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Research article

On degree–based topological indices of random polyomino chains

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Abstract: In this article, we study the degree-based topological indices in a random polyomino chain. The key purpose of this manuscript is to obtain the asymptotic distribution, expected value and variance for the degree-based topological indices in a random polyomino chain by using a martingale approach. Consequently, we compute the degree-based topological indices in a polyomino chain, hence some known results from the existing literature about polyomino chains are obtained as corollaries. Also, in order to apply the results, we obtain the expected value of several degree-based topological indices such as Sombor, Forgotten, Zagreb, atom-bond-connectivity, Randić and geometric-arithmetic index of a random polyomino chain.

Keywords: degree-based index; polyomino chains; random polyomino chains; martingale approach; asymptotic distribution; Sombor index; Randić index

1. Introduction

A numerical quantity TI associated with a graph G satisfying the equation $TI(G) = TI(G')$ for every graph G' isomorphic to G is called a graph invariant. In chemical graph theory, graph invariants that are applied in chemical investigations are known as topological indices. The goal of defining a topological index is to associate each chemical structure with a numerical value and thus investigate its properties. In fact, topological indices have found applications in Chemistry [1, 2], Computational Linguistics [3], Ecology [4]. Nowadays, a vast number of topological indices exist in the literature [5]. In this paper, we pay our attention to only degree-based topological indices; whose general form is:

$$TI(G) = \sum_{vu\in E(G)} f(d_v, d_u), \tag{1.1}$$

where f is some real valued function with the property $f(x, y) = f(y, x)$ for $x, y \in \{1, 2 \ldots\}$ and d_v is the degree of a node $v \in V(G)$. In the development of applications, degree-based topological indices have become a powerful tool, for instance, Forgotten index ($f(x, y) = x^2 + y^2$) reflects the structure-dependency of total π-electron energy E_π and measures the physical-chemical properties of molecular structures [6,7], the GA index ($f(x, y) = 2\frac{\sqrt{xy}}{x+y}$) can be used as predictive tool in QSPR/QSAR researches [8] and the atom-bond connectivity index ($f(x, y) = \sqrt{\frac{x+y-2}{xy}}$) has proven to be a valuable predictive index in study of heat of formation in alkanes [9].

On the other hand, a polyomino system is a finite 2-connected plane graph such that each interior face (say a cell) is surrounded by a regular square of length one. In a polyomino system, two squares are said to be adjacent if they share a side. A polyomino chain is a polyomino system in which the joining of the centres of its adjacent cells forms a path $c_1c_2 \ldots c_n$, where c_i is the centre of the i^{th} cell. Hence, in a polyomino chain every square is adjacent with at most two other squares. If a square has only one adjacent square, it is called terminal, if it has two adjacent squares having no vertex of degree 2, it is called medial, and if it has two adjacent squares such that it has a vertex of degree 2, it is called kink. A polyomino chain without kinks is called linear chain Li_n. A polyomino chain consisting of only kinks and terminal squares is known as zigzag chain Z_n (see Figure 1). A maximal linear chain (containing the terminal squares and kinks at its end) in the polyomino chains is called a segment of the polyomino chain.

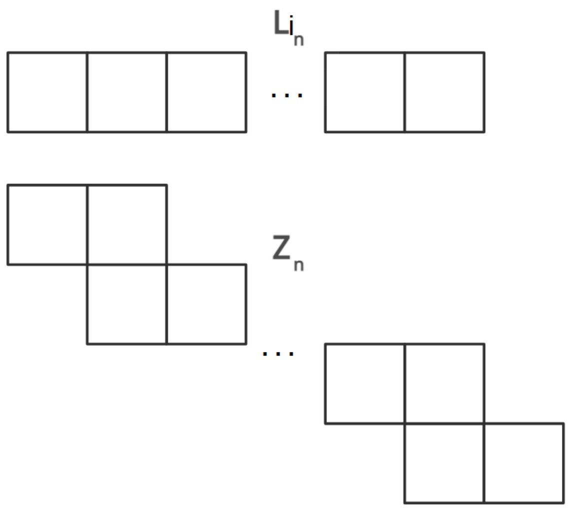

Figure 1. The linear chain and the zigzag chain.

The name polyomino was introduced in 1953 in analogy to dominoes by Solomon W. Golomb [10] and since then polyomino systems have been widely studied, as a matter of fact, in organic chemistry, especially in polycyclic aromatic compounds. At the present time, recent works on the polyomino chains include perfect matchings [11, 12], finding formulas for calculating several topological indices [13–16] and extremal problems [17–22]. Specifically, random polyomino chains have attracted substantial attention from researchers in recent years [23–27].

