Journal of Discrete Mathematics and Its Applications 10 (4) (2025) 375–392

Journal of Discrete Mathematics and Its Applications

Available Online at: http://jdma.sru.ac.ir

Research Paper

Gutman index of polyomino chains

Laila Azami, Nader Jafari-Rad*

Department of Mathematics, Faculty of Basic Sciences, Shahed University, Tehran, I. R. Iran.

Academic Editor: Ivan Gutman

Abstract. The Gutman index is a degree-distance-based topological descriptor of connected graphs. In this paper, we derive explicit analytic expressions for its expected value in polyomino chains built by sequentially attaching square tiles via one of two fixed local connection modes. This expectation is expressed as a cubic polynomial in the number of tiles n. We then identify which attachment patterns yield the extremal (maximum and minimum) values and compute the overall average of the Gutman index across all polyomino chains of length n. These results enhance the topological analysis of square-tiled networks with applications in chemical graph theory, polymer science, and materials design.

Keywords. Gutman index, graph, polyomino chains.
Mathematics Subject Classification (2020): 05C12, 05C50, 05C80.

1 Introduction

Chemical graph theory models molecular structures as simple, finite, connected graphs, with vertices representing atoms and edges representing chemical bonds [6,9,17]. Topological indices–numerical invariants built from vertex degrees and shortest-path distances–serve as key descriptors in quantitative structure–property/activity relationship studies (QSPR/QSAR) of organic compounds [1,2,8,13].
Let $G = (V, E)$ be a simple connected graph. For a vertex $v \in V$, its *degree*, denoted by $d(v)$, is the number of vertices that are adjacent to v. For any pair of vertices u, v, the *distance* $d(u, v)$

*Corresponding author (Email address: n.jafarirad@gmail.com).
Received 23 september 2025; Revised 07 October; Accepted 23 November 2025
First Publish Date: 01 December 2025

is the length of a shortest path between u and v. The *Wiener index*

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$$

was introduced to correlate molecular topology with boiling points and remains one of the most studied distance-based invariants [3,5,7,14].

The *Gutman index* refines the Wiener index by weighting each distance by the product of the incident vertex degrees:

$$\mathrm{Gut}(G) = \sum_{\{u,v\} \subseteq V(G)} d(u)d(v)d(u,v)$$

and has found widespread application in studies of polymeric and aromatic systems [4, 18,22].

A *polyomino system* is a finite 2-connected plane graph in which each interior face is a unit square, and two squares are adjacent if they share a side. A *polyomino chain* of length n is a polyomino system whose squares $H_1, H_2, \ldots, H_n$ can be ordered so that the centers of adjacent cells form a simple path $C_1, C_2, \ldots, C_n$. In such a chain, each square is adjacent to at most two others. A square with exactly one neighbor is called *terminal*, with two neighbors and no vertex of degree 2 is *medial*, and with two neighbors sharing a vertex of degree 2 is a *kink*. A chain without any kinks is a *linear chain*, while one consisting only of terminals and kinks is a *zigzag chain*. A maximal sequence of adjacent medials and terminals is called a *segment* of the chain. Figure 1 depicts the geometric configurations of polyomino chains L_n and Z_n,which serve as the structural basis for our Gutman index calculations.

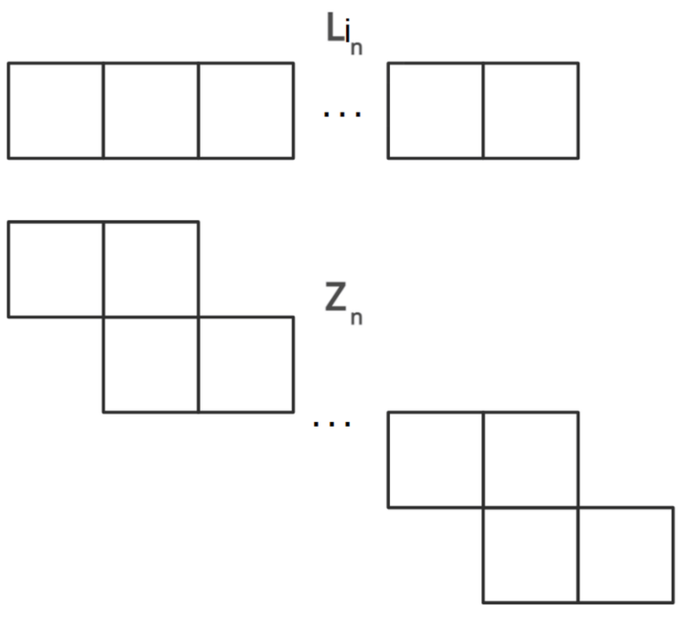

Figure 1. Polyomino chains of types L_n and Z_n.

In this paper, we focus on polyomino chains, where each new square attaches to one of the two available edges of the previous cell with prescribed probabilities. We derive closed form formulas for the expected Gutman index $E(\mathrm{Gut}(G_n))$ of a polyomino chain G_n with n cells. We identify the extremal attachment schemes that minimize or maximize this expectation and compute the average Gutman index over all non-isomorphic polyomino chains of a given length.

2 Gutman index of polyomino chains

Let PC_{n-1} denote a polyomino chain with $n-1$ squares. Adding one more square to PC_{n-1} yields the chain PC_n. Each new square can be attached to the previous square in one of two ways:

- Linearly, in which case the connection link L_n equals 1.

- Non-linearly, in which case $L_n = 2$.

