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Article

# Enumeration of the Additive Degree–Kirchhoff Index in the Random Polygonal Chains

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**Abstract:** The additive degree–Kirchhoff index is an important topological index. This paper we devote to establishing the explicit analytical expression for the simple formulae of the expected value of the additive degree–Kirchhoff index in a random polygon. Based on the result above, the additive degree–Kirchhoff indexes of all polygonal chains with extremal values and average values are obtained.

**Keywords:** additive degree–Kirchhoff index; random polygonal chains; expected value; extremal value; average value

**MSC:** 05C50

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## 1. Introduction

In this paper, we only consider simple and finite connected graphs. The topology and chemical index of the graph play important roles in describing the chemical molecular diagram and establishing the relationships between molecular structure and characteristics. It is a topological index closely related to the physical and chemical properties of compounds, so it is widely used to predict the physical and chemical properties and biological activity of compounds.

The molecular diagram in a chemical diagram is the structural diagram of a compound molecule. We let the vertices represent the atoms, and edges stand for the covalent bonds between atoms. Then, the molecular structure can be represented by this diagram, which is called the molecular diagram. For more detailed information, we can refer to [1–13] and the references cited therein.

The molecular topological index is a kind of topological invariant, which is a numerical parameter generated from a molecular structure, and the properties of molecules are indirectly expressed by molecular structure—that is, the relationship between molecular structure and performance can be established. The physical and chemical properties of molecules can be reflected by some topological indexes, which can be divided into many categories according to different parameters, such as point degree, adjacent point degree and the distance between two points. Let $G = (V(G), E(G))$ be a graph with the vertex set $V(G)$ and the edge set $E(G)$. 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 $v$.

In 1993, the resistance distance was found to be a novel distance function on the graph proposed by Klein and Randić [14]. $r(x, y)$ denotes the resistance distance between vertices $x$ and $y$ in $G$. For $x, y \subseteq V(G)$, the resistance distance between $x$ and $y$ in $G$, denoted by $r_G(x, y)$, is defined as the effective resistance between nodes $x$ and $y$ of the electrical network, for which nodes corresponding to vertices of $G$ and each edge of $G$ are replaced by resistors of unit resistance. The Kirchhoff index of $G$ is defined in analogy to the Wiener index as [15–21]

$$Kf(G) = \sum_{\{x,y\}\subseteq V_G} r(x,y). \tag{1}$$

In 2012, the additive degree–Kirchhoff index was introduced by Gutman, Feng and Yu. We refer the papers [22,23], in which it was defined as

$$Kf^+(G) = \sum_{\{x,y\}\subseteq V_G} (d(x)+d(y))r(x,y). \tag{2}$$

A random polygonal chain $G_n$ with $n$ polygons can be regarded as a polygonal chain $G_{n-1}$ with $n-1$ polygons to which a new terminal polygon $H_n$ has been adjoined by a cut edge; see Figure 1. For $n \geq 3$, the terminal polygon $H_n$ can be attached in $k$ ways, which results in the local arrangements we describe as $G_n^1, G_n^2, G_n^3, \ldots, G_n^k$. See Figure 2. A random polygonal chain $G_n(p_1, p_2, p_3, \ldots, p_{k-1})$ with $n$ polygons is a polygonal chain obtained by stepwise addition of terminal polygons. At each step $k(=3,4,\ldots,n)$, a random selection is made from one of the $k$ possible constructions:

- $G_{k-1} \to G_{2k}^1$ with probability $p_1$,
- $G_{k-1} \to G_{2k}^2$ with probability $p_2$,
- $G_{k-1} \to G_{2k}^3$ with probability $p_3$,
- $\vdots \quad \vdots \quad \vdots$
- $G_{k-1} \to G_{2k}^{k-1}$ 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 $p_1, p_2, p_3, \ldots, p_{k-1}$ are constants, unrelated to the step parameter $k$.

