https://toc.ui.ac.ir

Transactions on Combinatorics
ISSN (print): 2251-8657, ISSN (on-line): 2251-8665
Vol. xx No. x (202x), pp. xx–xx.

https://www.ui.ac.ir

EXPECTED GUTMAN INDEX OF MARKOV-DEPENDENT RANDOM POLYOMINO CHAINS

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Abstract. We introduce a Markov-dependent random model for polyomino chains in which each new square is attached linearly or as a kink according to a stationary two-state Markov chain. This model retains the geometric construction of classical random polyomino chains while allowing consecutive attachmenttypes to be dependent.

We develop a direct recursive method based on weighted distance sums associated with the two exposed edges of the terminal square. This method yields exact recursive relations for the auxiliary distance quantities and leads to a closed formula for the expected Gutman index. The independent Bernoulli model is recovered when the two transition probabilities are equal. The deterministic linear and zigzag polyomino chains are also obtained as limiting cases.

Our results show that the expected Gutman index depends not only on the stationary frequency of kink attachments, but also on the dependence between consecutive attachments.

1. Introduction

Topological indices are numerical graph invariants which are widely used in chemical graph theory and mathematical chemistry. They are used to describe structural properties of molecular graphs and

MSC(2020): Primary: 05C12; Secondary: 05C80, 05C92, 60J10.

Keywords: Gutman index, random polyomino chain, Markov chain, expected value, topological index.

Manuscript Type: Research Paper.

Communicated by Bijan Taeri.

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Received: 19 July 2026, Accepted: 28 September 2026, Published Online: dd mmmm yyyy.

Cite this article: L. Azami and N. Jafari Rad, Expected Gutman index of Markov-dependent random polyomino chains, *Trans. Comb.*, **x** no. x (202x) xx-xx. https://dx.doi.org/10.22108/toc.2026.149467.2373 .

to distinguish different molecular structures. The Wiener index is one of the earliest and most important distance-based topological indices [19]. Later, many other topological indices were introduced and studied, including the Hosoya index, the Randić index, and degree-distance indices [11, 14, 10, 7].

Let G be a connected graph with vertex set $V(G)$. The Gutman index of G is defined by

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

Here $d_G(u)$ denotes the degree of the vertex u, and $d_G(u,v)$ denotes the distance between the vertices u and v in G. Since the Gutman index contains both degree factors and distance factors, it reflects both local and global properties of the graph. Basic concepts on distances in graphs can be found in [3].

Polyomino chains form an important family of planar graphs. A polyomino is a finite connected union of unit squares joined edge to edge. A polyomino chain is a polyomino whose adjacency graph of squares is a path. The theory of polyominoes was introduced and developed in [8]. Because of their recursive chain structure, polyomino chains are suitable for step-by-step analysis. Several topological indices of polyomino chains have been studied in [1, 6, 20]. Random polyomino chains and related degree-based indices were studied in [15, 16].

The Gutman index of deterministic polyomino chains was studied in [2]. In that work, recursive formulas were obtained for the Gutman index of polyomino chains. Such formulas are useful because a polyomino chain can be constructed by adding one square at a time. Therefore, the change of the Gutman index can be studied through the contribution produced at each step.

Random chain models have also been considered in recent years. In these models, a graph is constructed according to a probabilistic rule, and one studies the expected value, variance, or limiting behavior of a topological index. Expected values of distance-based and degree-distance indices for random phenylene chains, spiro chains, polyphenylene chains, and polygonal chains were studied in [4, 5, 13, 12, 21]. Limiting behaviors for the Gutman index, the Schultz index, and related indices were investigated in [9, 17].

For random polyomino chains, a natural model is obtained by adding squares successively, where each new square is attached either linearly or as a kink. In the independent Bernoulli model, these choices are independent random variables. This assumption is mathematically convenient, but it does not describe possible dependence between consecutive attachment types. For example, a kink may tend to be followed by another kink, or the chain may tend to alternate between linear and kink attachments.

A Markov-chain approach has recently been used for studying Zagreb connection indices of random polyomino chains [16]. The Gutman index, however, combines degree and distance information and requires a different analysis.