A random polyomino chain ($RPC_n = RPC(n, p_1, p_2)$) could be constructed by the following way: for $n = 1$ and $n = 2$, RPC_n are shown in Figure 2. For $n \geq 3$, a new square can be attached in two ways, which results in RPC_n^1 and RPC_n^2 with probability p_1 and p_2 respectively, where $0 < p_1, p_2 < 1$ and $p_1 + p_2 = 1$, see Figure 3. For a random polyomino chain at time n, the value of a topological index is a random variable. Considering the arguments put forward in the previous paragraphs and by using a martingale approach, in this paper, we establish an asymptotic distribution for degree-based topological indices in a random polyomino chain. Moreover, their explicit analytical expressions of the expected value and variance are obtained. As a result, we show a general expression for calculating the degree-based topological indices for a polyomino chain. Finally, we compute the expected value of several degree-based topological indices, such as, Sombor, Forgotten, Zagreb index of a random polyomino chain.

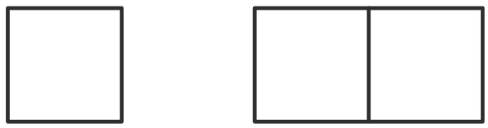

Figure 2. The graphs of RPC_1 and RPC_2.

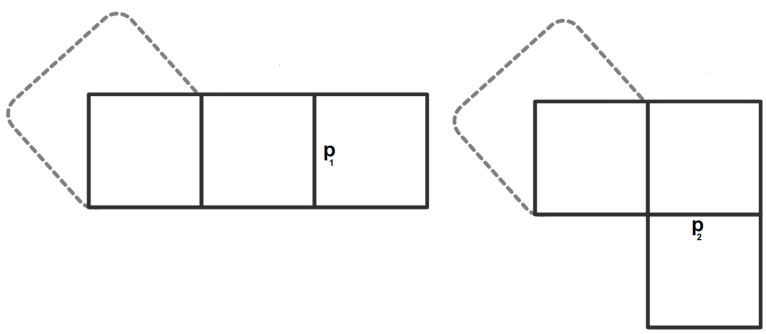

Figure 3. The two link ways for $RPC_n(n \geq 3)$.

2. Random polyomino chain

In this section, we state and prove our main results. First, let L_n denote the link selected at time $n \geq 3$, i.e., L_n denotes a random variable with range $\{1, 2\}$ where $p_i = \mathbb{P}(L_n = i)$. For $i, j \in \{1, 2\}$, $TI_n = TI(RPC_n)$, RPC_n^i denotes a random polyomino chain at time $n \geq 3$ such that $L_n = i$, $TI_{n,i} = TI(RPC_n^i)$, $RPC_n^{j,i}$ denotes a random polyomino chain at time $n \geq 4$ such that $L_{n-1} = j$ and $L_n = i$, $TI_{n,j,i} = TI(RPC_n^{j,i})$, $\alpha_{j,i} = TI_{4,j,i} - TI_{3,j}$, $\alpha_i = TI_{3,i} - TI_2$, $\alpha = \sum_{j=1}^{2} \sum_{i=1}^{2} \alpha_{j,i} p_j p_i$ and $\beta = \sum_{j=1}^{2} \sum_{i=1}^{2} \alpha_{j,i}^2 p_j p_i$.

Remark 1. Note that, by definition:

1. $\alpha_{1,1} = \alpha_1 = 3f(3, 3)$,
2. $\alpha_{1,2} = 3f(3, 4) + f(2, 4) + f(2, 3) - 2f(3, 3)$,
3. $\alpha_{2,1} = f(3, 4) - f(2, 4) + f(2, 3) + 2f(3, 3)$,
4. $\alpha_{2,2} = f(4, 4) + 2f(2, 4)$,
5. $\alpha_2 = 2f(3, 4) + 2f(2, 4) - f(3, 3)$.

Then, $\alpha_{2,1} - \alpha_{1,2} = \alpha_{1,1} - \alpha_2$. In particular, when $f(x, y) = x^a + y^a$ with $a \in \mathbb{R}$ and $x, y \in \{1, 2, \dots\}$ the following conditions are satisfied:

1. $\alpha_{1,1} = \alpha_{2,1}$,
2. $\alpha_{2,2} = \alpha_{1,2} = \alpha_2$.

Besides, in this case, $TI_n = \sum_{v \in V(RPC_n)} (d_v)^{a+1}$, due to the following identity

$$\sum_{vu \in E(G)} (d_v)^a + (d_u)^a = \sum_{v \in V(G)} (d_v)^{a+1},$$

the validity of the previous expression can be consulted, for instance in [28].