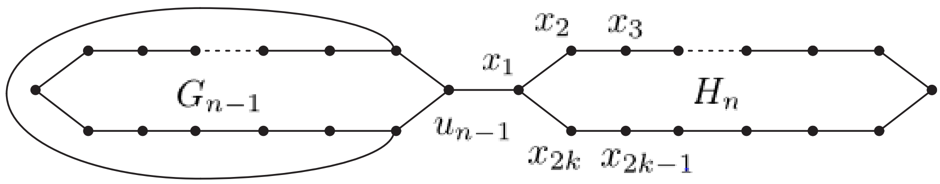


**Figure 1.** A polygonal chain $G_n$ with $n$ polygons.

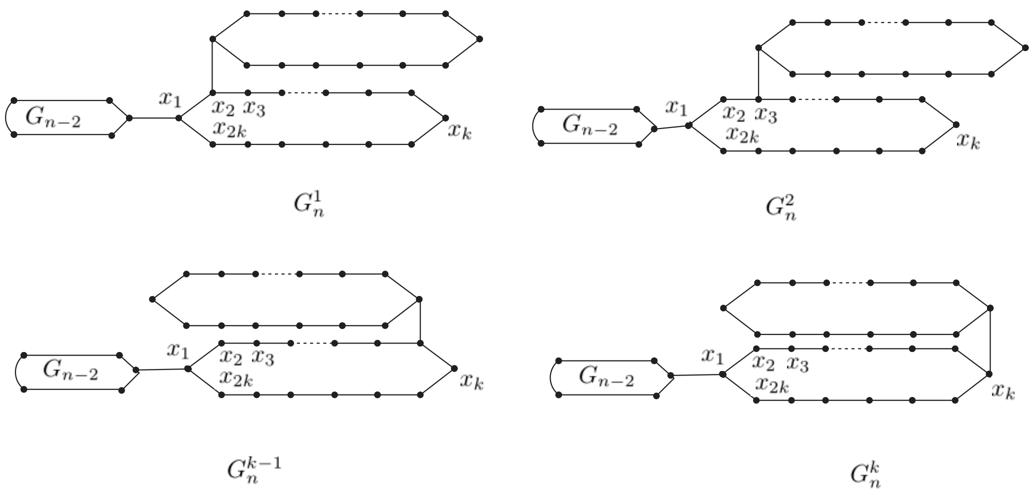


**Figure 2.** $k$ types of local arrangements in a polygonal chain.

Let $G_n$ be a polygonal chain with $n$ polygons $H_1, H_2, \ldots, H_n$. Set $u_k\omega_k$ as the cut edge of $G_n$ connecting $H_k$ and $H_{k+1}$ with $u_k \in V_{H_k}, \omega_k \in V_{H_{k+1}}$ for $k = 1,2,\cdots,n-1$. Clearly, both $\omega_k$ and $u_{k+1}$ are the vertices in $H_{k+1}$ and $d(\omega_k, u_{k+1}) \in \{1,2,3,\ldots,n\}$. In particular,

$G_n$ is the meta-chain $M_n$; the ortho-chains are $O_n^1, O_n^2, \ldots, O_n^{k-2}$; and the para-chain is $Ln$ 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., $p_k = 1$) for all $k \in \{1, 2, \ldots, n-2\}$, respectively. For convenience, let $\Theta_n$ be the set of all polygonal chains with $n$ polygons.

Huang, Kuang and Deng [24,25] obtained the expected values of the Kirchhoff index of random polyphenyl and spiro chains. Zhang and Li et al. [26], obtained the expected values of the expected values for the Schultz index, Gutman index, multiplicative degree–Kirchhoff index and additive degree–Kirchhoff index of a random polyphenylene chain. For more information, we can refer to [27–34]. The molecular diagram in this paper contains all the molecular diagrams of the previous study and is a general result. We calculate the explicit analytical expressions for the expected values of the additive degree–Kirchhoff index of a random polygonal chain. We also obtained the extremal values and average values of the additive degree–Kirchhoff index with respect to the set of all polygonal chains with $n$ polygons. It can be applied in practice more conveniently. These results can help biochemists with predicting and synthesizing new compounds and drugs.

## 2. The Additive Degree–Kirchhoff Index in a Random Polygonal Chain

In this section, we consider the expected value of additive degree–Kirchhoff index of the random polygonal chain. For a random polygonal chain $G_n$, the additive degree–Kirchhoff index is a random variable. In fact, $G_{n+1}$ is $G_n$ linked to a new terminal polygonal $H_{n+1}$ by an edge, where $H_{n+1}$ is spanned by vertices $x_1, x_2, x_3, \ldots, x_{2k}$, and the new edge is $u_n x_1$; see Figure 1. On the one hand, for all $v \in V_{G_n}$, one has

$$
\begin{aligned}
r(x_1, v) &= r(u_n, v) + 1, \\
r(x_2, v) &= r(u_n, v) + 1 + \frac{1 \cdot (2k-1)}{1 + (2k-1)} = r(u_n, v) + 1 + \frac{2k-1}{2k}, \\
r(x_3, v) &= r(u_n, v) + 1 + \frac{2 \cdot (2k-2)}{2 + (2k-2)} = r(u_n, v) + 1 + \frac{4k-4}{2k}, \\
&\vdots \qquad \vdots \qquad \vdots \\
r(x_k, v) &= r(u_n, v) + 1 + \frac{(k-1) \cdot (k+1)}{(k-1) + (k+1)} = r(u_n, v) + 1 + \frac{k^2-1}{2k}, \\
r(x_{k+1}, v) &= r(u_n, v) + 1 + \frac{k \cdot k}{k+k} = r(u_n, v) + 1 + \frac{k^2}{2k}, \\
r(x_{k+2}, v) &= r(u_n, v) + 1 + \frac{(k+1) \cdot (k-1)}{(k+1) + (k-1)} = r(u_n, v) + 1 + \frac{k^2-1}{2k}, \\
&\vdots \qquad \vdots \qquad \vdots \\
r(x_{2k-1}, v) &= r(u_n, v) + 1 + \frac{(2k-2) \cdot 2}{(2k-2) + 2} = r(u_n, v) + 1 + \frac{4k-4}{2k}, \\
r(x_{2k}, v) &= r(u_n, v) + 1 + \frac{(2k-1) \cdot 1}{(2k-1) + 1} = r(u_n, v) + 1 + \frac{2k-1}{2k}.
\end{aligned} \tag{3}
$$