In the present paper, we introduce a Markov-dependent random model for polyomino chains. The geometric construction is the same as in the deterministic and Bernoulli models. However, the attachment variables form a stationary two-state Markov chain. The state 0 represents a linear attachment, and the state 1 represents a kink attachment. Thus, the type of the next attachment may depend on the type of the preceding attachment.

The main contribution of this paper is a direct recursive method for computing the expected Gutman index in the Markov-dependent model. Instead of treating all local configurations separately, we introduce weighted distance sums associated with the two exposed edges of the terminal square. These auxiliary quantities satisfy exact recursive relations. By combining these relations with the deterministic recurrence for the Gutman index, we obtain a closed formula for the expected Gutman index.

The proposed model contains the independent Bernoulli model as a special case. Indeed, when the two transition probabilities are equal, the attachment variables become independent Bernoulli random variables. The deterministic linear and zigzag chains are also recovered as limiting cases.

The paper is organized as follows. Section 2 presents the preliminary definitions and the deterministic recursion for the Gutman index. In Section 3, we define the Markov-dependent random model. Section 4 introduces the auxiliary weighted distance sums associated with the two possible extensions of the terminal square. In Section 5, we derive their expected values. Section 6 contains the recurrence and the closed formula for the expected Gutman index. The independent Bernoulli special case is considered in Section 7. Section 8 discusses the deterministic linear and zigzag limiting cases. In Section 9, we interpret the dependence parameter and derive the correlation structure of the attachment variables. Finally, Section 10 contains concluding remarks.

2. Preliminaries and deterministic recursion

Throughout this paper, all graphs are finite, simple, and connected. Let G_n be a polyomino chain consisting of n unit squares $H_1, H_2, \ldots, H_n$. We take G_2 to be the polyomino chain formed by two edge-adjacent unit squares.

For every $n \geq 2$, the terminal square H_n can be extended in exactly two admissible ways. The first one continues the direction of the terminal segment and is called a linear attachment. The second one changes the direction of the terminal segment and is called a kink attachment.

Figure 1 fixes the geometric convention for the two possible extensions of the terminal square. Up to rotation and reflection, we may draw H_{n-1} immediately to the left of H_n. The right-hand exposed

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edge $e_n^{(0)}$ corresponds to a linear extension, whereas the lower exposed edge $e_n^{(1)}$ corresponds to a kink extension. The reflected kink configuration is treated as the same kink type.

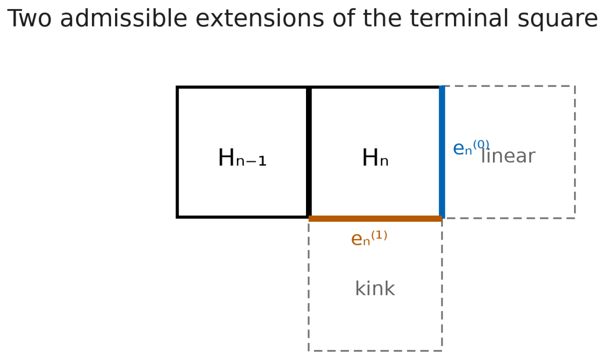

FIGURE 1. The two exposed edges associated with the terminal square H_n. Attaching a new square across the right-hand edge $e_n^{(0)}$ produces a linear extension, whereas attaching a new square across the lower edge $e_n^{(1)}$ produces a kink extension.

To remove any possible ambiguity, the two distinguished exposed edges are updated recursively. After a linear attachment, the roles of the linear and kink exposed edges are preserved. After a kink attachment, the direction of the previous kink exposed edge becomes the new linear direction, whereas the previous linear direction becomes the new kink direction. Hence, no additional left–right random choice is made in the model. The binary sequence $\eta_3, \eta_4, \ldots, \eta_n$ determines the resulting polyomino chain G_n uniquely up to a rigid motion of the square lattice. Let

$$e_n^{(0)} = \left\{x_n^{(0)}, y_n^{(0)}\right\}$$

denote the exposed edge associated with a linear attachment of a new square to G_n. Also, let

$$e_n^{(1)} = \left\{x_n^{(1)}, y_n^{(1)}\right\}$$

denote the exposed edge associated with a kink attachment of a new square to G_n.