Each polyomino chain consists of several segments. The first segment extends from the first square to the first kink, and each subsequent i-th segment spans from one kink to the next. The last segment extends from the last kink–or from the first square if there is no kink–to the final square. The i-th segment is denoted by s_i, as illustrated in the following figure.

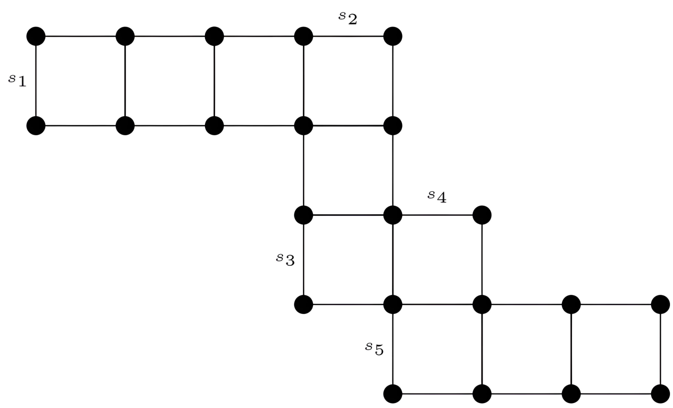

Figure 2. A polyomino chain consisting of 10 cells and 5 segments.

Two different configurations for connecting the n-th square to the $(n-1)$-th square are illustrated in Figures 3 and 4. In the first configuration (Figure 3), we have $L_n = 1$, while in the second configuration (Figure 4), we have $L_n = 2$.

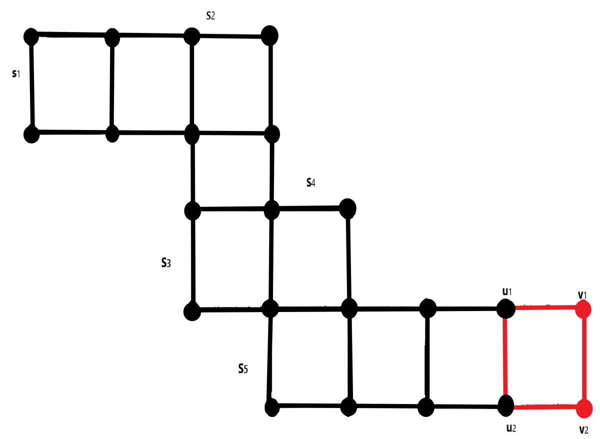

Figure 3. The n-th cell is added linearly to the polyomino chain $\mathrm{pc}_{n-1}(L_n = 1)$.

or

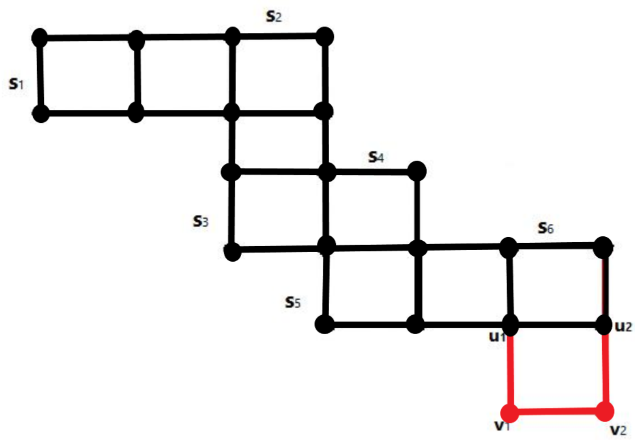

Figure 4. The n-th cell is added to pc_{n-1} via a kinked attachment $L_n = 2$.

By adding the n-th square, two new vertices v_1, v_2 with degree 2 are introduced, and the degrees of the existing vertices u_1, u_2 are also affected. Since the Gutman index depends on both vertex degrees and pairwise distances, the following set of vertices contributes to the Gutman index of the updated chain:

$$A = \{v_1, v_2, u_1, u_2\}.$$

Note: In the construction of polyomino chains, the configuration of the $(n-1)$-th square depends on the value of L_n.

- If $L_n = 1$, the $(n-1)$-th square adopts a medial configuration, meaning it is aligned linearly with its adjacent squares, forming a straight segment.

- If $L_n = 2$, the $(n-1)$-th square takes a kink configuration, indicating a change in direction that introduces a bend in the chain.

Geometrically, a medial square lies collinearly with its predecessor and successor, while a kink square forms a right angle with at least one of its neighbors, resulting in a corner-like structure within the chain.

In the following, we give a recursive relation for the Gutman index of PC_n based on PC_{n-1} (Theorem 1).

Theorem 2.1. *Let PC_n be a polyomino chain obtained by adding a new square to the end of PC_{n-1}. Then, the Gutman index of PC_n can be computed recursively as follows:*

$$Gut(G_n) = Gut(G_{n-1}) + 13 + 24n + 3I_{L_n=2} + 3 \sum_{\substack{u \in V(G) \setminus A \\ v \in \{u_1, u_2\}}} d(u)D(u,v),$$

where:

- *$I_{L_n=2}$ is the indicator function, equal to 1 if $L_n = 2$, and 0 otherwise.*
- *$d(u)$ denotes the degree of vertex u.*
- *$D(u,v)$ is the distance between vertices u and v in the graph.*
- *The set $A = \{v_1, v_2, u_1, u_2\}$ contains the vertices directly affected by the addition of the new square.*

Proof.