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

On the other hand,

$$
\begin{aligned}
\sum_{i=1}^{2k} d(x_i)r(x_1,x_i) &= \frac{4k^2-1}{3} = \frac{8k^3-2k}{6k},\\
\sum_{i=1}^{2k} d(x_i)r(x_2,x_i) &= \frac{4k^2-1}{3} + \frac{1\cdot(2k-1)}{2k} = \frac{8k^3+4k+3}{6k},\\
\sum_{i=1}^{2k} d(x_i)r(x_3,x_i) &= \frac{4k^2-1}{3} + \frac{2\cdot(2k-2)}{2k} = \frac{8k^3+10k-12}{6k},\\
&\vdots \qquad \vdots \qquad \vdots\\
\sum_{i=1}^{2k} d(x_i)r(x_k,x_i) &= \frac{4k^2-1}{3} + \frac{(k-1)\cdot(k+1)}{2k} = \frac{8k^3+3k^2-2k-3}{6k},\\
\sum_{i=1}^{2k} d(x_i)r(x_{k+1},x_i) &= \frac{4k^2-1}{3} + \frac{k\cdot k}{2k} = \frac{8k^2+3k-2}{6},\\
\sum_{i=1}^{2k} d(x_i)r(x_{k+2},x_i) &= \frac{4k^2-1}{3} + \frac{(k+1)\cdot(k-1)}{2k} = \frac{8k^3+3k^2-2k-3}{6k},\\
&\vdots \qquad \vdots \qquad \vdots\\
\sum_{i=1}^{2k} d(x_i)r(x_{2k-1},x_i) &= \frac{4k^2-1}{3} + \frac{(2k-2)\cdot 2}{2k} = \frac{8k^3+10k-12}{6k},\\
\sum_{i=1}^{2k} d(x_i)r(x_{2k},x_i) &= \frac{4k^2-1}{3} + \frac{(2k-1)\cdot 1}{2k} = \frac{8k^3+4k+3}{6k}.
\end{aligned}
\tag{5}
$$

**Theorem 1.** *For $n \geq 1$, the expected value for the additive degree–Kirchhoff index of the random polygonal chain $G_n$ is*

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

**Proof.** Recall that the random polygonal chain $G_{n+1}$ is obtained by attaching to $G_n$ a new terminal polygonal $H_{n+1}$ by an edge, where $H_{n+1}$ is spanned by vertices $x_1, x_2, x_3, \ldots, x_{2k}$, and the new edge is $u_n x_1$; we may use the same notation as that used at the beginning of last section. By (2), one has

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

Note that

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

Recall that $d(x_1) = 3$ and $d(x_i) = 2$ for $i \in \{2, 3, 4, \ldots, 2k\}$. From (3) and (4), we have

$$\begin{aligned}
&\sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} (d(v) + d(x_i))r(v, x_i) \\
=& \sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} d(v)r(v, x_i) + \sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} d(x_i)r(v, x_i) \\
=& \sum_{v\in V_{G_n}} d(v)[(r(u_n, v) + 1) + (r(u_n, v) + 1 + \frac{1\cdot(2k-1)}{2k}) \\
&+ (r(u_n, v) + 1 + \frac{2\cdot(2k-2)}{2k}) + (r(u_n, v) + 1 + \frac{3\cdot(2k-3)}{2k}) \\
&+ \cdots + (r(u_n, v) + 1 + \frac{(k-1)\cdot(k+1)}{2k}) + (r(u_n, v) + 1 + \frac{k\cdot k}{2k}) \\
&+ (r(u_n, v) + 1 + \frac{(k-1)\cdot(k+1)}{2k}) + \cdots + (r(u_n, v) + 1 + \frac{2\cdot(2k-2)}{2k}) \\
&+ (r(u_n, v) + 1 + \frac{1\cdot(2k-1)}{2k})] \\
&+ \sum_{v\in V_{G_n}} [3(r(u_n, v) + 1) + 2(r(u_n, v) + 1 + \frac{1\cdot(2k-1)}{2k}) \\
&+ 2(r(u_n, v) + 1 + \frac{2\cdot(2k-2)}{2k}) + 2(r(u_n, v) + 1 + \frac{3\cdot(2k-3)}{2k}) \\
&+ \cdots + 2(r(u_n, v) + 1 + \frac{(k-1)\cdot(k+1)}{2k}) + 2(r(u_n, v) + 1 + \frac{k\cdot k}{2k}) \\
&+ 2(r(u_n, v) + 1 + \frac{(k-1)\cdot(k+1)}{2k}) + \cdots + 2(r(u_n, v) + 1 + \frac{2\cdot(2k-2)}{2k}) \\
&+ 2(r(u_n, v) + 1 + \frac{1\cdot(2k-1)}{2k})] \\
=& 2k \sum_{v\in V_{G_n}} d(v)r(u_n, v) + \frac{4k^2 + 12k - 1}{6}[(4k+2)n - 1] \\
&+ (4k+1) \sum_{v\in V_{G_n}} r(u_n, v) + \frac{4k^2 + 12k + 2}{3} \times 2kn.
\end{aligned}$$