For vertices $u, v \in V(G_n)$, let $D_n(u, v)$ denote the distance between u and v in G_n. Let $d_n(u)$ denote the degree of the vertex u in G_n. Put

$$X_n = \mathrm{Gut}(G_n).$$

The following elementary facts will be used repeatedly.

Proposition 2.1. *For every $n \geq 2$, we have $|V(G_n)| = 2n + 2$, $|E(G_n)| = 3n + 1$ and,*

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$$\sum_{u\in V(G_n)} d_n(u) = 6n+2.$$

Proof. The graph G_2 has six vertices and seven edges. Each time a new square is attached to a polyomino chain, it shares exactly one edge with the preceding chain. Therefore, two new vertices and three new edges are added.

Hence, $|V(G_n)| = 6 + 2(n-2) = 2n+2$ and $|E(G_n)| = 7 + 3(n-2) = 3n+1$.

The handshaking lemma (see [18]) gives

$$\sum_{u\in V(G_n)} d_n(u) = 2|E(G_n)| = 6n+2.$$

This proves the result. □

For $n \geq 3$, let η_n denote the type of the attachment of H_n. We use the convention $\eta_n = 0$ for a linear attachment, and $\eta_n = 1$ for a kink attachment. At this stage, the variables η_n are only binary attachment labels. Their probabilistic behavior will be specified in the next section.

A recursive formula for the Gutman index of polyomino chains was obtained in [2]. It has the form

$$X_n = X_{n-1} + 13 + 24n + 3\eta_n + 3S_n, \qquad n \geq 3,$$

where S_n is the weighted distance contribution associated with the attachment of the square H_n.

A direct calculation for the initial chain gives $X_2 = 129$.

In Section 4, we introduce auxiliary weighted distance sums associated with the two exposed edges $e_n^{(0)}$ and $e_n^{(1)}$. These quantities provide a direct representation of the structural term S_n and lead to exact recursive formulas for the expected Gutman index.

3. Markov-dependent random model

In this section, we specify the probabilistic rule for the sequence of attachments. The geometric construction described in Section 2 remains unchanged. At each step, there are exactly two admissible attachment types: a linear attachment and a kink attachment. Let $(\eta_n)_{n\geq 3}$ be a time-homogeneous Markov chain with state space $\{0,1\}$. We use the convention that $\eta_n = 0$ when the square H_n is attached linearly, and $\eta_n = 1$when the square H_n is attached as a kink.

Assume that $P(\eta_{n+1} = 1 \mid \eta_n = 0) = b$ and $P(\eta_{n+1} = 1 \mid \eta_n = 1) = a$, where $0 < a < 1$ and $0 < b < 1$.

Let

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$$Q = (q_{ij})_{i,j\in\{0,1\}}$$

be the transition matrix of the Markov chain. Then $q_{00} = 1-b, q_{01} = b, q_{10} = 1-a$ and $q_{11} = a$. Let $\pi = (\pi_0, \pi_1)$ denote the stationary distribution of the Markov chain.

Proposition 3.1. *The stationary distribution of the Markov chain is given by* $\pi_0 = \frac{1-a}{1-a+b}$ *and* $\pi_1 = \frac{b}{1-a+b}$.

Proof. The stationarity equation is $\pi Q = \pi$. Its first component gives $\pi_0 = \pi_0(1-b) + \pi_1(1-a)$. Therefore, $\pi_0 b = \pi_1(1-a)$. Together with $\pi_0 + \pi_1 = 1$, this gives $\pi_0 = \frac{1-a}{1-a+b}$ and $\pi_1 = \frac{b}{1-a+b}$. This proves the result. □

From now on, we assume that the first attachment variable has the stationary distribution. Thus, $P(\eta_3 = i) = \pi_i, \qquad i \in \{0,1\}$. Consequently, for every $n \geq 3$, we have $P(\eta_n = 0) = \pi_0$ and $P(\eta_n = 1) = \pi_1$. Since η_n takes only the values 0 and 1, it follows that $\mathbb{E}(\eta_n) = \pi_1, \qquad n \geq 3$.