$$\begin{aligned}
\mathrm{Gut}(G_n) - \mathrm{Gut}(G_{n-1}) &= \mathrm{Gut}(G_n)_{u,v \subseteq A} + \mathrm{Gut}(G_n)_{\substack{u \notin A \\ v \in A}} - \mathrm{Gut}(G_{n-1})_{\substack{u \notin A \\ v \in \{u_1, u_2\}}} \\
&= \sum_{u,v \subseteq A} d(u)d(v)D(u,v) + \sum_{\substack{v \in V(G) \\ u \notin A}} d(u)d(v)D(u,v) \\
&\quad - \sum_{\substack{u \notin A \\ v \subseteq \{u_1, u_2\}}} d(u)d(v)D(u,v).
\end{aligned}$$

We now compute the above three summations. First note that

$$\sum_{u,v \subseteq A} d(u)d(v)D(u,v) = 49 + 9I_{L_n=2}.$$

We next compute $\sum_{\substack{v \in V(G) \\ u \notin A}} d(u)d(v)D(u,v)$. If $L_n = 1$, then

$$\begin{aligned}
\sum_{\substack{v \in V(G) \\ u \notin A}} d(u)d(v)D(u,v) &= \sum_{u \notin A} 3d(u)D(u,u_1) + \sum_{u \notin A} 3d(u)D(u,u_2) \\
&\quad + \sum_{u \notin A} 2d(u)D(u,v_1) + \sum_{u \notin A} 2d(u)D(u,v_2)
\end{aligned}$$

$$= \sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} 5d(u)D(u,v) + 4\sum_{u\notin A} d(u).$$

If $L_n = 2$, then

$$\sum_{\substack{v\in V(G)\\ u\notin A}} d(u)d(v)D(u,v) = \sum_{u\notin A} 4d(u)D(u,u_1)$$
$$+ \sum_{u\notin A} 3d(u)D(u,u_2) + \sum_{u\notin A} 2d(u)D(u,v_1)$$
$$+ \sum_{u\notin A} 2d(u)D(u,v_2) = \sum_{u\notin A} 6d(u)D(u,u_1)$$
$$+ \sum_{u\notin A} 5d(u)D(u,u_2) + 4\sum_{u\notin A} d(u).$$

Thus

$$\sum_{\substack{v\in V(G)\\ u\notin A}} d(u)d(v)D(u,v) = \sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} 5d(u)D(u,v) + \left[\sum_{u\notin A} d(u)D(u,u_1)\right] I_{L_n=2}$$
$$+ 4\sum_{u\notin A} d(u) \sum_{u\notin A} d(u) = 6n - 8 - I_{L_n=2}$$
$$= \sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} 5d(u)D(u,v) + \left[\sum_{u\notin A} d(u)D(u,u_1)\right] I_{L_n=2}$$
$$+ 4(6n - 8 - I_{L_n=2}) = \sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} 5d(u)D(u,v)$$
$$+ \left[\sum_{u\notin A} d(u)D(u,u_1)\right] I_{L_n=2} + 24n - 32 - 4I_{L_n=2}.$$

Now we compute

$$\sum_{\substack{u\notin A\\ v\subseteq\{u_1,u_2\}}} d(u)d(v)D(u,v).$$

If $L_n = 1$, then

$$\sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} d(u)d(v)D(u,v) = \sum_{u\notin A} 2d(u)D(u,u_1) + \sum_{u\notin A} 2d(u)D(u,u_2).$$

If $L_n = 2$, then

$$\sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} d(u)d(v)D(u,v) = \sum_{u\notin A} 3d(u)D(u,u_1) + \sum_{u\notin A} 2d(u)D(u,u_2).$$

Thus

$$\sum_{\substack{u\notin A\\ v\subseteq\{u_1,u_2\}}} d(u)d(v)D(u,v) = \sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} 2d(u)D(u,v) + \left[\sum_{u\notin A} d(u)D(u,u_1)\right] I_{L_n=2}.$$

Then

$$\begin{aligned}
\mathrm{Gut}(G_n) - \mathrm{Gut}(G_{n-1}) &= 49 + 9I_{L_n=2} + \sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} 5d(u)D(u,v)\\
&\quad + \left[\sum_{u\notin A} d(u)D(u,u_1)\right] I_{L_n=2} + 24n - 32 - 4I_{L_n=2}\\
&\quad - \left(\sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} 2d(u)D(u,v) + \left[\sum_{u\notin A} d(u)D(u,u_1)\right] I_{L_n=2}\right)\\
&= 13 + 24n + 3I_{L_n=2} + 3\sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} d(u)D(u,v).
\end{aligned}$$

□

We next introduce some definitions and Configurations.

Definition 2.2 (Local Configuration Impact on Gutman Index)**.** *In the polyomino chains, the summation*

$$\sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} d(u)D(u,v)$$

is influenced by the local configuration of the square whose vertices are involved in the computation, along with its two adjacent squares. Specifically, the contribution of the vertices belonging to the w-th square depends on which of the following eight configurations the triple $(w-1,w,w+1)$ *falls into:*

1. *medial – medial – medial*

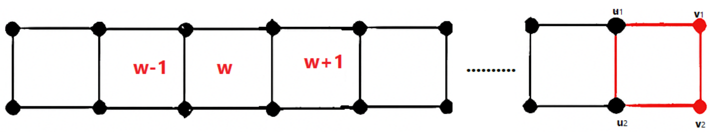

Figure 5. The triple $(w-1,w,w+1)$ is of type medial–medial–medial.