Note that $\sum_{i=1}^{2k} r(x_k, x_i) = \frac{8k^3-2k}{12k}$ for $k = 1, 2, 3, \cdots, 2k$. From (5), one has

$$\begin{aligned}
\sum_{\{x_i x_j\}\subseteq V_{H_{n+1}}} (d(x_i) + d(x_j))r(x_i, x_j) =& \frac{1}{2} \sum_{i=1}^{2k} \sum_{j=1}^{2k} (d(x_i) + d(x_j))r(x_i, x_j) \\
=& \sum_{i=1}^{2k} \sum_{j=1}^{2k} d(x_i)r(x_i, x_j) \\
=& \frac{8k^3 - 2k}{12k}[3 + 2 \times (2k-1)] \\
=& \frac{16k^3 + 4k^2 - 4k - 1}{6}.
\end{aligned}$$

Then,

$$Kf^+(G_{n+1}) = Kf^+(G_n) + (4k+2) \sum_{v\in V_{G_n}} r(u_n, v) + 2k \sum_{v\in V_{G_n}} d(v)r(u_n, v) + \frac{16k^3 + 52k^2 + 14k - 1}{3} n + \frac{8k^3 - 8k}{3}. \quad (6)$$

For a random polygonal chain $G_n$, the number $\sum_{v\in V_{G_n}} d(v)r(u_n,v)$ is a random variable. We may denote its expected value by

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

For a random polygonal chain $G_n$, the number $\sum_{v\in V_{G_n}} r(u_n,v)$ is a random variable. We may denote its expected value by

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

By a expectation operator and by substituting $R_n$ and $D_n$ into (6), we can obtain a recurrence relation for the expected value for the additive degree–Kirchhoff index of a random polygonal chain $G_n$ as follows:

$$E(Kf^+(G_{n+1})) = E(Kf^+(G_n)) + (4k+2)D_n + 2kR_n + \frac{16k^3+52k^2+14k-1}{3}n + \frac{8k^3-8k}{3}.$$

Consider the following $k$ possible cases.
**Case 1.** $G_n \longrightarrow G^1_{n+1}$. In this case, $u_n$ coincides with the vertex $x_2$ or $x_{2k}$. Consequently, $\sum_{v\in V_{G_n}} r(u_n,v)$ is given by $\sum_{v\in V_{G_n}} r(x_2,v)$ or $\sum_{v\in V_{G_n}} r(x_{2k},v)$ with probability $p_1$.
**Case 2.** $G_n \longrightarrow G^2_{n+1}$. In this case, $u_n$ coincides with the vertex $x_3$ or $x_{2k-1}$. Consequently, $\sum_{v\in V_{G_n}} r(u_n,v)$ is given by $\sum_{v\in V_{G_n}} r(x_3,v)$ or $\sum_{v\in V_{G_n}} r(x_{2k-1},v)$ with probability $p_2$.
**Case 3.** $G_n \longrightarrow G^3_{n+1}$. In this case, $u_n$ coincides with the vertex $x_4$ or $x_{2k-2}$. Consequently, $\sum_{v\in V_{G_n}} r(u_n,v)$ is given by $\sum_{v\in V_{G_n}} r(x_4,v)$ or $\sum_{v\in V_{G_n}} r(x_{2k-2},v)$ with probability $p_3$.