When $a = b = p$, the conditional distribution of η_{n+1} does not depend on the value of η_n. Since $P(\eta_3 = 1) = p$, the sequence $\eta_3, \eta_4, \ldots$ becomes a sequence of independent Bernoulli random variables with parameter p. Thus, the Markov-dependent model contains the independent Bernoulli model as a special case.

In the next section, we introduce the weighted distance sums associated with the two exposed edges of the terminal square.

4. Auxiliary weighted distance sums

In this section, we introduce two auxiliary weighted distance sums. These quantities are attached to the two possible extensions of the terminal square.

Let $x_n^{(0)}$ and $y_n^{(0)}$ be the two vertices of the exposed edge used for a linear extension of G_n. Let $x_n^{(1)}$ and $y_n^{(1)}$ be the two vertices of the exposed edge used for a kink extension of G_n.

For $i = 0, 1$, define

$$F_n^{(i)} = \sum_{v\in V(G_n)} d_n(v)\left(D_n(v, x_n^{(i)}) + D_n(v, y_n^{(i)})\right).$$

Thus, $F_n^{(0)}$ corresponds to the linear exposed edge, and $F_n^{(1)}$ corresponds to the kink exposed edge.

For the initial chain G_2, direct calculation gives $F_2^{(0)} = 42$. Also, $F_2^{(1)} = 36$.

Proposition 4.1. *For every $n \geq 2$, the following two recurrences hold:*

$$F_{n+1}^{(0)} = (1-\eta_{n+1})F_n^{(0)} + \eta_{n+1}F_n^{(1)} + 12n + 14.$$

https://dx.doi.org/10.22108/toc.2026.149467.2373

$$F_{n+1}^{(1)} = F_n^{(1)} + 12n + 8.$$

Proof. When the square H_{n+1} is attached to G_n, two new vertices of degree 2 are added. The two vertices of the common edge increase their degrees by one, and all other degrees remain unchanged.

If the new attachment is linear, the next linear exposed edge is determined by the previous linear exposed edge. If the new attachment is a kink, the next linear exposed edge is determined by the previous kink exposed edge. The total additional weighted distance contribution is $12n + 14$. Hence,

$$F_{n+1}^{(0)} = (1 - \eta_{n+1})F_n^{(0)} + \eta_{n+1}F_n^{(1)} + 12n + 14.$$

For the next kink exposed edge, the corresponding additional weighted distance contribution is $12n + 8$. Therefore,

$$F_{n+1}^{(1)} = F_n^{(1)} + 12n + 8.$$

This proves the proposition. □

Proposition 4.2. *For every $n \geq 2$, the structural term satisfies*

$$S_{n+1} = (1 - \eta_{n+1})F_n^{(0)} + \eta_{n+1}F_n^{(1)} - 4 - \eta_{n+1}.$$

Proof. For a linear attachment, the structural contribution is $F_n^{(0)} - 4$. For a kink attachment, the structural contribution is $F_n^{(1)} - 5$. Combining these two cases gives

$$S_{n+1} = (1 - \eta_{n+1})F_n^{(0)} + \eta_{n+1}F_n^{(1)} - 4 - \eta_{n+1}.$$

This proves the proposition. □

Theorem 4.3. *For every $n \geq 2$, the Gutman index satisfies*

$$X_{n+1} = X_n + 24(n + 1) + 1 + 3(1 - \eta_{n+1})F_n^{(0)} + 3\eta_{n+1}F_n^{(1)}.$$

Proof. By the deterministic recursion, $X_{n+1} = X_n + 13 + 24(n + 1) + 3\eta_{n+1} + 3S_{n+1}$. Substituting the formula for S_{n+1} gives

$$X_{n+1} = X_n + 24(n + 1) + 1 + 3(1 - \eta_{n+1})F_n^{(0)} + 3\eta_{n+1}F_n^{(1)}.$$

This proves the theorem. □

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5. Expected values of the auxiliary quantities

Put $s = 1 - b$. The second recurrence in the preceding section does not contain a random variable. Hence, the quantity $F_n^{(1)}$ is deterministic.

