frac{n}{3})p_2 \\ &+(8k^3 + 16k^2 + 10k + 2)\frac{n^3}{3} - (4k^2 + 6k + 2)n^2 + (4k^3 - 4k^2 + 8k + 7)\frac{n}{3} - 1. \end{aligned}$$

Thus,

$$\frac{\partial E(G(Gut_n))}{\partial p_2} = (N_1 - N_2)\frac{n^3}{3} + (N_1 - N_2)n^2 - 2(N_1 - N_2)\frac{n}{3} > 0.$$

So $E(G(Gut_n))$ achieves the minimum value, when $p_2 = 0$ (*i.e.* $p_1 = 1$), that is $G_n \cong M_n$. □

3. The Schultz index in a random polygonal chain

In this section, we will consider the expected values of Schultz index of the random polygonal chain. In fact, G_{n+1} is G_n linked to a new terminal polygonal H_{n+1} by an edge, the H_{n+1} is made up with vertices $x_1, x_2, x_3, \ldots, x_{2k}$, and the new edge is $u_n x_1$; see Figure 1.

Theorem 3.1 The $E(S(G_n))(n \geq 1)$ of the random polygonal chain G_n is

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

Proof. Recall the random polygonal chain G_{n+1} is G_n linked a new terminal polygonal H_{n+1} by an edge, the H_{n+1} is made up with vertices $x_1, x_2, x_3, \ldots, x_{2k}$, and the new edge is $u_n x_1$; see Figure 1. By(1.3),

$$\begin{aligned} S(G_{n+1}) =& \sum_{\{u,v\}\subseteq V_{G_n}} (d(u) + d(v))d(u,v) + \sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} (d(v) + d(x_i))d(v, x_i) \\ &+ \sum_{\{x_i x_j\}\subseteq V_{H_{n+1}}} (d(x_i) + d(x_j))d(x_i, x_j). \end{aligned}$$

Note that

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

Recall that $d(x_1) = 3$ and $d(x_i) = 2$ ($i \in \{2, 3, 4, \ldots, 2k\}$). On the basis of (2.1)-(2.3), We get

$$\begin{aligned} \sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} (d(v) + d(x_i))d(v, x_i) &= \sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} d(v)d(v, x_i) + \sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} d(x_i)d(v, x_i) \\ &= \sum_{v\in V_{G_n}} d(v)[(d(u_n, v) + 1) + (d(u_n, v) + 2) + (d(u_n, v) + 3) \\ &\quad + \cdots + (d(u_n, v) + k + 1) + (d(u_n, v) + k) + \ldots + (d(u_n, v) + 2)] \\ &\quad + \sum_{v\in V_{G_n}} [3(d(u_n, v) + 1) + 2(d(u_n, v) + 2) + 2(d(u_n, v) + 3) \\ &\quad + \cdots + 2(d(u_n, v) + k + 1) + 2(d(u_n, v) + k) + \cdots + 2(d(u_n, v) + 2)] \end{aligned}$$

$$
\begin{aligned}
&= \sum_{v\in V_{G_n}} d(v)[2kd(u_n,v) + (k^2+2k)] \\
&\quad + \sum_{v\in V_{G_n}} [(4k+1)d(u_n,v) + (2k^2+4k+1)] \\
&= 2k\sum_{v\in V_{G_n}} d(v)d(u_n,v) + (k^2+2k)[(4k+2)n-1] \\
&\quad + (4k+1)\sum_{v\in V_{G_n}} d(u_n,v) + (2k^2+4k+1)\cdot 2kn \\
&= 2k\sum_{v\in V_{G_n}} d(v)d(u_n,v) + (4k+1)d(u_n,v) \\
&\quad + (8k^3+18k^2+6k)n - (k^2+2k).
\end{aligned}
$$

From (2.4), one has

$$
\begin{aligned}
\sum_{\{x_ix_j\}\subseteq V_{H_{n+1}}} (d(x_i)+d(x_j))d(x_i,x_j) &= \frac{1}{2}\sum_{i=1}^{2k}\sum_{j=1}^{2k}(d(x_i)+d(x_j))d(x_i,x_j) \\
&= \sum_{i=1}^{2k}\sum_{j=1}^{2k} d(x_i)d(x_i,x_j) \\
&= 2k^2 + (2k^2+1) + \cdots + (2k^2+k-1) + (2k^2+k) \\
&\quad + (2k^2+k-1) + \cdots + (2k^2+1) \\
&= [(2k^2+1) + (2k^2+k-1)](k-1) + 4k^2 + k \\
&= 4k^3 + k^2.
\end{aligned}
$$