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

**Case k − 3.** $G_n \longrightarrow G^{k-3}_{n+1}$. In this case, $u_n$ coincides with the vertex $x_{k-2}$ or $x_{k+4}$. Consequently, $\sum_{v\in V_{G_n}} r(u_n,v)$ is given by $\sum_{v\in V_{G_n}} r(x_{k-2},v)$ or $\sum_{v\in V_{G_n}} r(x_{k+4},v)$ with probability $p_{k-3}$.
**Case k − 2.** $G_n \longrightarrow G^{k-2}_{n+1}$. In this case, $u_n$ coincides with the vertex $x_{k-1}$ or $x_{k+3}$. Consequently, $\sum_{v\in V_{G_n}} r(u_n,v)$ is given by $\sum_{v\in V_{G_n}} r(x_{k-1},v)$ or $\sum_{v\in V_{G_n}} r(x_{k+3},v)$ with probability $p_{k-2}$.
**Case k − 1.** $G_n \longrightarrow G^{k-1}_{n+1}$. In this case, $u_n$ coincides with the vertex $x_k$ or $x_{k+2}$. Consequently, $\sum_{v\in V_{G_n}} r(u_n,v)$ is given by $\sum_{v\in V_{G_n}} r(x_k,v)$ or $\sum_{v\in V_{G_n}} r(x_{k+2},v)$ with probability $p_{k-1}$.
**Case k.** $G_n \longrightarrow G^k_{n+1}$, then $u_n$ is the vertex $x_{k+1}$. Consequently, $\sum_{v\in V_{G_n}} r(u_n,v)$ is given by $\sum_{v\in V_{G_n}} r(x_{k+1},v)$ with probability $1-p_1-p_2-p_3-\ldots-p_{k-3}-p_{k-2}-p_{k-1}$.

According to the above $k$ cases, we may obtain the expected value $R_n$ as

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

By applying the expectation operator to the above equation, and noting that $E(R_n) = R_n$, we obtain

$$
\begin{aligned}
R_n =& R_{n-1} + \{(2k^2 + 5k + 2) - \sum_{i=1}^{k-1} [(2k^2 + 5k + 2) - \frac{2k + i \cdot (2k - i)}{k} (2k+1)] p_i \} n \\
&+ \sum_{i=1}^{k-1} [(2k^2 + 5k + 2) - \frac{2k + i \cdot (2k - i)}{k} (2k+1)] p_i - \frac{2k^2 + 15k + 10}{3}.
\end{aligned}
$$

Let

$$
V = \sum_{i=1}^{k-1} [(2k^2 + 5k + 2) - \frac{2k + i \cdot (2k - i)}{k} (2k+1)] p_i.
$$

Hence,

$$
R_n = R_{n-1} + [(2k^2 + 5k + 2) - V] n + V - \frac{2k^2 + 15k + 10}{3}.
$$

The boundary condition is

$$
R_1 = E(\sum_{v \in V_{G_n}} d(v) r(u_1, v)) = \frac{4k^2 - 1}{3}.
$$

According to the above recurrence relation and the boundary condition, we have

$$
\begin{aligned}
R_n =& \{ \frac{(2k^2+5k+2)}{2} - \frac{1}{2}\sum_{i=1}^{k-1}[(2k^2+5k+2) - \frac{2k+i\cdot(2k-i)}{k}(2k+1)]p_i \} n^2 \\
&+ \{ \frac{1}{2}\sum_{i=1}^{k-1}[(2k^2+5k+2) - \frac{2k+i\cdot(2k-i)}{k}(2k+1)]p_i + \frac{2k^2-15k-14}{6} \} n + 1.
\end{aligned}
$$

Thus,

$$
R_n = [\frac{(2k^2+5k+2)}{2} - \frac{1}{2}V]n^2 + [\frac{1}{2}V + \frac{2k^2-15k-14}{6}]n + 1.
$$

According to the above and the above $k$ cases, we may obtain the expected value $D_n$ as

$$
\begin{aligned}
D_n =& p_1 \sum_{v\in V_{G_n}} r(x_2,v) + p_2 \sum_{v\in V_{G_n}} r(x_3,v) + p_3 \sum_{v\in V_{G_n}} r(x_4,v) \\
&+ \cdots + p_{k-3} \sum_{v\in V_{G_n}} r(x_{k-2},v) + p_{k-2} \sum_{v\in V_{G_n}} r(x_{k-1},v) + p_{k-1} \sum_{v\in V_{G_n}} r(x_k,v) \\
&+ (1-p_1-p_2-p_3-\ldots-P_{k-3}-P_{k-2}-p_{k-1}) \sum_{v\in V_{G_n}} r(x_{k+1},v) \\
=& p_1[\sum_{v\in V_{G_{n-1}}} r(u_{n-1},v) + (1+\frac{1\cdot(2k-1)}{2k})\times 2k(n-1) + \frac{4k^2-1}{6}] \\
&+ p_2[\sum_{v\in V_{G_{n-1}}} r(u_{n-1},v) + (1+\frac{2\cdot(2k-2)}{2k})\times 2k(n-1) + \frac{4k^2-1}{6}] \\
&+ p_3[\sum_{v\in V_{G_{n-1}}} r(u_{n-1},v) + (1+\frac{3\cdot(2k-3)}{2k})\times 2k(n-1) + \frac{4k^2-1}{6}] \\
&+ \ldots \\
&+ p_{k-3}[\sum_{v\in V_{G_{n-1}}} r(u_{n-1},v) + (1+\frac{(k-3)\cdot(k+3)}{2k})\times 2k(n-1) + \frac{4k^2-1}{6}] \\
&+ p_{k-2}[\sum_{v\in V_{G_{n-1}}} r(u_{n-1},v) + (1+\frac{(k-2)\cdot(k+2)}{2k})\times 2k(n-1) + \frac{4k^2-1}{6}] \\
&+ p_{k-1}[\sum_{v\in V_{G_{n-1}}} r(u_{n-1},v) + (1+\frac{(k-1)\cdot(k+1)}{2k})\times 2k(n-1) + \frac{4k^2-1}{6}] \\
&+ (1-p_1-p_2-\ldots-p_{k-2}-p_{k-1})[\sum_{v\in V_{G_{n-1}}} r(u_{n-1},v) + (1+\frac{k\cdot k}{2k})\times 2k(n-1) + \frac{4k^2-1}{6}].
\end{aligned}
$$