Theorem 1. *Let $RPC_n = RPC(n, p_1, p_2)$ be a random polyomino chain, then for $n \geq 3$*

$$\mathbb{E}(TI_n) = \mathbb{E}(TI_3) + \alpha(n - 3),$$

$$V(TI_n) = V(TI_3) + (\beta - \alpha^2)(n - 3),$$

where

$$\mathbb{E}(TI_3) = TI_2 + \sum_{i=1}^{2} \alpha_i p_i,$$

$$V(TI_3) = \sum_{i=1}^{2} \alpha_i^2 p_i - \left(\sum_{i=1}^{2} \alpha_i p_i \right)^2.$$

Proof. For $n \geq 4$, it follows from the definition of a random polyomino chain and by the definition of $TI(G)$ in Equation (1.1) the following almost-sure recursive relation of TI_n conditional on $\mathbb{F}_{n-1}$ and the random vector (L_{n-1}, L_n)

$$TI_{n,L_{n-1},L_n} - TI_{n-1} = TI_{4,L_{n-1},L_n} - TI_{3,L_{n-1}},$$

where $\mathbb{F}_{n-1}$ denotes the σ-field generated by the history of the growth of the random polyomino chain in the first $n - 1$ stages. Now for $n \geq 4$, we take the expectation with respect to (L_{n-1}, L_n) to get

$$\begin{aligned} \mathbb{E}(TI_n \mid \mathbb{F}_{n-1}) &= \sum_{j=1}^{2} \sum_{i=1}^{2} (TI_{n-1} + \alpha_{j,i}) p_j p_i \\ &= TI_{n-1} + \sum_{j=1}^{2} \sum_{i=1}^{2} \alpha_{j,i} p_j p_i, \end{aligned}$$

where, $\alpha_{j,i} = TI_{4,j,i} - TI_{3,j}$. Then, taking expectation, we obtain a recurrence relationship for $\mathbb{E}(TI_n)$ with $n \geq 4$,

$$\mathbb{E}(TI_n) = \mathbb{E}(TI_{n-1}) + \sum_{j=1}^{2}\sum_{i=1}^{2}\alpha_{j,i}p_j p_i. \tag{2.1}$$

We solve Equation (2.1) with the initial value $\mathbb{E}(TI_3)$ and we obtain the result stated in the theorem,

$$\mathbb{E}(TI_n) = \mathbb{E}(TI_3) + \alpha(n-3),$$

where $\alpha = \sum_{j=1}^{2}\sum_{i=1}^{2}\alpha_{j,i}p_j p_i$. For $n \geq 4$, the expression for $\mathbb{E}(TI_n^2)$ follows in a similar manner,

$$\begin{aligned}
\mathbb{E}(TI_n^2 \mid \mathbb{F}_{n-1}) &= \sum_{j=1}^{2}\sum_{i=1}^{2}(TI_{n-1} + \alpha_{j,i})^2 p_j p_i \\
&= \sum_{j=1}^{2}\sum_{i=1}^{2} TI_{n-1}^2 p_j p_i + 2TI_{n-1}\alpha_{j,i}p_j p_i + \alpha_{j,i}^2 p_j p_i \\
&= TI_{n-1}^2 + 2\alpha TI_{n-1} + \beta,
\end{aligned}$$

where $\beta = \sum_{j=1}^{2}\sum_{i=1}^{2}\alpha_{j,i}^2 p_j p_i$, thus

$$\begin{aligned}
\mathbb{E}(TI_n^2) &= \mathbb{E}(TI_{n-1}^2) + 2\alpha\mathbb{E}(TI_{n-1}) + \beta \\
&= \mathbb{E}(TI_{n-1}^2) + 2\alpha\mathbb{E}(TI_3) + 2\alpha^2(n-4) + \beta,
\end{aligned}$$

then iterating, for $n \geq 3$ it is obtained that

$$\mathbb{E}(TI_n^2) = \mathbb{E}(TI_3^2) + (2\alpha\mathbb{E}(TI_3) + \beta)(n-3) + \alpha^2(n-3)(n-4).$$

For $n \geq 3$, the variance of TI_n is obtained immediately by taking the difference between $\mathbb{E}(TI_n^2)$ and $\mathbb{E}(TI_n)^2$,

$$\begin{aligned}
V(TI_n) &= V(TI_3) + \beta(n-3) + \left((n-3)(n-4) - (n-3)^2\right)\alpha^2 \\
&= V(TI_3) + (\beta - \alpha^2)(n-3).
\end{aligned}$$

Finally, note that

$$\begin{aligned}
\mathbb{E}(TI_3) &= \mathbb{E}(\mathbb{E}(TI_3 \mid L_3)) \\
&= \sum_{i=1}^{2}(TI_2 + \alpha_i)p_i \\
&= TI_2 + \sum_{i=1}^{2}\alpha_i p_i,
\end{aligned}$$

where $\alpha_i = TI_{3,i} - TI_2$. In the same manner, we have

$$V(TI_3) = \sum_{i=1}^{2} \alpha_i^2 p_i - \left(\sum_{i=1}^{2} \alpha_i p_i \right)^2 ,$$

proving the theorem. ■

Observe that the following statements are equivalent

1. $\beta - \alpha^2 = 0$.
2. $\alpha_{1,1} = \alpha_{1,2} = \alpha_{2,2} = \alpha_{2,1}$.
3. For $n \geq 2$, $TI_n = TI_2 + \alpha(n-2)$ almost surely.
4. $f(3,4) = (2f(4,4) + f(2,4))/3$, $f(3,3) = (f(4,4) + 2f(2,4))/3$ and $f(2,3) = (-f(4,4) + 4f(2,4))/3$.