Then

$$
S(G_{n+1}) = S(G_n) + (4k+2)\sum_{v\in V_{G_n}} d(u_n,v) + 2k\sum_{v\in V_{G_n}} d(v)d(u_n,v) + (8k^3+18k^2+6k)n + (4k^3-2k). \quad (3.1)
$$

For a random polygonal chain G_n, the number $\sum_{v\in V_{G_n}} d(u_n,v)$ is a random variable. We let

$$
B_n := E(\sum_{v\in V_{G_n}} d(u_n,v)).
$$

Substituting B_n into (3.1), we obtain the recurrence formula of $E(S(G_n))$,

$$
E(S(G_{n+1})) = E(S(G_n)) + (4k+2)B_n + 2kA_n + (8k^3+20k^2+12k+2)n + (4k^3-4k-1).
$$

Continue to consider the following k possible ways.
Way 1. $G_n \longrightarrow G^1_{n+1}$. In this way, u_n same as the vertex x_2 or x_{2k}. Then, $\sum_{v\in V_{G_n}} d(u_n,v)$ is described as $\sum_{v\in V_{G_n}} d(x_2,v)$ or $\sum_{v\in V_{G_n}} d(x_{2k},v)$ with probability p_1.
Way 2. $G_n \longrightarrow G^2_{n+1}$. In this way, u_n same as the vertex x_3 or x_{2k-1}. Then, $\sum_{v\in V_{G_n}} d(u_n,v)$ is described as $\sum_{v\in V_{G_n}} d(x_3,v)$ or $\sum_{v\in V_{G_n}} d(x_{2k-1},v)$ with probability p_2.

Way 3. $G_n \longrightarrow G_{n+1}^3$. In this way, u_n same as the vertex x_4 or x_{2k-2}. Then, $\sum_{v\in V_{G_n}} d(u_n, v)$ is described as $\sum_{v\in V_{G_n}} d(x_4, v)$ or $\sum_{v\in V_{G_n}} d(x_{2k-2}, v)$ with probability p_3.

$\vdots \quad \vdots \quad \vdots$

Way k-3. $G_n \longrightarrow G_{n+1}^{k-3}$. In this way, u_n same as the vertex x_{k-2} or x_{k+4}. Then, $\sum_{v\in V_{G_n}} d(u_n, v)$ is described as $\sum_{v\in V_{G_n}} d(x_{k-2}, v)$ or $\sum_{v\in V_{G_n}} d(x_{k+4}, v)$ with probability p_{k-3}.
Way k-2. $G_n \longrightarrow G_{n+1}^{k-2}$. In this way, u_n same as the vertex x_{k-1} or x_{k+3}. Then, $\sum_{v\in V_{G_n}} d(u_n, v)$ is described as $\sum_{v\in V_{G_n}} d(x_{k-1}, v)$ or $\sum_{v\in V_{G_n}} d(x_{k+3}, v)$ with probability p_{k-2}.
Way k-1. $G_n \longrightarrow G_{n+1}^{k-1}$. In this way, u_n same as the vertex x_k or x_{k+2}. Then, $\sum_{v\in V_{G_n}} d(u_n, v)$ is described as $\sum_{v\in V_{G_n}} d(x_k, v)$ or $\sum_{v\in V_{G_n}} d(x_{k+2}, v)$ with probability p_{k-1}.
Way k. $G_n \longrightarrow G_{n+1}^{k}$, then u_n is the vertex x_{k+1}. Then, $\sum_{v\in V_{G_n}} d(u_n, v)$ is described as $\sum_{v\in V_{G_n}} d(x_{k+1}, v)$ with probability $1 - p_1 - p_2 - p_3 - \cdots - p_{k-3} - p_{k-2} - p_{k-1}$.