By applying the expected operator to the above equation, and noting that $E(D_n) = D_n$, we obtain

$$
D_n = D_{n-1} + \{(k^2+2k) - \sum_{i=1}^{k-1}[k^2 - i(2k-i)]p_i\}n + \sum_{i=1}^{k-1}[k^2-i(2k-i)]p_i - \frac{2k^2+12k+1}{6}.
$$

Let

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

Hence,

$$
D_n = D_{n-1} + [(k^2+2k) - U]n + U - \frac{2k^2+12k+1}{6}.
$$

The boundary condition is

$$D_1 = E(\sum_{v \in V_{G_1}} r(u_1, v)) = \frac{4k^2 - 1}{6}.$$

According to the above recurrence relation and the boundary condition, we have

$$D_n = [\frac{k^2 + 2k}{2} - \sum_{i=1}^{k-1} \frac{k^2 - i(2k-i)}{2} p_i] n^2 + [\sum_{i=1}^{k-1} \frac{k^2 - i(2k-i)}{2} p_i + \frac{k^2 - 6k - 1}{6}] n.$$

Thus,

$$D_n = [\frac{k^2 + 2k}{2} - \frac{1}{2}U] n^2 + [\frac{1}{2}U - \frac{k^2 - 6k - 1}{6}] n.$$

Therefore,

$$\begin{aligned} E(Kf^+(G_{n+1})) =& E(Kf^+(G_n)) + (4k+2)D_n + 2kR_n + \frac{16k^3 + 52k^2 + 14k - 1}{3} n + \frac{8k^3 - 8k}{3} \\ =& E(Kf^+(G_n)) + (4k+2)\{[\frac{k^2 + 2k}{2} - \frac{1}{2}U] n^2 + [\frac{1}{2}U - \frac{k^2 - 6k - 1}{6}] n\} \\ &+ 2k\{[\frac{(2k^2 + 5k + 2)}{2} - \frac{1}{2}V] n^2 + [\frac{1}{2}V + \frac{2k^2 - 15k - 14}{6}] n + 1\} \\ &+ \frac{16k^3 + 52k^2 + 14k - 1}{3} n + \frac{8k^3 - 8k}{3}. \end{aligned}$$

and the boundary condition is $E(Kf^+(G_1)) = \frac{8k^3 - 2k}{3}$.

According to the above recurrence relation and the boundary condition, we have

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

Let

$$T = \sum_{i=1}^{k-1} [4k^3 + 2k^2 - (4k+2)(i \cdot (2k-i))] p_i.$$

$$F_i = [4k^3 + 2k^2 - (4k+2)(i \cdot (2k-i))].$$

Hence,

$$E(Kf^+(G_n)) = [(4k^3 + 10k^2 + 4k) - T] \frac{n^3}{3} + [\frac{4k^3 - 2k^2 - 10k - 1}{3} + T] n^2 - [(8k^3 - 4k - 1) + 2T] \frac{n}{3}.$$

as desired. □

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 1, we can receive the additive degree–Kirchhoff indexes 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

$$
\begin{aligned}
Kf^+(M_n) &= \frac{16k^2+4k-2}{3}n^3 + \frac{16k^3-20k^2-10k+5}{3}n^2 - \frac{8k^3-4k^2-4k+3}{3}n, \\
Kf^+(O_n^1) &= \frac{24k^2-4k-8}{3}n3 + \frac{16k^3-44k^2+14k+23}{3}n^2 - \frac{8k^3-20k^2+12k+15}{3}n, \\
Kf^+(O_n^2) &= \frac{32k^2-20k-18}{3}n^3 + \frac{16k^3-68k^2+62k+53}{3}n^2 - \frac{8k^3-36k^2+44k+35}{3}n, \\
\vdots \qquad & \qquad \vdots \qquad\qquad \vdots \\
Kf^+(O_n^{k-3}) &= \frac{4k^3+10k^2-12k-8}{3}n^3 + \frac{4k^3-2k^2+38k+23}{3}n^2 - \frac{8k^2+28k+15}{3}n, \\
Kf^+(O_n^{k-2}) &= \frac{4k^3+10k^2-2}{3}n^3 + \frac{4k^3-2k^2+2k+5}{3}n^2 - \frac{8k^2+4k+3}{3}n, \\
Kf^+(L_n) &= \frac{4k^3+10k^2+4k}{3}n^3 + \frac{4k^3-2k^2-10k-1}{3}n^2 - \frac{8k^2-4k-1}{3}n. \\
Kf^+(O_n^i) &= [(4k^3+10k+4k)-F_{i+1}]\frac{n^3}{3} + [\frac{4k^3-2k^2-10k-1}{3}+F_{i+1}]n^2 - [(8k^2-4k-1)+2F_{i+1}]\frac{n}{3}.
\end{aligned}
$$