2. *medial – kink – medial*

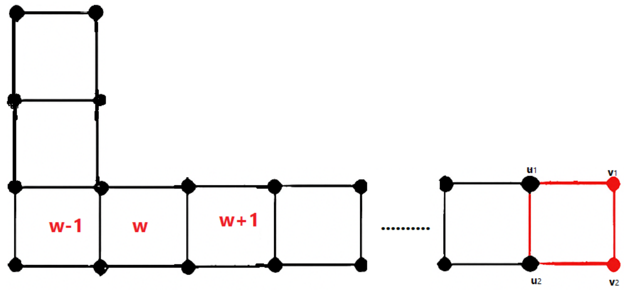

Figure 6. The triple $(w-1, w, w+1)$ is of type medial – kink – medial.

3. *medial –medial–kink*

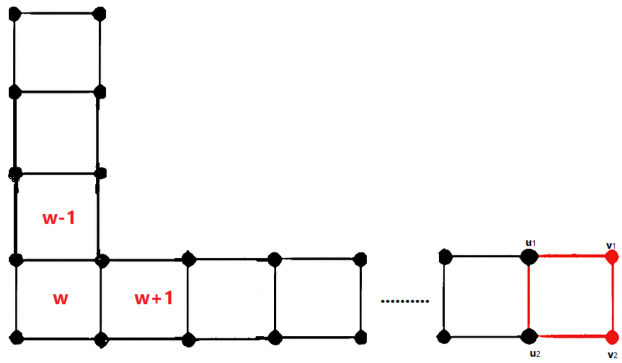

Figure 7. The triple $(w-1, w, w+1)$ is of type medial–medial–kink.

4. *kink – medial –medial*

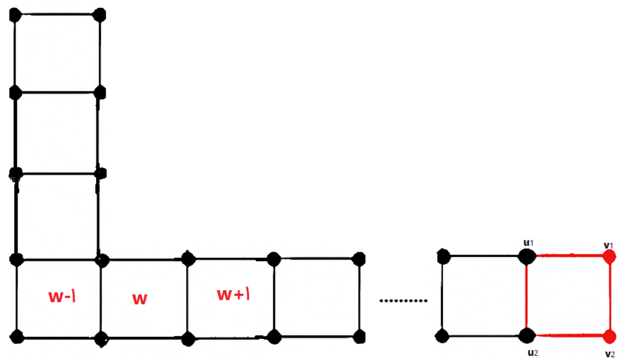

Figure 8. The triple $(w-1, w, w+1)$ is of type kink–medial–medial.

5. *kink – kink – medial*

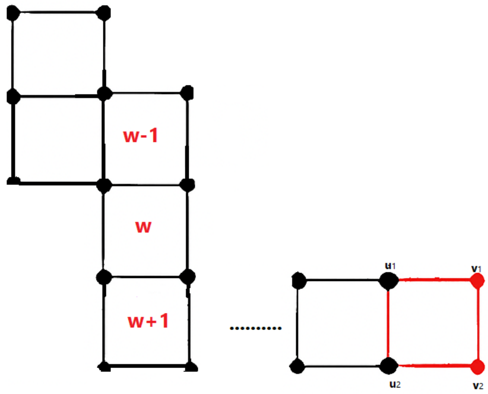

Figure 9. The triple $(w-1, w, w+1)$ is of type kink–kink–medial.

6. *medial – kink – kink*

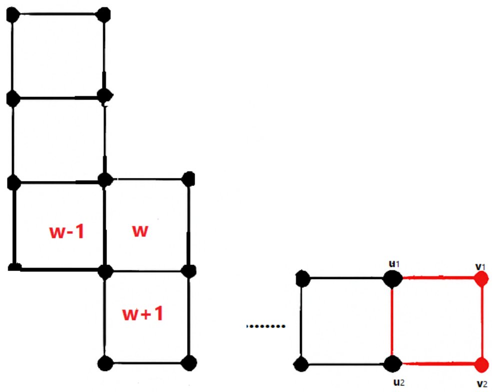

Figure 10. The triple $(w-1, w, w+1)$ is of type medial–kink–kink.

7. *kink – medial – kink*

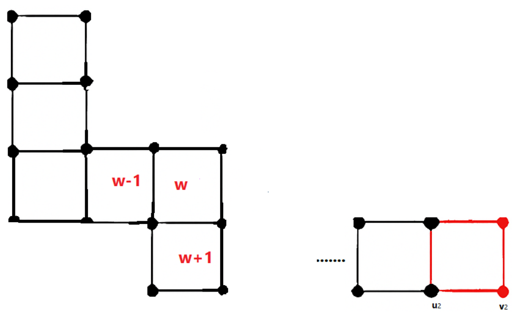

Figure 11. The triple $(w-1, w, w+1)$ is of type kink–medial–kink.

8. *kink – kink – kink*

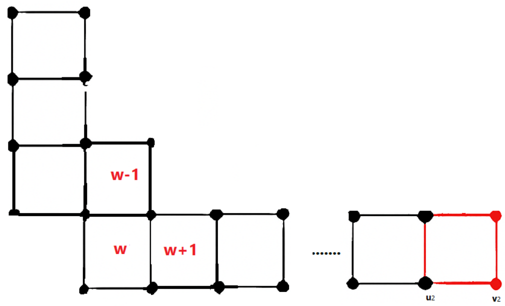

Figure 12. The triple $(w-1, w, w+1)$ is of type kink–kink–kink.

These configurations, illustrated in Figure 13, play a crucial role in determining the local structural impact on the Gutman index.