On the basis of the above k ways, we get

$$
\begin{aligned}
B_n =& p_1 \sum_{v\in V_{G_n}} d(x_2, v) + p_2 \sum_{v\in V_{G_n}} d(x_3, v) + p_3 \sum_{v\in V_{G_n}} d(x_4, v) \\
&+ \cdots + p_{k-3} \sum_{v\in V_{G_n}} d(x_{k-2}, v) + p_{k-2} \sum_{v\in V_{G_n}} d(x_{k-1}, v) + p_{k-1} \sum_{v\in V_{G_n}} d(x_k, v) \\
&+ (1 - p_1 - p_2 - p_3 - \cdots - P_{k-3} - P_{k-2} - p_{k-1}) \sum_{v\in V_{G_n}} d(x_{k+1}, v) \\
=& p_1[\sum_{v\in V_{G_{n-1}}} d(u_{n-1}, v) + 2 \times 2k(n-1) + k^2] \\
&+ p_2[\sum_{v\in V_{G_{n-1}}} d(u_{n-1}, v) + 3 \times 2k(n-1) + k^2] \\
&+ p_3[\sum_{v\in V_{G_{n-1}}} d(u_{n-1}, v) + 4 \times 2k(n-1) + k^2] \\
&+ \cdots \\
&+ p_{k-3}[\sum_{v\in V_{G_{n-1}}} d(u_{n-1}, v) + (k-2) \times 2k(n-1) + k^2] \\
&+ p_{k-2}[\sum_{v\in V_{G_{n-1}}} d(u_{n-1}, v) + (k-1) \times 2k(n-1) + k^2] \\
&+ p_{k-1}[\sum_{v\in V_{G_{n-1}}} d(u_{n-1}, v) + k \times 2k(n-1) + k^2] \\
&+ (1 - p_1 - p_2 - p_3 - \cdots - p_{k-3} - p_{k-2} - p_{k-1})[\sum_{v\in V_{G_{n-1}}} d(u_{n-1}, v) + (k+1) \times 2k(n-1) + k^2].
\end{aligned}
$$

Substitute the expectation for the above equation,, and let $E(B_n) = B_n$, we obtain

$$
B_n = B_{n-1} + \{(2k^2 + 2k) - \sum_{i=1}^{k-1} [2k^2 + 2k - (i+1) \cdot 2k] p_i\} n
$$

$$+\sum_{i=1}^{k-1}[2k^2+2k-(i+1)\cdot 2k]p_i-(k^2+2k).$$

Let

$$Z=\sum_{i=1}^{k-1}[2k^2+2k-(i+1)\cdot 2k]p_i.$$

Hence,

$$B_n=B_{n-1}+[(2k^2+2k)-Z]n+Z-(k^2+2k).$$

By the calculation

$$B_1=E(\sum_{v\in V_{G_1}}d(u_1,v))=k^2.$$

Based on the above results, we have

$$B_n=\{(k^2+k)-\frac{1}{2}\sum_{i=1}^{k-1}[2k^2+2k-(i+1)\cdot 2k]p_i\}n^2+\{\frac{1}{2}\sum_{i=1}^{k-1}[2k^2+2k-(i+1)\cdot 2k]p_i-k\}n.$$

Thus,

$$B_n=[(k^2+k)-\frac{1}{2}Z]n^2+[\frac{1}{2}Z-k]n.$$

and

$$A_n=[(2k\cdot k+3k+1)-\frac{1}{2}M]n^2+[\frac{1}{2}M-(3k+2)]n+1.$$

Therefore,

$$\begin{aligned}E(S(G_{n+1}))=&E(S(G_n))+(4k+2)B_n+2kA_n+(8k^3+20k^2+12k+2)n+(4k^3-4k-1)\\=&E(S(G_n))+(4k+2)\{[(k^2+k)-\frac{1}{2}Z]n^2+[\frac{1}{2}Z-k]n\}\\&+2k\{[(2k\cdot k+3k+1)-\frac{1}{2}M]n^2+[\frac{1}{2}M-(3k+2)]n+1\}\\&+(8k^3+20k^2+12k+2)n+(4k^3-4k-1)\end{aligned}$$

and $E(S(G_1))=4k^3$.

Finally, we get the expected expression

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

Let

$$X = 2\sum_{i=1}^{k-1}[4k^3 - (4i-2)k^2 - 2ik]p_i$$

$$Y_i = 2[4k^3 - (4i-2)k^2 - 2ik]$$

Hence,

$$E(S(G_n)) = [(8k^3+12k^2+4k) - X]\frac{n^3}{3} + [X - (2k^2+2k)]n^2 + [(4k^3-6k^2+2k) - 2X]\frac{n}{3}.$$