Through observation and direct calculation, we have

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

**Corollary 1.** *For a random polygonal chain $G_n$ $(n \geq 3)$, the para-chain $L_n$ realizes the maximum of $E(Kf^+(G_n))$, and the meta-chain $M_n$ realizes that of the minimum.*

**Proof.** By Theorem 1, we have

$$
\begin{aligned}
E(Kf^+(G_n)) = \sum_{i=1}^{k-1}(-F_i\frac{n^3}{3} + F_in^2 - 2F_i\frac{n}{3})p_i + (4k^3+10k^2+4k)\frac{n^3}{3} \\
+\frac{4k^3-2k^2-10k-1}{3}n^2 - \frac{8k^2-4k-1}{3}n.
\end{aligned}
$$

Note that $n \geq 3$, so by taking the partial derivative, one has

$$
\begin{aligned}
\frac{\partial E(Kf^+(G_n))}{\partial p_i} &= -F_i\frac{n^3}{3} + F_in^2 - \frac{2}{3}F_in < 0. \\
\frac{\partial E(Kf^+(G_n))}{\partial p_1} &= -(4k^3-6k^2+2)\frac{n^3}{3} + (4k^3-6k^2+2)n^2 - \frac{2}{3}\cdot(4k^3-6k^2+2)n < 0, \\
\frac{\partial E(Kf^+(G_n))}{\partial p_2} &= -(4k^3-14k^2+8k+8)\frac{n^3}{3} + (4k^3-14k^2+8k+8)n^2 - \frac{2}{3}\cdot(4k^3-14k^2+8k+8)n < 0, \\
\frac{\partial E(Kf^+(G_n))}{\partial p_3} &= -(4k^3-22k^2+24k+18)\frac{n^3}{3} + (4k^3-22k^2+24k+18)n^2 - \frac{2}{3}(4k^3-22k^2+24k+18)n < 0, \\
\vdots \qquad & \qquad \vdots \qquad\qquad \vdots \\
\frac{\partial E(Kf^+(G_n))}{\partial p_{k-1}} &= -(4k+2)\frac{n^3}{3} + (4k+2)n^2 - \frac{2}{3}\cdot(4k+2)n < 0.
\end{aligned}
$$

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

$$E(Kf^+(G_n)) = \sum_{i=1}^{k-2}(-F_i\frac{n^3}{3} + F_in^2 - 2F_i\frac{n}{3})p_i + (-F_{k-1}\frac{n^3}{3} + F_{k-1}n^2 - 2F_{k-1}\frac{n}{3})(1 - p_1 - p_2 - \cdots - p_{k-2})$$
$$+ (4k^3 + 10k^2 + 4k)\frac{n^3}{3} + \frac{4k^3 - 2k^2 - 10k - 1}{3}n^2 - \frac{8k^2 - 4k - 1}{3}n.$$

Therefore,

$$\frac{\partial E(Kf^+(G_n))}{\partial p_i} = -(F_i - F_{k-1})\frac{n^3}{3} + (F_i - F_{k-1})n^2 - \frac{2}{3}(F_i - F_{k-1})n < 0.$$
$$\frac{\partial E(Kf^+(G_n))}{\partial p_1} = -(4k^3 - 6k^2 - 4k)\frac{n^3}{3} + (4k^3 - 6k^2 - 4k)n^2 - \frac{2}{3}\cdot(4k^3 - 6k^2 - 4k)n < 0,$$
$$\frac{\partial E(Kf^+(G_n))}{\partial p_2} = -(4k^3 - 14k^2 + 4k + 6)\frac{n^3}{3} + (4k^3 - 14k^2 + 4k + 6)n^2 - \frac{2}{3}\cdot(4k^3 - 14k^2 + 4k + 6)n < 0,$$
$$\vdots \qquad \vdots \qquad \vdots$$
$$\frac{\partial E(Kf^+(G_n))}{\partial p_{k-2}} = -(12k + 6)\frac{n^3}{3} + (12k + 6)n^2 - \frac{2}{3}\cdot(12k + 6)n < 0.$$