Consequently, when $\beta - \alpha^2 = 0$, $\frac{TI_n}{n}$ converges almost surely to α as $n \to \infty$. It is worth noting that by using the equivalences stated above we can conclude that, TI_n is a deterministic sequence almost surely if and only if $\alpha_{1,1} = \alpha_{1,2} = \alpha_{2,2} = \alpha_{2,1}$. Hence, by Remark 1 if $f(x, y) = x^a + y^a$ with $a \in \mathbb{R}$ we have that TI_n is a deterministic sequence almost surely if and only if $2 \cdot 3^{a+1} = 4^{a+1} + 2^{a+1}$, $a \in \mathbb{R}$. The last equation has two unique solutions $a = 0, -1$, since for $a \in (-1, 0)$, x^{a+1} is a strictly concave function on $\mathbb{R}^+$ hence $(\frac{4+2}{2})^{a+1} > \frac{4^{a+1}+2^{a+1}}{2}$ and for $a > 0$ or $a < -1$, x^{a+1} is a strictly convex function on $\mathbb{R}^+$ hence $(\frac{4+2}{2})^{a+1} < \frac{4^{a+1}+2^{a+1}}{2}$. Therefore, TI_n is a deterministic sequence almost surely if and only if $a \in \{0, -1\}$. This fact makes sense since

$$\sum_{vu \in E(RPC_n)} (d_v)^0 + (d_u)^0 = \sum_{v \in V(RPC_n)} (d_v)^1 = 2|E(RPC_n)| = 2 + 6n,$$

and

$$\sum_{vu \in E(RPC_n)} (d_v)^{-1} + (d_u)^{-1} = \sum_{v \in V(RPC_n)} (d_v)^0 = |V(RPC_n)| = 2 + 2n.$$

Now, we exploit a martingale formulation to investigate the asymptotic behavior of TI_n when $\beta - \alpha^2 > 0$.

Proposition 2. *For $n \geq 3$, $\{M_n = TI_n - \alpha(n-3)\}_n$ is a martingale with respect to $\mathbb{F}_n$.*

Proof. Observe that $\mathbb{E}(|M_n|) < +\infty$. For $n \geq 4$, by Theorem 1,

$$\begin{aligned}
\mathbb{E}(M_n \mid \mathbb{F}_{n-1}) &= \mathbb{E}(TI_n - \alpha(n-3) \mid \mathbb{F}_{n-1}) \\
&= \mathbb{E}(TI_n \mid \mathbb{F}_{n-1}) - \alpha(n-3) \\
&= TI_{n-1} + \alpha - \alpha(n-3) \\
&= TI_{n-1} - \alpha(n-4) \\
&= M_{n-1}.
\end{aligned}$$

The proof is completed. ■

We use the notation $\xrightarrow{D}$ to denote convergence in distribution and $\xrightarrow{P}$ to denote convergence in probability. Here, $\mathrm{N}\left(\mu, \sigma^2\right)$ denotes a random variable with normal distribution with mean μ and variance σ^2.

Theorem 3. *As $n \to \infty$,*

$$\frac{TI_n - (n-3)\alpha}{\sqrt{n}} \xrightarrow{D} N(0, \beta - \alpha^2).$$

Proof. For $k \geq 4$ and $j, i \in \{1, 2\}$, we have

$$|\nabla M_k| = |\nabla TI_k - \alpha| \leq 2 \max_{(j,i)}\{|\alpha_{j,i}|\},$$

where $\nabla M_k = M_k - M_{k-1}$ and $\nabla TI_k = TI_k - TI_{k-1}$. That is, given $\varepsilon > 0$, there exists an $N_0(\varepsilon) > 0$ such that, the sets $\left\{|\nabla M_k| > \varepsilon\sqrt{n}\right\}$ are empty for all $n > N_0(\varepsilon)$. Then, we conclude that

$$U_n := \frac{1}{n}\sum_{k=4}^{n} \mathbb{E}\left((\nabla M_k)^2\, \mathbb{I}_{\{|\nabla M_k| > \varepsilon\sqrt{n}\}} \mid \mathbb{F}_{k-1}\right),$$

converges to 0 almost surely, hence, $U_n \xrightarrow{P} 0$. Then, the Lindeberg's condition is verified. Next, the conditional variance condition is given by

$$V_n := \frac{1}{n}\sum_{k=4}^{n} \mathbb{E}\left((\nabla M_k)^2 \mid \mathbb{F}_{k-1}\right) \xrightarrow{P} \beta - \alpha^2.$$