as desired. □

Specially, If we set $(p_1, p_2, p_3, \ldots, p_{k-1}) = (1,0,0,\ldots,0), (0,1,0,\ldots,0), (0,0,1,\ldots,0), \cdots, (0,\ldots,1,0,0), (0,\ldots,0,1,0), (0,\ldots,0,0,1), (0,\ldots,0,0,0)$, respectively, and by Theorem 3.1, we can receive the Schultz index of the meta-chain M_n, the ortho-chain O_n^1, $O_n^2, \ldots, O_n^{k-2}$ and the para-chain L_n, as

$$\begin{aligned}
S(M_n) &= (16k^2+8k)\frac{n^3}{3} + (8k^3-6k^2-6k)n^2 - (12k^3-2k^2-10k)\frac{n}{3},\\
S(O_n^1) &= (24k^2+12k)\frac{n^3}{3} + (8k^3-14k^2-10k)n^2 - (12k^3-18k^2-18k)\frac{n}{3},\\
S(O_n^2) &= (32k^2+16k)\frac{n^3}{3} + (8k^3-22k^2-14k)n^2 - (12k^3-34k^2-26k)\frac{n}{3},\\
&\vdots \qquad\qquad \vdots \qquad\qquad \vdots\\
S(O_n^{k-3}) &= (8k^3-4k^2-4k)\frac{n^3}{3} + (14k^2+6k)n^2 + (4k^3-38k^2-14k)\frac{n}{3},\\
S(O_n^{k-2}) &= (8k^3+4k^2)\frac{n^3}{3} + (6k^2+2k)n^2 + (4k^3-22k^2-6k)\frac{n}{3},\\
S(L_n) &= (8k^3+12k^2+4k)\frac{n^3}{3} - (2k^2+2k)n^2 + (4k^3-6k^2+2k)\frac{n}{3}.\\
S(O_n^i) &= [(8k^3+12k^2+4k) - Y_{i+1}]\frac{n^3}{3} + [Y_{i+1} - (2k^2+2k)]n^2 + [(4k^3-6k^2+2k) - 2Y_{i+1}]\frac{n}{3}.
\end{aligned}$$

Obviously

$$S(M_n) + S(L_n) = S(O_n^1) + S(O_n^2) + \ldots + S(O_n^{k-2}).$$

Corollary 3.2 For a random polygonal chain G_n ($n \geq 3$), the para-chain L_n gets to the maximum and the meta-chain M_n gets to the minimum of $E(S(G_n))$.

Proof. By Theorem 3.1

$$E(S(G_n)) = \sum_{i=1}^{k-1}(-Y_i\frac{n^3}{3} + Y_i n^2 - 2Y_i\frac{n}{3})p_i + (8k^3+12k^2+4k)\frac{n^3}{3}$$
$$-(2k^2+2k)n^2 + (4k^3-6k^2+2k)\frac{n}{3}.$$

When $n \geq 3$, take the partial derivative of $E(S(G_n))$

$$
\begin{aligned}
\frac{\partial E(S(G_n))}{\partial p_i} &= -Y_i\frac{n^3}{3} + Y_i n^2 - \frac{2}{3}Y_i n < 0.\\
\frac{\partial E(S(G_n))}{\partial p_1} &= -(8k^3-4k^2-4k)\frac{n^3}{3} + (8k^3-4k^2-4k)n^2 - 2(8k^3-4k^2-4k)\frac{n}{3},\\
\frac{\partial E(S(G_n))}{\partial p_2} &= -(8k^3-12k^2-8k)\frac{n^3}{3} + (8k^3-12k^2-8k)n^2 - 2(8k^3-12k^2-8k)\frac{n}{3} < 0,\\
\frac{\partial E(S(G_n))}{\partial p_3} &= -(8k^3-20k^2-12k)\frac{n^3}{3} + (8k^3-20k^2-12k)n^2 - 2(8k^3-20k^2-12k)\frac{n}{3} < 0,\\
&\vdots \qquad\qquad \vdots \qquad\qquad \vdots\\
\frac{\partial E(S(G_n))}{\partial p_{k-1}} &= -(8k^2+4k)\frac{n^3}{3} + (8k^2+4k)n^2 - 2(8k^2+4k)\frac{n}{3} < 0.
\end{aligned}
$$