Proposition 5.1. *For every $n \geq 2$, we have $F_n^{(1)} = 6n^2 + 2n + 8$.*

Proof. The initial value is $F_2^{(1)} = 36$. Also, $F_{n+1}^{(1)} - F_n^{(1)} = 12n + 8$. The formula follows by summing these increments from 2 to $n - 1$. $\square$

For $n \geq 3$, define $U_n = \mathbb{E}\left((1 - \eta_n)F_n^{(0)}\right)$. The next lemma gives the value of $F_n^{(0)}$ on the event that the n-th attachment is a kink.

Lemma 5.2. *For every $n \geq 3$, on the event $\eta_n = 1$, we have $F_n^{(0)} = F_n^{(1)} + 6$.*

Proof. The first recurrence for the auxiliary sums gives $F_n^{(0)} = F_{n-1}^{(1)} + 12(n - 1) + 14$. The second recurrence gives $F_n^{(1)} = F_{n-1}^{(1)} + 12(n-1) + 8$. Subtracting the second identity from the first one proves the result. $\square$

Proposition 5.3. *For every $n \geq 3$, we have*

$$U_n = \pi_0 \left(6n^2 + 2n + 14 + \frac{6(1 - s^{n-2})}{b}\right).$$

Proof. For $n = 3$, the first recurrence for the auxiliary sums gives $F_3^{(0)} = 80$ on the event $\eta_3 = 0$. Hence, $U_3 = 80\pi_0$. This is the stated formula for $n = 3$. For $n \geq 3$, the event $\eta_{n+1} = 0$ has conditional probability s when $\eta_n = 0$ and conditional probability $1 - a$ when $\eta_n = 1$. Therefore,

$$U_{n+1} = sU_n + (1 - a)\mathbb{E}\left(\eta_n F_n^{(0)}\right) + \pi_0(12n + 14).$$

By the preceding lemma and the stationarity of the Markov chain,

$$\mathbb{E}\left(\eta_n F_n^{(0)}\right) = \pi_1 \left(F_n^{(1)} + 6\right).$$

Moreover, the stationary probabilities satisfy $(1 - a)\pi_1 = b\pi_0$. Consequently,

$$U_{n+1} = sU_n + \pi_0 \left(b\left(F_n^{(1)} + 6\right) + 12n + 14\right).$$

Substituting the formula for $F_n^{(1)}$ and using induction gives

$$U_n = \pi_0 \left(6n^2 + 2n + 14 + \frac{6(1 - s^{n-2})}{b}\right).$$

https://dx.doi.org/10.22108/toc.2026.149467.2373

This proves the result. □

For $n \geq 2$, define

$$T_n = \mathbb{E}\left((1-\eta_{n+1})F_n^{(0)} + \eta_{n+1}F_n^{(1)}\right).$$

Theorem 5.4. *For every $n \geq 2$, we have*

$$T_n = 6n^2 + 2n + 14 - 6\pi_1 + \frac{6s\pi_0(1-s^{n-2})}{b}.$$

Proof. The formula can be verified directly for $n = 2$. Let $n \geq 3$. By conditioning on η_n, we obtain

$$T_n = sU_n + (1-a)\mathbb{E}\left(\eta_n F_n^{(0)}\right) + \pi_1 F_n^{(1)}.$$

Using the preceding lemma, the stationarity identity, and the formula for U_n, we get

$$T_n = sU_n + b\pi_0\left(F_n^{(1)} + 6\right) + \pi_1 F_n^{(1)}.$$

Substituting the explicit expressions for U_n and $F_n^{(1)}$ gives

$$T_n = 6n^2 + 2n + 14 - 6\pi_1 + \frac{6s\pi_0(1-s^{n-2})}{b}.$$

This proves the result. □

6. Expected Gutman index

Recall that

$$T_n = \mathbb{E}\left((1-\eta_{n+1})F_n^{(0)} + \eta_{n+1}F_n^{(1)}\right).$$

The previous section gives

$$T_n = 6n^2 + 2n + 14 - 6\pi_1 + \frac{6s\pi_0(1-s^{n-2})}{b}.$$

By the linearity property of the expectation we have the following.