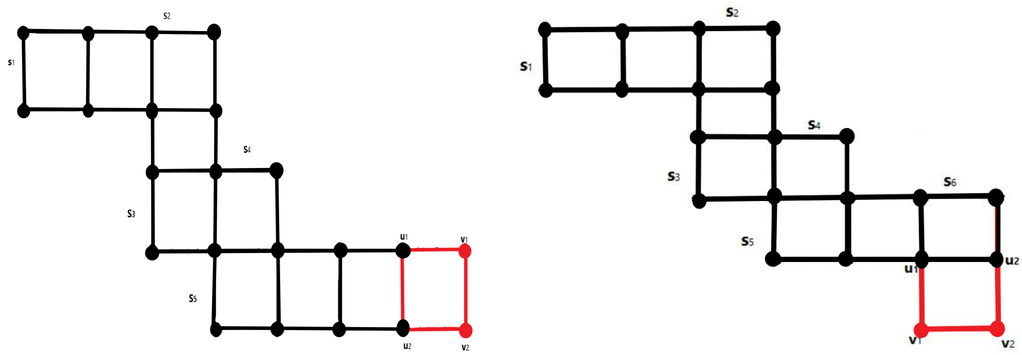

Figure 13. The triple $(w-1, w, w+1)$ is of type kink–medial–medial.

Theorem 2.3. *In a polyomino chain of length n, consider three consecutive medial squares. Let w be the index of the central square, and let B be the set of its vertices. For each ordered pair (u, v) satisfying*

$$u \in B \quad \text{and} \quad v \in \{u_1, u_2\}.$$

Then the contribution from square w is

$$\frac{1}{2} \sum_{\substack{v \in \{u_1, u_2\} \\ u \in B}} d(u) D(u, v) = 12(n-w) - 6I_{w \in s_t},$$

where, s_t denotes the final segment of the chain,

$$I_{w \in s_t} = \begin{cases} 1 & \text{if } w \in s_t, \\ 0 & \text{otherwise.} \end{cases}$$

and the factor $\frac{1}{2}$ accounts for each vertex being shared by two adjacent squares.

Proof. According to Figures 6 and 7, we distinguish two cases depending on whether the central square w belongs to the final segment s_t.

Case 1: $w \in s_t$.

From Figure 6, we compute

$$\frac{1}{2}\sum_{\substack{v\in\{u_1,u_2\}\\ u\in B}} d(u)D(u,v) = \frac{3}{2}[4(n-w)+2(n-w+1)+2(n-w-1)] = 12(n-w).$$

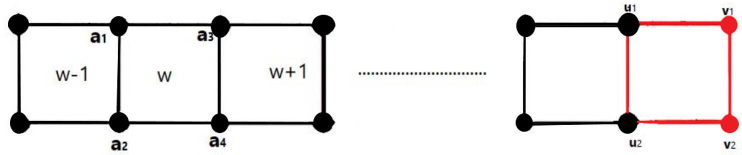

Figure 14. The configutartion of Case 1.

Case 2: $w \notin s_t$.

From Figure 7, one similarly obtains

$$\begin{aligned}\frac{1}{2}\sum_{\substack{v\in\{u_1,u_2\}\\ u\in B}} d(u)D(u,v) &= \frac{3}{2}(n-w-2)+\frac{9}{2}(n-w-1)+\frac{9}{2}(n-w)+\frac{3}{2}(n-w+1)\\ &= 12(n-w)-6.\end{aligned}$$

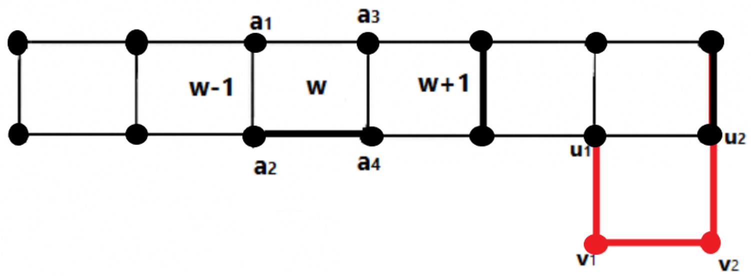

Figure 15. The configutartion of Case 2.

Combining both cases yields the unified formula:

$$\frac{1}{2}\sum_{\substack{v\in\{u_1,u_2\}\\ u\in B}} d(u)D(u,v) = 12(n-w) - 6I_{w\in s_t}.$$ □

Theorem 2.4. *In a polyomino chain of length n, consider three consecutive squares that form a kink (i.e., the central square turns 90°). Let w be the index of the central square, and let B be the set of its* *vertices. For each ordered pair (u,v) with*

$$u \in B \quad \text{and} \quad v \in \{u_1,u_2\},$$

define

- *$d(u)$ as the degree of vertex u divided by the number of squares sharing u,*
- *$D(u,v)$ as the distance between u and v.*

Then the total contribution for square w is

$$\sum_{\substack{v\in\{u_1,u_2\}\\ u\in B}} d(u)D(u,v) = 12(n-w)-6.$$

Proof. From the configuration shown below, the eight contributions sum as follows:

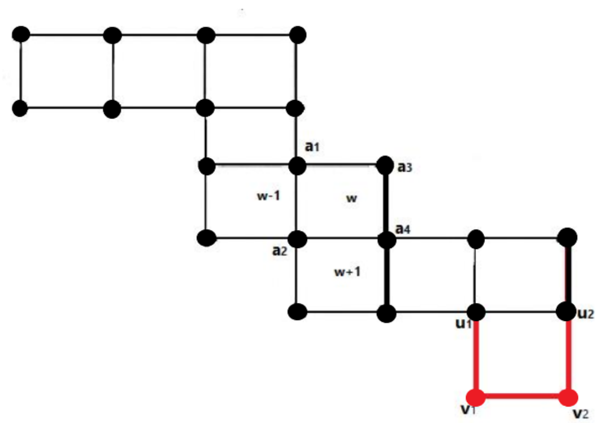

Figure 16. The configutartion.

$$\begin{aligned}\sum_{\substack{v\in\{u_1,u_2\}\\ u\notin A}} d(u)D(u,v) &= \frac{4}{3}(n-w)+\frac{4}{3}(n-w+1)+\frac{4}{3}(n-w-1)+\frac{4}{3}(n-w-1)\\ &\quad+\frac{4}{3}(n-w)+\frac{4}{3}(n-w-2)+2(n-w-1)+2(n-w)\\ &= 12(n-w)-6.\end{aligned}$$

□

Corollary 2.5 (Gutman Index of Linear Polyomino Chains)**.** *Let G_n be a linear polyomino chain of n squares. For $n \geq 4$, its Gutman index satisfies the recurrence*

$$Gut(G_n) = Gut(G_{n-1}) + 66n + 1 + 36\sum_{w=2}^{n-2}(n-w), \quad n \geq 4$$

Evaluating the summation and imposing the base value $Gut(G_3) = 328$ yield the closed-form expression

$$Gut(G_n) = 6n^3 + 15n^2 + 10n + 1.$$

Proof. By Theorems 1 and 2, every square except the first and the last lies in the configuration covered by Theorem 2. Hence for $n \geq 4$ one obtains

$$\mathrm{Gut}(G_n) - \mathrm{Gut}(G_{n-1}) = 13 + 24n + 3I_{L_n=2} + 3 \sum_{\substack{v \in \{u_1, u_2\} \\ u \notin A}} d(u)D(u,v). \tag{*}$$

Here $I_n = 0$ since the chain is linear, and has length at least 4. Moreover, for the two vertices of degree 2 one checks directly that

$$\sum_{\substack{v \in \{u_1, u_2\} \\ u \notin A}} d(u)D(u,v) = 14n - 4.$$

Substituting into (*) gives

$$\mathrm{Gut}(G_n) = \mathrm{Gut}(G_{n-1}) + 66n + 1 + 36 \sum_{w=2}^{n-2} (n - w), \quad n \geq 4.$$

We proceed by extending the recurrence relation and simplifying it as follows.

1. Sum simplification:

$$\sum_{w=2}^{n-2} (n - w) = \sum_{k=2}^{n-2} k = \frac{(n-2)(n-1)}{2} - 1.$$

2. Plug into the recurrence:

$$\mathrm{Gut}(G_n) = \mathrm{Gut}(G_{n-1}) + 66n + 1 + 18(n-2)(n-1) - 36.$$

3. Solve the first-order recurrence:

$$\mathrm{Gut}(G_n) = \mathrm{Gut}(G_{n-1}) + 18n^2 + 12n + 1, \quad \mathrm{Gut}(G_3) = 328 \Rightarrow$$

$$\mathrm{Gut}(G_n) = 6n^3 + 15n^2 + 10n + 1.$$

□

Corollary 2.6 (Gutman Index of Zigzag Polyomino Chains). *Let G_n be a zigzag polyomino chain consisting of n squares, where $n \geq 6$. Then the Gutman index of G_n is given by the recurrence:*

$$Gut(G_n) = Gut(G_{n-1}) + 24n + 16 + 3 \left[\sum_{w=3}^{n-3} (12(n-w) - 6) + 26n - 23 \right].$$

Moreover, the closed-form expression is:

$$Gut(G_n) = Gut(G_5) + 6n^3 + 3n^2 - 89n + 11255.$$

Proof. In a zigzag polyomino chain, all internal squares (i.e., squares with indices $w = 3, \ldots, n-1$) form kink-kink-kink configurations. Let B denote the set of vertices belonging to square w. According to Theorem 3, the contribution of each such square w to the Gutman index is:

$$\sum_{\substack{v \in \{u_1, u_2\} \\ u \in B}} d(u)D(u,v) = 12(n-w) - 6.$$

This expression accounts for the normalized degrees of vertices (i.e., degrees divided by the number of squares sharing each vertex) and their distances to the reference vertices u_1 and u_2.

$$\mathrm{Gut}(G_n) - \mathrm{Gut}(G_{n-1}) = 16 + 24n + 3\sum_{w=3}^{n-1} d(u)D(u,v)$$

$$\mathrm{Gut}(G_n) = \mathrm{Gut}(G_{n-1}) + 16 + 24n + 3\sum_{w=3}^{n-1} (12(n-w) - 6)$$

$$= \mathrm{Gut}(G_{n-1}) + 16 + 24n + 3\left(\sum_{w=3}^{n-1} (12(n-w) - 6) + 26n - 23\right).$$

We simplify the summation:

$$\mathrm{Gut}(G_n) = \mathrm{Gut}(G_{n-1}) + 24n + 16 + 3\left[6n(n-5) - 6 + 26n - 23\right].$$

$$\mathrm{Gut}(G_n) = \mathrm{Gut}(G_5) + \sum_{k=6}^{n} \left[18k^2 - 12k - 71\right].$$

Now, we telescope this recurrence from the base case $\mathrm{Gut}(G_5)$:

$$\mathrm{Gut}(G_n) = \mathrm{Gut}(G_5) + 6n^3 + 3n^2 - 89n + 11255. \qquad \square$$

Theorem 2.7 (Extremal Bounds for the Gutman Index)**.** *Let G_n be any polyomino chain with $n \geq 3$ squares. Denote by L_n the linear chain (no kinks) and by Z_n the zigzag chain (every internal square is a kink) of length n. Then*

$$\mathrm{Gut}(Z_n) \leq \mathrm{Gut}(G_n) \leq \mathrm{Gut}(L_n)$$

with equality on the right if and only if $G_n \cong L_n$, and equality on the left if and only if $G_n \cong Z_n$.