When $p_1 = p_2 = \ldots = p_{k-1} = 0$ (i.e. $p_k = 1$), the para-chain L_n gets to the maximum of $E(S(G_n))$, that is $G_n \cong L_n$. If $p_1 + p_2 + p_3 + \ldots + p_{k-1} = 1$, let $p_{k-1} = 1 - p_1 - p_2 - \ldots - p_{k-2}$ $(0 \leq p_1 \leq 1,\ 0 \leq p_2 \leq 1, \ldots, 0 \leq p_{k-1} \leq 1)$, we have

$$
\begin{aligned}
E(S(G_n)) = &\sum_{i=1}^{k-2}(-Y_i\frac{n^3}{3} + Y_i n^2 - 2Y_i\frac{n}{3})p_i + (-Y_{k-1}\frac{n^3}{3} + Y_{k-1}n^2 - 2Y_{k-1}\frac{n}{3})(1 - p_1 - p_2 - \cdots - p_{k-2})\\
&+ (8k^3+12k^2+4k)\frac{n^3}{3} - (2k^2+2k)n^2 - (4k^3-6k^2+2k)\frac{n}{3}.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\frac{\partial E(S(G_n))}{\partial p_i} &= -(Y_i - Y_{k-1})\frac{n^3}{3} + (Y_i - Y_{k-1})n^2 - \frac{2}{3}(Y_i - Y_{k-1})n < 0.\\
\frac{\partial E(S(G_n))}{\partial p_1} &= -(8k^3-12k^2-8k)\frac{n^3}{3} + (8k^3-12k^2-8k)n^2 - \frac{2}{3}(8k^3-12k^2-8k)n < 0,\\
\frac{\partial E(S(G_n))}{\partial p_2} &= -(8k^3-20k^2-12k)\frac{n^3}{3} + (8k^3-20k^2-12k)n^2 - \frac{2}{3}(8k^3-20k^2-12k)n < 0,\\
\frac{\partial E(S(G_n))}{\partial p_3} &= -(8k^3-28k^2-16k)\frac{n^3}{3} + (8k^3-28k^2-16k)n^2 - \frac{2}{3}(8k^3-28k^2-16k)n < 0,\\
&\vdots \qquad\qquad \vdots \qquad\qquad \vdots\\
\frac{\partial E(S(G_n))}{\partial p_{k-2}} &= -(8k^2+4k)\frac{n^3}{3} + (8k^2+4k)n^2 - \frac{2}{3}(8k^2+4k)n < 0.
\end{aligned}
$$

So $p_1 = p_2 = \ldots = p_{k-2} = 0$ (i.e. $p_{k-1} = 1$), $E(S(G_n))$can't attain the minimum value. With the same calculations as above, If $p_1 + p_2 + p_3 + \ldots + p_i = 1$, let $p_i = 1 - p_1 - p_2 - \ldots - p_{i-1}$ $(0 \leq p_1 \leq 1,\ 0 \leq p_2 \leq 1, \ldots, 0 \leq p_{i-1} \leq 1)$, $(i \geq 3)$, we have

$$
\begin{aligned}
E(S(G_n)) = &\sum_{i=1}^{k-3}(-Y_i\frac{n^3}{3} + Y_i n^2 - 2Y_i\frac{n}{3})p_i + (-Y_{k-2}\frac{n^3}{3} + Y_{k-2}n^2 - 2Y_{k-2}\frac{n}{3})(1 - p_1 - p_2 - \cdots - p_{k-3})\\
&+ (8k^3+12k^2+4k)\frac{n^3}{3} - (2k^2+2k)n^2 + (4k^3-6k^2+2k)\frac{n}{3}.
\end{aligned}
$$

Therefore,

$$\frac{\partial E(S(G_n))}{\partial p_i} = -(Y_i - Y_{k-2})\frac{n^3}{3} + (Y_i - Y_{k-2})n^2 - \frac{2}{3}(Y_i - Y_{k-2})n < 0, (k-3 \geq 3).$$

only when $p_1 + p_2 = 1$, they may get to the minimum value. Then let $p_1 = 1 - p_2$ $(0 \leq p_2 \leq 1)$

$$\begin{aligned} E(S(G_n)) =& (-Y_1\frac{n^3}{3} + Y_1 n^2 - 2Y_1\frac{n}{3})(1-p_2) + (-Y_2\frac{n^3}{3} + Y_2 n^2 - 2Y_2\frac{n}{3})p_2 \\ &+ (8k^3 + 12k^2 + 4k)\frac{n^3}{3} - (2k^2 + 2k)n^2 + (4k^3 - 6k^2 + 2k)\frac{n}{3}. \end{aligned}$$