Theorem 6.1. *For every $n \geq 2$, we have*

$$\mathbb{E}(X_{n+1}) = \mathbb{E}(X_n) + 18n^2 + 30n + 67 - 18\pi_1 + \frac{18s\pi_0(1-s^{n-2})}{b}.$$

Proof. By the deterministic recursion obtained in Section 4, we have

$$X_{n+1} = X_n + 24(n+1) + 1 + 3(1-\eta_{n+1})F_n^{(0)} + 3\eta_{n+1}F_n^{(1)}.$$

Taking expectations gives $\mathbb{E}(X_{n+1}) = \mathbb{E}(X_n) + 24(n+1) + 1 + 3T_n$. Substituting the formula for T_n gives

$$\mathbb{E}(X_{n+1}) = \mathbb{E}(X_n) + 18n^2 + 30n + 67 - 18\pi_1 + \frac{18s\pi_0(1-s^{n-2})}{b}.$$

This proves the result. □

Theorem 6.2. *For every $n \geq 2$, the expected Gutman index is given by*

$$\mathbb{E}(X_n) = 6n^3 + 6n^2 + 55n - 53 - 18\pi_1(n-2) + \frac{18s\pi_0}{b}\left(n - 2 - \frac{1-s^{n-2}}{b}\right).$$

Proof. For the initial chain, direct calculation gives $X_2 = 129$. Iterating the preceding recurrence from 2 to $n-1$ gives

$$\mathbb{E}(X_n) = X_2 + \sum_{k=2}^{n-1}\left(18k^2 + 30k + 67 - 18\pi_1 + \frac{18s\pi_0(1-s^{k-2})}{b}\right).$$

We use the identities

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

$$\sum_{k=2}^{n-1} k^2 = \frac{n(n-1)(2n-1)}{6} - 1,$$

and

$$\sum_{k=2}^{n-1} s^{k-2} = \frac{1-s^{n-2}}{b}.$$

Substituting these identities and simplifying gives

$$\mathbb{E}(X_n) = 6n^3 + 6n^2 + 55n - 53 - 18\pi_1(n-2) + \frac{18s\pi_0}{b}\left(n - 2 - \frac{1-s^{n-2}}{b}\right).$$

This proves the result. □

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The leading term of the expected Gutman index is $6n^3$. Thus, the Markov dependence changes lower-order terms of the expected Gutman index, while the cubic leading term remains the same.

7. The independent Bernoulli special case

In this section, we recover the independent Bernoulli model from the Markov-dependent model.

Assume that $a = b = p$, where $0 < p < 1$. Put $q = 1 - p$. Then the two rows of the transition matrix are equal. Therefore, the conditional distribution of η_{n+1} does not depend on η_n. Since the initial variable has the stationary distribution, the variables $\eta_3, \eta_4, \eta_5, \ldots$ are independent Bernoulli random variables with parameter p. In this case, we have $\pi_0 = q$, $\pi_1 = p$, and $s = q$.

Proposition 7.1. *For every $n \geq 2$, the expected Gutman index in the independent Bernoulli model satisfies*

$$\mathbb{E}(X_{n+1}) = \mathbb{E}(X_n) + 18n^2 + 30n + 67 - 18p + \frac{18q^2(1 - q^{n-2})}{p}.$$

Proof. The recurrence for the Markov-dependent model is

$$\mathbb{E}(X_{n+1}) = \mathbb{E}(X_n) + 18n^2 + 30n + 67 - 18\pi_1 + \frac{18s\pi_0(1 - s^{n-2})}{b}.$$

Substituting $\pi_0 = q$, $\pi_1 = p$, $s = q$, and $b = p$ gives the result. $\square$

Theorem 7.2. *For every $n \geq 2$, the expected Gutman index of the independent Bernoulli random polyomino chain is*

$$\mathbb{E}(X_n) = 6n^3 + 6n^2 + 55n - 53 - 18p(n-2) + \frac{18q^2}{p}\left(n - 2 - \frac{1 - q^{n-2}}{p}\right).$$

Proof. The closed formula for the Markov-dependent model is

$$\mathbb{E}(X_n) = 6n^3 + 6n^2 + 55n - 53 - 18\pi_1(n-2) + \frac{18s\pi_0}{b}\left(n - 2 - \frac{1 - s^{n-2}}{b}\right).$$

Substituting $\pi_0 = q$, $\pi_1 = p$, $s = q$, and $b = p$ gives the stated formula. $\square$

The formula in the theorem is stated for $0 < p < 1$. The endpoint cases $p = 0$ and $p = 1$ correspond to the deterministic linear and zigzag polyomino chains, respectively. These cases are considered in the next section.