Proof. **Preliminaries from the paper**
Attachment model and notation: Starting from, attach the n-th square either linearly ($L_n = 1$) or as a kink ($L_n = 2$). The four locally affected vertices are

$$A = \{v_1, v_2, u_1, u_2\}.$$

Incremental formula (Theorem 1):

$$\mathrm{Gut}(G_n) - \mathrm{Gut}(G_{n-1}) = 13 + 24n + 3I_{(L_n=2)} + 3 \sum_{v \in \{u_1,u_2\}} \sum_{u \in V(G_n)\setminus A} d(u)D(u,v). \tag{1}$$

Local triple and square-vertex set: For an internal index $w \in \{2,\dots,n-2\}$, let B_w be the set of the four vertices of square w, and consider its triple $(w-1, w, w+1)$.
Local contribution bounds (from Theorems 2 and 3)
For fixed step n and an internal square w, define the local contribution

$$C_w(G_{n-1}, n) := \sum_{v \in \{u_1,u_2\}} \sum_{u \in B_w} d(u)D(u,v).$$

Theorems 2 and 3 imply the sharp two-sided bound

$$12(n-w) - 16 \le C_w(G_{n-1}, n) \le 12(n-w) \tag{2}$$

with equality cases:

- Upper bound $C_w = 12(n-w)$ holds exactly when the triple $(w-1, w, w+1)$ is medial-medial-medial and the middle square w lies in the final segment S_t.
- Lower bound $C_w = 12(n-w) - 6$ holds whenever the triple is kinked (as in a zigzag), and also for medial-medial-medial triples when $w \notin S_t$.

Equivalently, introduce the binary defect

$$\delta_w(G_{n-1}) := \begin{cases} 0, & \text{if } (w-1,w,w+1) \text{ is MMM and } w \in S_t, \\ 1, & \text{otherwise} \end{cases}$$

so that

$$C_w(G_{n-1}, n) = 12(n-w) - 6\delta_w(G_{n-1}). \tag{3}$$

Summing over internal squares,

$$S_n(G_{n-1}) := \sum_{w=2}^{n-2} C_w(G_{n-1}, n) = \sum_{w=2}^{n-2} 12(n-w) - 6\sum_{w=2}^{n-2} \delta_w(G_{n-1}). \tag{4}$$

Two extremal shapes are immediate:

- Linear chain L_{n-1}: all internal triples are MMM within S_t, hence $\delta_w(L_{n-1}) = 0$ for all w, so
$$S_n(L_{n-1}) = \sum_{w=2}^{n-2} 12(n-w).$$
- Zigzag chain Z_{n-1}: all internal triples are kinked, hence $\delta_w(Z_{n-1}) = 1$ for all w, so
$$S_n(Z_{n-1}) = \sum_{w=2}^{n-2} (12(n-w) - 6) = S_n(L_{n-1}) - 6(n-3).$$

Therefore, for any G_{n-1},

$$S_n(Z_{n-1}) \leq S_n(G_{n-1}) \leq S_n(L_{n-1}). \tag{5}$$

with equality if $G_{n-1} = Z_{n-1}$ or L_{n-1}, respectively.

Stepwise extremality of the increment

From (1) and (4),

$$\Delta_n(G) = \mathrm{Gut}(G_n) - \mathrm{Gut}(G_{n-1}) = 13 + 24n + 3I_{(L_n=2)} + 3S_n(G_{n-1}). \tag{6}$$

Using (5),

$$\Delta_n(Z) \leq \Delta_n(G) \leq \Delta_n(L), \tag{7}$$

where the stepwise equalities hold precisely when G_{n-1} is zigzag/linear and the attachment preserves that shape at step n (i.e., $L_n = 2$ for zigzag, $L_n = 1$ for linear). Any deviation forces at least one strict inequality in (7).

A quantified gap follows from the explicit sums above:

$$\Delta_n(L) - \Delta_n(Z) = 3(S_n(L_{n-1}) - S_n(Z_{n-1})) - 3 = 18(n-3) - 3 > 0 \quad (n \geq 4). \tag{8}$$

Telescoping and equality conditions

Telescoping (for any fixed base G_3):

$$\mathrm{Gut}(G_n) = \mathrm{Gut}(G_3) + \sum_{k=4}^{n} \Delta_k(G).$$

Summing (7) from $k = 4$ to n yields

$$\mathrm{Gut}(Z_n) \leq \mathrm{Gut}(G_n) \leq \mathrm{Gut}(L_n).$$

- Upper equality holds if $\Delta_n(G) = \Delta_n(L)$ for all k, i.e., if the chain is linear at every step: $G_n \cong L_n$.
- Lower equality holds if $\Delta_n(G) = \Delta_n(Z)$ for all k, i.e., if the chain is zigzag at every step: $G_n \cong Z_n$. □

Conclusion

This paper uses the linear-kink attachment model and a finely separated incremental description of the Gutman index change to build a local-to-global framework that reduces eight local configurations to two canonical contributions distinguished by a fixed ”defect.” This structure directly yields cubic closed-form expressions in n for the linear chain L_n and the zigzag chain Z_n and proves them uniquely extremal. The argument hinges on stepwise extremality of each index increment followed by a telescoping sum. Finally, the segment-based bookkeeping together with the defect decomposition provides an efficient template for constrained, weighted, and probabilistic extensions.