Since,

$$\begin{aligned}
\frac{1}{n}\sum_{k=4}^{n} \mathbb{E}\left((\nabla M_k)^2 \mid \mathbb{F}_{k-1}\right) &= \frac{1}{n}\sum_{k=4}^{n} \mathbb{E}\left((\nabla TI_k - \alpha)^2 \mid \mathbb{F}_{k-1}\right) \\
&= \frac{1}{n}\sum_{k=4}^{n}\sum_{j=1}^{2}\sum_{i=1}^{2}(\alpha_{j,i} - \alpha)^2 p_j p_i \\
&= \frac{n-3}{n}\sum_{j=1}^{2}\sum_{i=1}^{2}(\alpha_{j,i} - \alpha)^2 p_j p_i.
\end{aligned}$$

Therefore, by the Martingale Central Limit Theorem [29], we thus obtain the stated result. ■

Finally, in order to apply the results obtained in this section, we compute the expected value of several important topological indices for a random polyomino chain (see Table 1).

Table 1. The information of interest associated with each topological index: $\mathbb{E}(TI_n) = (Ap_1^2 + Bp_1 + C)n - 3Ap_1^2 + (D - 3B)p_1 + E$.

TI	A	B	C	D	E
first Zagreb index	0	-2	20	-2	-6
second Zagreb index	-1	-4	32	-4	-24
first hyper-Zagreb index	-2	-26	136	-26	-106
second hyper-Zagreb index	-21	-120	384	-92	-560
modified first Zagreb index	0	-13/144	5/16	-13/144	43/72
Albertson index	-2	-2	4	-6	-2
extended index	1/6	-2/3	7/2	-7/12	5/12
sigma index	2	-10	8	-10	-10
Sombor index	395/3349	-225/113	2599/178	-2102/1065	-2108/441
Randić index	-34/2413	184/3229	1138/1189	224/4583	1338/1279
reciprocal Randić index	-255/2588	-426/763	985/102	-509/870	-665/257
sum-connectivity index	-33/2872	449/6784	461/394	382/6307	1092/1283
reciprocal sum-connectivity index	302/14565	-731/1829	5216/675	-42/107	-59/1243
harmonic index	-11/420	23/210	11/12	2/21	457/420
atom-bond-connectivity (ABC) index	183/6023	-432/7583	991/489	-130/3373	691/796
augmented Zagreb index	-1636/757	2399/1751	944/27	515/269	-1814/137
forgotten index	0	-18	72	-18	-58
geometric-arithmetic index	-307/9318	353/2396	883/306	380/2817	637/565
arithmetic-geometric index	413/10692	-365/2282	3499/1121	-976/6871	969/1126
inverse sum indeg index	-19/210	-8/105	14/3	-2/21	-116/105

3. Polyomino chain

In this section, the goal is to obtain explicit analytical expressions to calculate $TI(PC_n)$ where PC_n is a polyomino chain with n squares. Let $m \geq 1$ and $i \in \{1, 2, \ldots, m\}$ note that a polyomino chain PC_n consists of a sequence of segments $s_1, s_2, \ldots, s_m$ (see Figure 4) with lengths $l(s_i) = l_i$ such that $\sum_{i=1}^{m} l_i = n + m - 1$, where l_i is calculated by the number of squares in s_i.

Theorem 4. *Let PC_n be a polyomino chain having $n \geq 3$ squares and $m \geq 1$ segment(s) s_i with $i = 1, 2, \ldots, m$. Then*

$$\begin{aligned} TI(PC_n) = \; & 3f(3,3)n + (4f(3,4) + 2f(2,3) - 6f(3,3))m \\ & + (f(2,4) - f(2,3) + f(3,3) - f(3,4))(I_1 + I_m) \\ & + (f(4,4) + 2f(2,4) - 4f(3,4) - 2f(2,3) + 3f(3,3))\gamma \\ & + 2f(2,2) + 2f(2,3) + f(3,3) - 4f(3,4), \end{aligned}$$

where, $I_i = \begin{cases} 1 & if \quad l_i = 2 \\ 0 & if \quad l_i \neq 2 \end{cases}$ *and* $\gamma = \sum_{i=2}^{m-1} I_i$.