8. Deterministic limiting cases

The deterministic linear and zigzag polyomino chains are obtained when all attachment variables are fixed. These cases are degenerate extensions of the random model. Let L_n denote the linear polyomino chain with n squares. Suppose that $\eta_k = 0$ for every $k \geq 3$. Then every new square is attached linearly. Hence, $G_n = L_n$.

Proposition 8.1. *For every $n \geq 2$, we have*

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

Proof. When every attachment is linear, the recurrence for the Gutman index becomes $X_{n+1} = X_n + 18n^2+48n+31$. Since $X_2 = 129$, summing the recurrence from 2 to $n-1$ gives $X_n = 6n^3+15n^2+10n+1$. Since $G_n = L_n$, the result follows. □

Let Z_n denote the zigzag polyomino chain with n squares. Suppose that $\eta_k = 1$ for every $k \geq 3$. Then every new square is attached as a kink. Hence,

$G_n = Z_n$.

Proposition 8.2. *For every $n \geq 2$, we have*

$$\mathrm{Gut}(Z_n) = 6n^3 + 6n^2 + 37n - 17.$$

Proof. When every attachment is a kink, the recurrence for the Gutman index becomes $X_{n+1} = X_n + 18n^2 + 30n + 49$. Together with $X_2 = 129$, this gives $X_n = 6n^3 + 6n^2 + 37n - 17$. Since $G_n = Z_n$, the result follows. □

The formulas above are satisfied with the limiting forms of the independent Bernoulli formula. More precisely, the linear formula is obtained as p tends to 0, whereas the zigzag formula is obtained as p tends to 1.

9. Dependence parameter and correlation

The stationary probability of a kink and the dependence between consecutive attachments can be described separately.

Put $p = \pi_1$. Put $q = 1 - p$. Define $\rho = a - b$.

Proposition 9.1. *The transition probabilities satisfy $a = p + q\rho$. $b = p(1 - \rho)$. Consequently, $1 - a = q(1 - \rho)$ and $1 - b = q + p\rho$.*

Proof. The stationarity relation is $p = qb+pa$. Since $\rho = a-b$, we obtain $p = b+p\rho$. Hence, $b = p(1-\rho)$. Therefore, $a = b + \rho = p + q\rho$. The remaining two identities follow directly. □

https://dx.doi.org/10.22108/toc.2026.149467.2373

Proposition 9.2. *For fixed $p \in (0,1)$ and $q = 1-p$, the parameter ρ is admissible if and only if*

$$\rho < 1, \qquad \rho > -\frac{p}{q}, \qquad \rho > -\frac{q}{p}.$$

Proof. By Proposition 9.1, we have $a = p + q\rho$ and $b = p(1-\rho)$. The condition $a > 0$ is equivalent to $\rho > -\frac{p}{q}$. The condition $a < 1$ is equivalent to $\rho < 1$. The condition $b > 0$ is also equivalent to $\rho < 1$. Finally, the condition $b < 1$ is equivalent to $\rho > -\frac{q}{p}$. Therefore, $0 < a < 1$ and $0 < b < 1$ hold if and only if the stated inequalities for ρ are satisfied. □

Corollary 9.3. *For every $n \geq 2$, the expected Gutman index can be expressed in terms of p and ρ as*

$$\mathbb{E}(X_n) = 6n^3 + 6n^2 + 55n - 53 - 18p(n-2) + 18q \sum_{j=1}^{n-3} (n-2-j)(q+p\rho)^j.$$

For $n = 2$ and $n = 3$, the summation term is understood to be zero.

Proof. For $n = 2$ and $n = 3$, the result follows directly from Theorem 6.2.