Thus,

$$\frac{\partial E(S(G_n))}{\partial p_2} = (Y_1 - Y_2)\frac{n^3}{3} - (Y_1 - Y_2)n^2 + \frac{2}{3}(Y_1 - Y_2)n > 0.$$

So $E(S(G_n))$ achieves the minimum value, when $p_2 = 0$ (*i.e.* $p_1 = 1$), that is $G_n \cong M_n$. □

4. The average values for the the Gutman index and Schultz index

Recall that Θ_n is the set of all polygonal chains with n polygons. We give the average value for the Gutman index and Schultz index with respect to Θ_n.

$$Gut_{avr}(\Theta_n) = \frac{1}{|\Theta_n|}\sum_{G\in\Theta_n} Gut(G), \quad S_{avr}(\Theta_n) = \frac{1}{|\Theta_n|}\sum_{G\in\Theta_n} S(G).$$

For achieving the average value $Gut_{avr}(\Theta_n)$, $S_{avr}(\Theta_n)$, It takes $p_1 = p_2 = \ldots = p_k = \frac{1}{k}$ in the expected value for the Gutman index and Schultz index of the random polygonal chain (i.e.$E(Gut(G_n))$, $E(S(G_n))$). According to Theorem 2.1 and 3.1,

Theorem 4.1 The $Gut_{avr}(\Theta_n)(n \geq 1)$ and $S_{avr}(\Theta_n)(n \geq 1)$ for the the Gutman index and Schultz index of the random chain G_n are

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

$$\begin{aligned} S_{avr}(\Theta_n) =& \{(8k^3 + 12k^2 + 4k) - \frac{2}{k}\sum_{i=1}^{k-1}[4k^3 - (4i-2)k^2 - 2ik]p_i\}\frac{n^3}{3} \\ &+ \{\frac{2}{k}\sum_{i=1}^{k-1}[4k^3 - (4i-2)k^2 - 2ik]p_i - (2k^2 + 2k)\}n^2 \\ &+ \{(4k^3 - 6k^2 + 2k) - \frac{2\cdot 2}{k}\sum_{i=1}^{k-1}[4k^3 - (4i-2)k^2 - 2ik]p_i\}\frac{n}{3}. \end{aligned}$$

After verification, the equations are established,

$$Gut_{avr}(\Theta_n) = \frac{1}{k}Gut(M_n) + \frac{1}{k}Gut(O_n^1) + \frac{1}{k}Gut(O_n^2) + \ldots + \frac{1}{k}Gut(O_n^{k-2}) + \frac{1}{k}Gut(L_n).$$
$$S_{avr}(\Theta_n) = \frac{1}{k}S(M_n) + \frac{1}{k}S(O_n^1) + \frac{1}{k}S(O_n^2) + \ldots + \frac{1}{k}S(O_n^{k-2}) + \frac{1}{k}S(L_n).$$

5. Conclusion

In this paper, we establish the explicit analytical expressions for the expected values of the Gutman index, Schultz index of a random polygonal chain . We also get the extremal values and average values of Gutman and Schultz indices. All these results will contribute to the study of the topological index of graphs and can better predict the physicochemical properties of more novel compounds, which can be applied to the research of drugs, macromolecular polymers and new materials [20,31–33].

In chemical graph theory, the matter of polygonal chain is being widely studied by researchers. The molecular structures of polygonal chemicals are various and its physicochemical properties also become more and more important, and refer to [34–37]. It is possible to establish exact formulas for the expected values of some indices of a random polygon chain with n regular polygons[38–41].

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Conflict of interest

The authors declare that they have no competing interests.

References

1. A. I. Pavlyuchko, E. V. Vasiliev, L. A. Gribov, Quantum chemical estimation of the overtone contribution to the IR spectra of hydrocarbon halogen derivatives, *J. Struct. Chem.*, (2010), 1045–1051. https://doi.org/10.1007/s10947-010-0161-5

2. D. R. Flower, On the properties of bit string-based measures of chemical similarity, *J. Chem. Inf. Comput. Sci.*, **38** (1998), 379–386. https://doi.org/10.1021/ci970437z

3. H. L. Donald, M. A. Whitehead, Molecular geometry and bond energy. III. Cyclooctatetraene and related compounds, *J. Am. Chem. Soc.*, **91** (1969), 238–242. https://doi.org/10.1021/ja01030a003