Proof. Note that PC_n is a realization of RPC_n, then we know the value of L_k for $k = 3, 4, \ldots, n$. Therefore, by using the ideas presented in Section 2 we have,

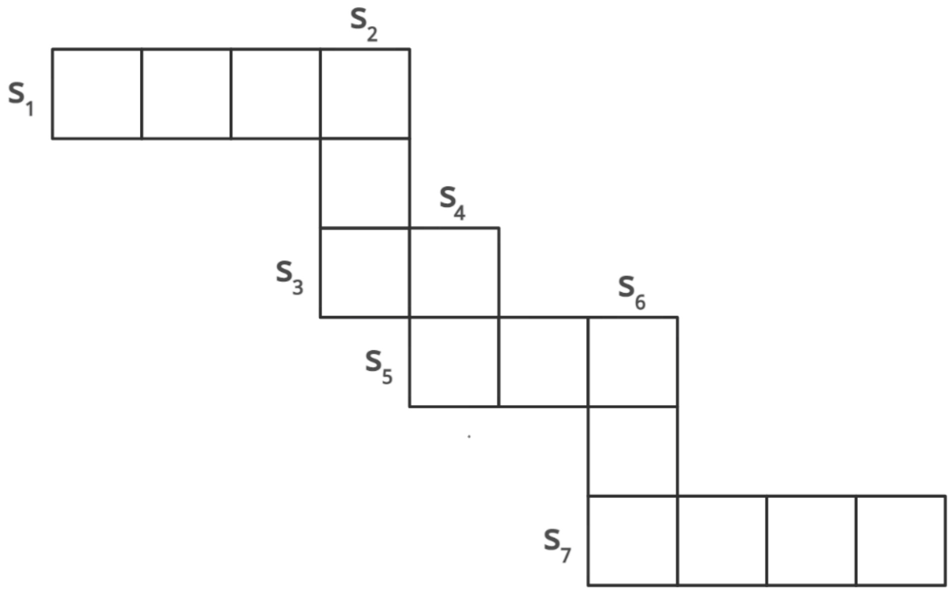

Figure 4. Segments of a polyomino chain.

$$
\begin{aligned}
TI(PC_n) &= TI_2 + \alpha_2 I_1 + \alpha_{1,1}(1 - I_1) + \sum_{k=4}^{n} \alpha_{L_{k-1},L_k} \\
&= TI_2 + (\alpha_2 - \alpha_{1,1}) I_1 + \alpha_{1,1} + \sum_{j=1}^{2} \sum_{i=1}^{2} X_{j,i}\alpha_{j,i},
\end{aligned}
$$

where $X_{j,i} = |\{k \in \{4, 5, \ldots, n\} \mid L_{k-1} = j \text{ and } L_k = i \text{ in } PC_n\}|$ and $I_1 = I_{\{l_1=2\}}$. Now, if at time k $(3 \leq k \leq n)$, $L_k = 2$ then the last segment in PC_{k-1} is finished (so, a new segment is initiated in PC_k) and if at time k, $L_k = 1$ then a square is added to the last segment in PC_{k-1}. Hence, $X_2 = |\{k \in \{3, 4, \ldots, n\} \mid L_k = 2 \text{ in } PC_n\}| = m - 1$ and $X_1 = |\{k \in \{3, 4, \ldots, n\} \mid L_k = 1 \text{ in } PC_n\}| = n - 2 - (m - 1) = n - m - 1$. Moreover, $X_{1,2} = |\{i \in \{1, 2, \ldots, m - 1\} \mid l_i \neq 2 \text{ in } PC_n\}|$ and $X_{2,1} = |\{i \in \{2, 3, \ldots, m\} \mid l_i \neq 2 \text{ in } PC_n\}|$. We may write this as: $X_{1,2} = m - \gamma - 1 - I_1$ and $X_{2,1} = m - \gamma - 1 - I_m$, where,

$$
I_i = \begin{cases} 1 & if \quad l_i = 2 \\ 0 & if \quad l_i \neq 2 \end{cases} \quad \text{and } \gamma = \sum_{i=2}^{m-1} I_i.
$$

Consequently, $X_{1,1} = n - 2m + \gamma - 1 + I_1 + I_m$ and $X_{2,2} = \gamma$, because of the following identities

$$
X_{1,1} + X_{2,1} = X_1 - 1 + I_1,
$$

$$
X_{2,2} + X_{1,2} = X_2 - I_1.
$$

Finally, we arrive at the desired result by replacing the values of $X_{j,i}$, $\alpha_{j,i}$ and α_2. ■

Remark 2. 1. By using that $\sum_{i=1}^{m} l_i = n + m - 1$, it is verified that, $X_{1,1} = \sum_{l_i \neq 2} (l_i - 3)$.