Now let $n \geq 4$ and put $m = n-2$. Since $b = 1-s$, we have

$$\frac{s}{b}\left(m - \frac{1-s^m}{b}\right) = \sum_{j=1}^{m-1} (m-j)s^j.$$

By Proposition 9.1, $s = q + p\rho, \pi_0 = q$ and $\pi_1 = p$. Substituting these identities into Theorem 6.2 gives the desired formula. □

Proposition 9.4. *Fix $p \in (0,1)$. For every $n \geq 4$, the expected Gutman index $\mathbb{E}(X_n)$ is a strictly increasing function of the dependence parameter ρ on its admissible interval.*

Proof. By the preceding corollary,

$$\mathbb{E}(X_n) = 6n^3 + 6n^2 + 55n - 53 - 18p(n-2) + 18q \sum_{j=1}^{n-3} (n-2-j)(q+p\rho)^j.$$

For fixed p, we have $q = 1-p > 0$. Moreover, the admissibility conditions imply $q + p\rho = 1-b > 0$. Each term $(n-2-j)(q+p\rho)^j$ is strictly increasing in ρ for $1 \leq j \leq n-3$. Since $n \geq 4$, the sum contains at least one term. Therefore, $\mathbb{E}(X_n)$ is strictly increasing in ρ. □

For fixed p and $n \geq 4$, the independent Bernoulli model corresponds to $\rho = 0$. Hence, positive admissible values of ρ increase the expected Gutman index relative to the independent model with the same stationary kink probability. Negative admissible values of ρ decrease the expected Gutman index.

Proposition 9.5. *For every $k \geq 3$ and every $h \geq 0$, we have*

$$\mathrm{Cov}(\eta_k, \eta_{k+h}) = pq\rho^h.$$

Moreover,

$$\mathrm{Corr}(\eta_k, \eta_{k+h}) = \rho^h.$$

Proof. Put $u_h = P(\eta_{k+h} = 1 \mid \eta_k = 1)$. Then $u_0 = 1$. The Markov property gives $u_{h+1} = b + (a-b)u_h$. Since $a - b = \rho$ and $p = b + \rho p$, it follows that $u_{h+1} - p = \rho(u_h - p)$. Hence, $u_h = p + q\rho^h$.Therefore,

$$P(\eta_k = 1, \eta_{k+h} = 1) = p(p + q\rho^h).$$

Subtracting p^2 gives

$$\mathrm{Cov}(\eta_k, \eta_{k+h}) = pq\rho^h.$$

Since $\mathrm{Var}(\eta_k) = pq$, the correlation formula follows. □

When $\rho = 0$, we have $a = b = p$. Thus, the Markov-dependent model reduces to the independent Bernoulli model. Positive values of ρ describe persistence of attachment types, whereas negative values describe a tendency to alternate between linear and kink attachments.

10. **Conclusion**

In this paper, we introduced a Markov-dependent random model for polyomino chains. In this model, each new square is attached either linearly or as a kink, and the sequence of attachment types is governed by a stationary two-state Markov chain.

We developed a direct recursive method for studying the expected Gutman index. Two auxiliary weighted distance sums associated with the linear and kink exposed edges were introduced. Their recursive relations allowed us to obtain an explicit recurrence and a closed formula for the expected Gutman index.

The obtained formula shows that the expected Gutman index depends on the stationary probability of kink attachments and on the transition probabilities of the Markov chain. Hence, the dependence between consecutive attachment types affects the lower-order terms of the expected Gutman index.

We also verified that the model contains the independent Bernoulli random polyomino chain as a special case. Moreover, the deterministic linear and zigzag polyomino chains are recovered when all attachments are linear or all attachments are kinks, respectively.

The dependence parameter ρ provides an interpretation of the correlation structure of the attachment process. In particular, positive values of ρ correspond to persistence of attachment types, whereas negative values correspond to a tendency to alternate between linear and kink attachments.

https://dx.doi.org/10.22108/toc.2026.149467.2373

Possible directions for future research include the study of variance and limiting behavior of the Gutman index under Markov dependence. It would also be interesting to consider higher-order Markov models and other distance-based topological indices of random polyomino chains.

Declaration of competing interest. The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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https://dx.doi.org/10.22108/toc.2026.149467.2373