Thus, $p_1 = p_2 = \ldots = p_{k-2} = 0$ (i.e., $p_{k-1} = 1$), and $E(Kf^+(G_n))$ cannot attain the minimum value. With the same calculations as the same above, if $p_1 + p_2 + p_3 + \ldots + p_i = 1$, let $p_i = 1 - p_1 - p_2 - \ldots - p_{i-1}$ $(0 \leq p_1 \leq 1,\ 0 \leq p_2 \leq 1, \ldots, 0 \leq p_{i-1} \leq 1)$, $(i \geq 3)$. Then, we have

$$E(Kf^+(G_n)) = \sum_{i=1}^{k-3}(-F_i\frac{n^3}{3} + F_in^2 - 2F_i\frac{n}{3})p_i + (-F_{k-2}\frac{n^3}{3} + F_{k-2}n^2 - 2F_{k-2}\frac{n}{3})(1 - p_1 - p_2 - \cdots - p_{k-3})$$
$$+ (4k^3 + 10k^2 + 4k)\frac{n^3}{3} + \frac{4k^3 - 2k^2 - 10k - 1}{3}n^2 - \frac{8k^2 - 4k - 1}{3}n.$$

Therefore,

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

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

$$E(Kf^+(G_n)) = (-F_1\frac{n^3}{3} + F_1n^2 - 2F_1\frac{n}{3})(1 - p_2) + (-F_2\frac{n^3}{3} + F_2n^2 - 2F_2\frac{n}{3})p_2$$
$$+ (4k^3 + 10k^2 + 4k)\frac{n^3}{3} + \frac{4k^3 - 2k^2 - 10k - 1}{3}n^2 - \frac{8k^2 - 4k - 1}{3}n.$$

Thus,
$$\frac{\partial E(Kf^+(G_n))}{\partial p_2} = (F_1 - F_2)\frac{n^3}{3} - (F_1 - F_2)n^2 + \frac{2}{3}(F_1 - F_2)n > 0.$$

Thus, $E(Kf^+(G_n))$ achieves the minimum value when $p_2 = 0$ (i.e., $p_1 = 1$); that is, $G_n \cong M_n$. $\square$

## 3. The Average Value for the Additive Degree–Kirchhoff Index

Recall that $\Theta_n$ is the set of all polygonal chains with $n$ polygons. In this section, we give the average value for the additive degree–Kirchhoff index with respect to $\Theta_n$.

$$Kf^+_{avr}(\Theta_n) = \frac{1}{|\Theta_n|}\sum_{G\in\Theta_n} Kf^+(G).$$

In order to achieve the average value $Kf^{+}_{avr}(\Theta_n)$, it takes $p_1 = p_2 = \cdots = p_k = \frac{1}{k}$ in the expected value for the additive degree–Kirchhoff index of the random polygonal chain $E(Kf^{+}(G_n))$. According to Theorem 1, we have:

**Theorem 2.** *For $n \geq 1$, the average value for the the additive degree–Kirchhoff indexes with respect to $\Theta_n$ are*

$$E(Kf^{+}(G_n)) = [(4k^3 + 10k^2 + 4k) - \frac{1}{k}\sum_{i=1}^{k-1} F_i]\frac{n^3}{3} + [\frac{4k^3 - 2k^2 - 10k - 1}{3} + \frac{1}{k}\sum_{i=1}^{k-1} F_i]n^2 - [(8k^3 - 4k - 1) + \frac{2}{k}\sum_{i=1}^{k-1} W_i]\frac{n}{3}.$$

After verification, the equations are established:

$$Kf^{+}_{avr}(\Theta_n) = \frac{1}{k}Kf^{+}(M_n) + \frac{1}{k}Kf^{+}(O^1_n) + \frac{1}{k}Kf^{+}(O^2_n) + \cdots + \frac{1}{k}Kf^{+}(O^{k-2}_n) + \frac{1}{k}Kf^{+}(L_n).$$

## 4. Concluding Remarks

Most of the published papers are about the study of polyphenylene and cyclooctatetraene chains; the results are not generic. In this paper, we obtained the explicit analytical expression for the expected values of the additive degree–Kirchhoff index as a random polygonal chain. We also obtained the extremal values and average values of the index. All the research can better predict the physicochemical properties of more novel compounds, which can be applied to the research of drugs, macromolecular polymers and new materials.

In chemical graph theory, the matter of a 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 [35–37]. The graph invariant not only presents vast potential for structure–activity and structure–property relationships, but also offers precious leads for the advancement of safe and potent curative of multiple nature as well. By this paper is possible to establish exact formulas for the expected values of some indices of a random polygon chain with $n$ regular polygons.

In reverse engineering of pharmaceuticals and nanomaterials—refer to [38–41]—scientists hope to create certain drugs or test the performance of a nanometer material. They can use the method of this study by extending it to a certain topological index (corresponding to certain features of drugs or material) with expected values, extremal values and average values, getting the structures of the target compounds from the point of view of mathematics and then synthesizing the targeted chemicals.

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