2. On the other hand, by definition if $f(x, y) = x^a + y^a$ with $a \in \mathbb{R}$ then the coefficients of γ and $I_1 + I_m$ in Theorem 4 are zero and the coefficient of m is zero, i.e., the general expression showed in Theorem 4 is independent of m if and only if $2 \cdot 3^{a+1} = 4^{a+1} + 2^{a+1}$ if and only if $a \in \{0, -1\}$.
3. Finally, by the way, in [30] the authors established a general expression for calculating the bond incident degree (BID) indices of a polyomino chain; which follows from Theorem 4. *BID* indices form a subclass of the class all degree-based topological indices.

By definition if $PC_n = Li_n$, we deduce that $m = 1$ and $l_1 = n$ and if $PC_n = Z_n$, then $m = n - 1$ and $l_i = 2$ for $i = 1, 2, \ldots, m$. Therefore, the following corollary may be obtained directly by Theorem 4.

Corollary 1. *Let Li_n and Z_n be linear and zigzag chains respectively with $n \geq 3$ squares. Then*

$$TI(Li_n) = 3f(3,3)n + 4f(2,3) + 2f(2,2) - 5f(3,3),$$

$$TI(Z_n) = (2f(2,4) + f(4,4))n + 4f(2,3) - 3f(4,4) + 2f(3,4) - 4f(2,4) + 2f(2,2).$$

It is worth noting that in 2020, Buragohain et al. [31] introduced a novel generalized topological index for some chemical structures defined as

$$ISI_{(\alpha,\beta)}(G) = \sum_{uv \in E(G)} (d(u)d(v))^{\alpha}(d(u) + d(v))^{\beta}.$$

In [13] the authors studied the generalized $ISI_{(\alpha,\beta)}$-index and (α,β)-Zagreb index of a linear chain. By using Corollary 1 the results showed in [13] can be obtained. In addition, taking $f(x, y) = x^2 + y^2$ in Equation (1.1), we obtain the Forgotten index. Recently, in [15] the computation of the Forgotten index in a polyomino chain was given as follows:

Corollary 2. *Let $n \geq 2$ and PC_n be a polyomino chain with $m \geq 1$ segment(s). Then* $F(PC_n) = 54n + 18m - 40$.

Note that, the general expression obtained in Corollary 2 is independent of γ, I_1 and I_m; which makes sense because of Remark 2. In a similar manner, we can obtain the above result from Theorem 4. Finally, in the following results by using Theorem 4 we will compute $TI(PC_n)$ of several kinds of polyomino chains.

Corollary 3. *For the polyomino chain with $n \geq 3$ squares and 2 segments s_1 and s_2 satisfy $l_1 = 2$ and $l_2 = n - 1$, PC_n^1, we have the following:*

$$TI(PC_3^1) = 2f(3,4) + 4f(2,3) + 2f(2,4) + 2f(2,2),$$

and for $n \geq 4$

$$TI(PC_n^1) = 3f(3,3)n + 3f(3,4) + 5f(2,3) - 10f(3,3) + f(2,4) + 2f(2,2).$$

Corollary 4. *For the polyomino chain with $n \geq 5$ squares and $m \geq 3$ segments $s_1, s_2, \ldots, s_m$ satisfy $l_1 = l_m = 2$ and $l_2, l_3, \ldots, l_{m-1} \geq 3$, PC_n^2, we have the following:*

$$TI(PC_n^2) = 3f(3,3)n + (4f(3,4) + 2f(2,3) - 6f(3,3))m + 3f(3,3) - 6f(3,4) + 2f(2,4) + 2f(2,2).$$

Corollary 5. *For the polyomino chain with $n \geq 6$ squares and $m \geq 3$ segments $s_1, s_2, \ldots, s_m$ satisfy $l_1 = 2$ and $l_2, l_3, \ldots, l_m \geq 3$ or $l_m = 2$ and $l_1, l_2, \ldots, l_{m-1} \geq 3$, PC_n^3, we have the following:*

$$TI(PC_n^3) = 3f(3,3)n + (4f(3,4) + 2f(2,3) - 6f(3,3))m + 2f(2,2) + f(2,3) + 2f(3,3) - 5f(3,4) + f(2,4).$$

Corollary 6. *For the polyomino chain with $n \geq 7$ squares and $m \geq 3$ segments $s_1, s_2, \ldots, s_m$ satisfy $l_1, l_2, \ldots, l_m \geq 3$, PC_n^4, we have the following:*

$$TI(PC_n^4) = 3f(3,3)n + (4f(3,4) + 2f(2,3) - 6f(3,3))m + 2f(2,2) + 2f(2,3) + f(3,3) - 4f(3,4).$$

Actually, the authors in [32–34] calculated several topological indices, such as, redefined Zagreb index, harmonic index and inverse sum index for L_n, Z_n and PC_n^i with $i = 1, 2$; which are deduced from Corollaries 1, 3 and 4. Besides, in [7, 35, 36] the authors computed Forgotten, Randić and generalized Zagreb index for L_n, Z_n and PC_n^i with $i = 1, 2, 3, 4$; hence we can deduce the results above mentioned by using Corollaries 1, 3, 4, 5 and 6. In fact the results showed in [7] can be verified directly by Corollary 2.