4. E. Estrada, D. Bonchev, P. Zhang, Chemical Graph Theory, *Discrete Math. Appl.*, (2013), 1–24. https://doi.org/10.1201/b16132-92

5. J. A. Bondy, U. S. R. Murty, Graph Theory, Springer, New York, 2008.

6. F. Buckley, F. Harary, Distance in Graphs, Addison-Wesley, Reading, 1989. https://doi.org/10.1007/978-0-8176-4789-6-3

7. H. Hosoya, Topological index, A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.*, **44**(1971), 2332–2339. https://doi.org/10.1246/bcsj.44.2332

8. M. Garavelli, F. Bernardi, A. Cembran, Cyclooctatetraene Computational Photo- and Thermal Chemistry: A reactivity model for conjugated hydrocarbons, *J. Am. Chem. Soc.*, **124** (2002), 13770–13789. https://doi.org/10.1021/ja020741v

9. R. C. Entringer, D. E. Jackson, D. A. Snyder, Distance in graphs, *Czechoslovak Math. J.*, **26** (1976), 283–296.

10. A. L. Chen, F. J. Zhang, Wiener index and perfect matchings in random phenylene chains, *MATCH Commun. Math. Comput. Chem.*, **61** (2009), 623–630. https://doi.org/10.1117/12.676730

11. H. Deng, Wiener indices of spiro and polyphenyl hexagonal chains, *Math. Computer Model.*, **55** (2012), 634–644. https://doi.org/10.1016/j.mcm.2011.08.037

12. L. Ma, H. Bian, B. J. Liu, H. Z. Yu, The expected values of the Wiener indices in the random phenylene and spiro chains, *Ars Combin.*,**130** (2017), 267–274.

13. Q. N. Zhou, L. G. Wang, Y. Lu, Wiener index and Harary index on Hamilton-connected graphs with large minimum degree, *Discrete Appl. Math.*, **247** (2018), 180–185. https://doi.org/10.1016/j.dam.2018.03.063

14. Wiener, Structrual determination of paraffin boiling points, *J. Am. Chem. Soc.*, , **69** (1947), 17–20. https://doi.org/10.1021/ja01193a005

15. S. Mukwembi, S. Munyira, MunyiraDegree distance and minimum degree, *Bull. Aust. Math. Soc.*, **87** (2013), 255–271. https://doi.org/10.1017/S0004972712000354

16. S. L. Wei, W. C. Shiu, Enumeration of Wiener indices in random polygonal chains, *J. Math. Anal. Appl.*, **469** (2018), 537–548. https://doi.org/10.1016/j.jmaa.2018.09.027

17. W. Yang, F. Zhang, Wiener index in random polyphenyl chains, *MATCH Commun. Math. Comput. Chem.*, **68** (2012), 371–376. https://doi.org/10.1155/2012/128492

18. L. L. Zhang, Q. S. Li, S. C. Li, M. J. Zhang, The expected values for the Schultz index, Gutman index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random polyphenylene chain, *J. Discrete Appl. Math.*, **282** (2020), 243–256. https://doi.org/10.1016/j.dam.2019.11.007

19. J. F. Qi, M. L. Fang, X. Y. Geng, The expected value for the Wiener index in the Random Spiro Chains, *Polycycl. Aromat. Comp.*. https://doi.org/10.1080/10406638.2022.2038218

20. A. Heydari, On the modified Schultz index of $C_4C_8(S)$ nanotubes and nanotorus, *Digest. J. Nanomater. Biostruct.*, **5** (2010), 51–56. https://doi.org/10.1063/1.3279788

21. M. R. Farahani, Hosoya, Schultz, modified Schultz polynomials and their topological indices of benzene molecules: First members of polycyclic aromatic hydrocarbons (PAHs), *Int. J. Theor. Chem.*, **1** (2013), 9–16.