Open Problems

1. **Expectation in a biased random attachment model** In the sequential growth model where each new square attaches linearly with probability $1-p$ and as a kink with probability p, derive an exact closed-form expression for $\mathbb{E}[\mathrm{Gut}(G_n)]$ as a cubic polynomial in n whose coefficients depend explicitly on p. Analyze how the "segment restart" triggered by a kink influences the local defect term in the expectation.

2. **Variance, higher moments, and limit laws** Compute $\mathrm{Var}(\mathrm{Gut}(G_n))$ and, more generally, obtain formulas for its second and third moments under the same biased model. Investigate whether a central-limit theorem holds for the normalized Gutman index as $n \to \infty$ for fixed $p \in (0,1)$.

3. **Extension to other tilings** Adapt the local-to-global and defect-decomposition approach to polyhex (hexagonal) and polyiamond (triangular) chains. Determine whether a fixed local penalty still governs the transition between maximal and minimal configurations, and derive the corresponding closed-form laws and extremal shapes.

Funding

No funding was received.

Data Availability Statement

No data is used by the authors in this article.

Conflicts of Interests

The authors declare that there is no conflict of interest.

References

[1] J. A. Bondy, U. S. R. Murty, Graph theory, Springer, New York, 2008. https://www.zib.de/userpage/groetschel/teaching/WS1314/BondyMurtyGTWA.pdf
[2] F. Buckley, F. Harary, Distance in graphs, Addison-Wesley, Reading, 1989.
[3] 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://match.pmf.kg.ac.rs/electronic_versions/Match61/n3/match61n3_623-630.pdf
[4] X. Cheng, X. Li, Extremal general Gutman index of trees, MATCH Commun. Math. Comput. Chem. 89 (2023) 567–582. https://doi.org/10.46793/match.89-3.567C
[5] H. Deng, Wiener indices of spiro and polyphenyl hexagonal chains, Math. Comput. Model. 55 (2012) 634–644. https://doi.org/10.48550/arXiv.1006.5488

[6] 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/10.3389/fchem.2022.1067874
[7] R. C. Entringer, D. E. Jackson, D. A. Snyder, Distance in graphs, Czechoslovak Math. J. 26 (1976) 283–296. http://eudml.org/doc/12941
[8] E. Estrada, D. Bonchev, P. Zhang, Chemical graph theory, Discrete Math. Appl. (2013) 1–24. https://doi.org/10.1201/b16132-92
[9] 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
[10] S. W. Golomb, Polyominoes, Princeton Univ. Press, Princeton, 1994.
[11] A. Granados, A. Portilla, Y. Quintana, E. Touris, Bounds for the Gutman-Milovanovic index and some applications, J. Math. Chem. 63 (2025) 406–418. https://doi.org/10.1007/s10910-024-01677-7
[12] F. Guo, H. Wang, M. Yang, S. Wang, The limiting behaviors for the Gutman index and the Schultz index in a random $(2k-1)$-polygonal chain, Filomat 37 (2023) 2487–2501. https://doi.org/10.2298/FIL2407487G
[13] 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
[14] 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.
[15] Y. Mao, K. C. Das, Steiner Gutman index, MATCH Commun. Math. Comput. Chem. 79 (2018) 779–794. https://match.pmf.kg.ac.rs/electronic_versions/Match79/n3/match79n3_779-794.pdf
[16] E. D. Molina, J. M. Rodriguez-Garcia, J. M. Sigarreta, S. J. Torralbas Fitz, On the Gutman-Milovanovic index and chemical applications, AIMS Mathematics 10 (2025) 1998–2020. https://doi.org/10.3934/math.2025094
[17] 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. 51 (2010) 1045–1051. https://doi.org/10.1007/s10947-010-0161-5
[18] J. F. Qi, M. L. Fang, X. Y. Geng, The expected value for the Wiener index in the random spiro chains, Polycycl. Aromat. Comp. (2022). https://doi.org/10.1080/10406638.2022.2038218
[19] S. C. Sigarreta, S. M. Sigarreta, H. Cruz-Suarez, On degree-based topological indices of random polyomino chains, Math. Biosci. Eng. 19 (2022) 8760–8773. https://doi.org/10.3934/mbe.2022406
[20] S. Sigarreta, H. Cruz-Suarez, Zagreb connection indices on polyomino chains and random polyomino chains, Mathematics 12 (2024) 57. https://doi.org/10.48550/arXiv.2405.12389
[21] C. Tao, S. Tang, X. Geng, The limiting behaviors of the Gutman and Schultz indices in random 2k-sided chains, Axioms 13 (2024) 518. https://doi.org/10.3390/axioms13080518
[22] 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

Citation: L. Azami, N. Jafari Rad, Gutman index of polyomino chains, J. Disc. Math. Appl. 10(4) (2025) 375–392.
https://doi.org/10.22061/jdma.2025.12559.1168