On the other hand, here a polyomino chain of dimension $n \geq 1$ with $k = k_1 + k_2 + k_3$ where k_1 is the number of kinks, k_2 is the number of medials and k_3 is the number of terminals in a unit of polyomino chain will be denoted by $PC_{n,k}$. In Figure 5, a general representation of a polyomino chain $PC_{n,k}$ is depicted. Let $k \geq 3$, by definition of $PC_{n,k}$, we have: $m = 2n$, $\gamma = n - 1$, $I_m = 1$ and $I_1 = I_{\{k=3\}}$. Hence, in the following corollary, we will compute $TI(PC_{n,k})$ for $k \geq 3$ by using Theorem 4.

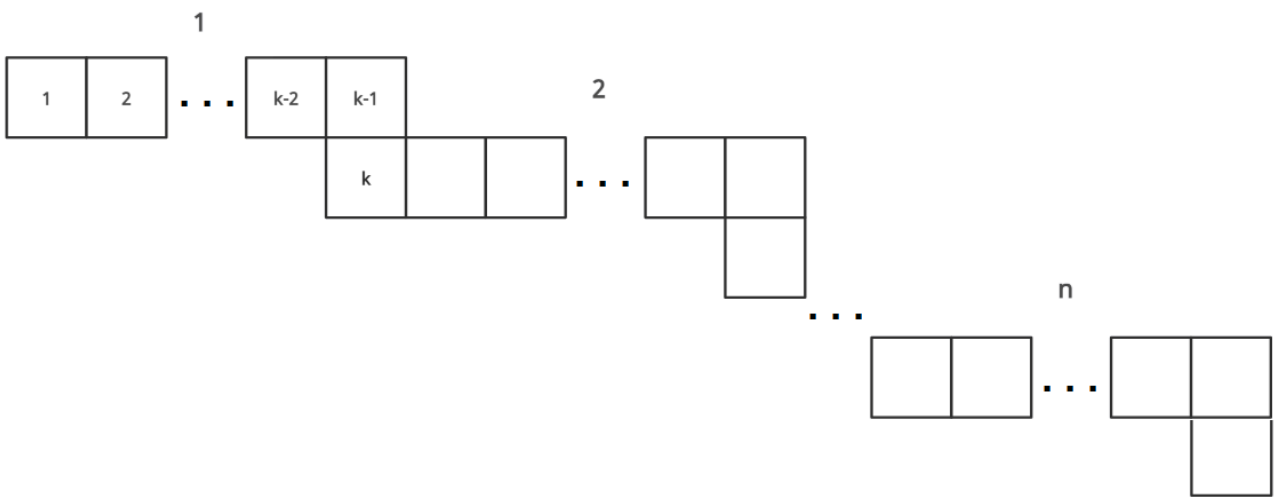

Figure 5. General representation of $PC_{n,k}$.

Remark 3. Note that, by definition $PC_{n,1} = Li_n$ and $PC_{n,2} = Z_{2n}$.

Corollary 7. *Let $k \geq 3$, $n \geq 1$, then we have*

$$\begin{aligned} TI(PC_{n,k}) = \; & (3(k-3)f(3,3) + 4f(3,4) + 2f(2,3) + f(4,4) + 2f(2,4))n \\ & + (f(2,4) - f(2,3) + f(3,3) - f(3,4))I_{\{k=3\}} \\ & + 2f(2,2) + 3f(2,3) - f(3,3) - f(3,4) - f(2,4) - f(4,4). \end{aligned}$$

In fact, in [37] Hayat et al. computed the exact analytical expressions of the ABC, GA, ABC_4 and GA_5 index for $PC_{n,k}$ with $k = 3, 4, 5$. These results can be obtained as a consequence of Corollary 7.

4. Conclusion

In this paper, we proposed a martingale approach to the study of topological indices in random polyomino chains. The expected value and variance have been determined and we formulated a martingale to characterize the asymptotic behavior of the topological indices. Moreover, we considered some particular topological indices, such as, the first Zagreb, Sombor, harmonic, geometric-arithmetic and second Zagreb index for a random polyomino chain. In fact, from the derived results, several known results about polyomino chains were obtained as corollaries. We believe the results obtained in this paper can provide theoretical support for the chemical research. By the way, the extremal random polyomino chains with respect to several well-known degree-based topological indices have been discussed in our next paper. Finally, it would be interesting to extend the work of this paper to k-polygonal chains. We expect to develop it in the future.

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Conflict of interest

The authors declare there is no conflict of interest.

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