22. Z. Xiao, S. Chen, The modified Schultz index of armchair polyhex nanotubes, *J. Comput. Theor. Nanosci.*, **6** (2009), 1109–1114. https://doi.org/10.1166/jctn.2009.1150

23. G. H. Huang, M. J. Kuang, H. Y. Deng, The expected values of Kirchhoff indices in the random polyphenyl and spiro chains, *Ars Math. Contemp.*, **9** (2015), 197–207. https://doi.org/10.26493/1855-3974.458.7b0

24. W. C. Evans, D. Evans, Hydrocarbons and derivatives, in *Trease and Evans' Pharmacognosy* (eds. W. C. Evans and D. Evans), (2009) 173–193. https://doi.org/10.1016/B978-0-7020-2933-2.00019-8

25. W. B. Person, G. C. Pimentel, K. S. Pitzer, The Structure of Cyclooctatetraene, *J. Am. Chem. Soc.*, **74** (1952), 3437–3438. https://doi.org/10.1021/ja01133a524

26. E. Booth, G. Strobel, B. Knighton, J. Sears, B. Geary, R. Avci, A rapid column technique for trapping and collecting of volatile fungal hydrocarbons and hydrocarbon derivatives, *Biotechnol. Letters.*, (2011), 1963–1972. https://doi.org/10.1007/s10529-011-0660-2

27. S. Chen, Modified Schultz index of zig-zag polyhex nanotubes, *J. Comput. Theor. Nanosci.*, **6** (2009), 1499–1503. https://doi.org/10.1166/jctn.2009.1201

28. P. Zhao, B. Zhao, X. Chen, Y. Bai, Two classes of chains with maximal and minimal total $\pi-$ *electron* energy, *MATCH Commun. Math. Comput. Chem.*, **62** (2009), 525–536.

29. X. Chen, B. Zhao, P. Zhao, Six-membered ring spiro chains with extremal Merrifild-Simmons index and Hosoya index, *MATCH Commun. Math. Comput. Chem.*, **62** (2009), 657–665.https://doi.org/10.1111/j.1467-9892.2008.00605

30. Y. Bai, B. Zhao, P. Zhao, Extremal Merrifield-Simmons index and Hosoya index of polyphenyl chains, *MATCH Commun. Math. Comput. Chem.*, **62** (2009), 649–656. https://doi.org/10.1111/j.1467-9892.2008.00605.x

31. I. Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.*, **34** (1994), 1087–1089. https://doi.org/10.1021/ci00021a009

32. R. J. Schwamm, M. D. Anker, M. Lein, R. vs. Addition: The reaction of an Aluminyl Anion with 1,3,5,7-Cyclooctatetraene, *J. Chem.*, **58** (2019), 1489–1493. https://doi.org/10.1002/ange.201811675

33. R. Todeschini, V. Consonni, Handbook of Molecular Descriptors,Wiley-VCH, 2000.

34. G. Luthe, J. A. Jacobus, L. W. Robertson, Receptor interactions by polybrominated diphenyl ethers versus polychlobrinated biphenyls: a theoretical structure-activity assessment, *Environ. Toxicol. Pharm.*, **25** (2008), 202–210. https://doi.org/10.1016/j.etap.2007.10.017

35. M. Traetteberg, G. Hagen, S. J. Cyvin, IV. 1,3,5,7-Cyclooctatetraene, *Zeitschrift Für Naturforschung B.*, **25** (1970), 134–138. https://doi.org/10.1515/znb-1970-0201

36. N. Milas, J. Nolan, Jr. Petrus, H. L. Otto, Notes-Ozonization of Cyclooctatetraene, *J. Org. Chem.*, **23** (1958), 624–625. https://doi.org/10.1021/jo01098a611

37. W. B. Person, G. C. Pimentel, K. S. Pitzer, The Structure of Cyclooctatetraene, *J. Am. Chem. Soc.*, **74** (1952), 3437–3438. https://doi.org/10.1021/ja01133a524

38. F. S. Mathews, W. N. Lipscomb, The structure of Silver Cyclooctatetraene Nitrate, *J. Phys. Chem.*, **63** (1959), 845–850. https://doi.org/10.1021/j150576a017

39. R. C. Tendick, J. T. O'Beck, M. R. Nimmo, T. Y. Francis Record, Hydrocarbon conversion system and method with a plurality of sources of compressed oxygen-containing gas, *Free Patents Online*, (2002).

40. Q. R. Li, Q. Yang, H. Yin, S. Yang, Analysis of by-products from improved Ullmann reaction using TOFMS and GCTOFMS, *J. Univ. Sci. Technol. China.*, **34** (2004), 335–341.https://doi.org10.2174/0929866043478455

41. S. Tepavcevic, A. T. Wroble, M. Bissen, D. J. Wallace, Y. Choi, L. Hanley, Photoemission studies of polythiophene and polyphenyl films produced via surface polymerization by ion-assisted deposition, *J. Phys. Chem. B.*, **109** (2005), 7134–7140. https://doi.org/10.1021/jp0451445