Topological indices in Random Spiro Chains

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Abstract: Let \( G = (V(G), E(G)) \) denote a graph, many important topological indices can be defined as

\[
TI(G) = \sum_{v \in V(G)} h(d_v)^a,
\]

or

\[
TI(G) = \sum_{vu \in E(G)} f(d_v, d_u)^a.
\]

In this paper, we study these kinds of topological indices in random spiro chains via a martingale approach. In which their explicit analytical expressions of the exact distribution, expected value and variance are obtained. As \( n \) goes to \( \infty \), the asymptotic normality of topological indices of a random spiro chain is established through the Martingale Central Limit Theorem. In particular, we compute the Nirmala, Sombor, Randić and Zagreb index for a random spiro chain along with their comparative analysis.

1 Introduction

A graph \( G \) is determined by two sets \((V(G), E(G))\), the set of nodes \((V(G))\) and edges \((E(G))\). The edges and nodes are interpreted according to the problem to be modeled. In particular, a molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds of a molecule, where a simple graph is a graph without directed, weighted or multiple edges, and without self-loops. Topological indices numerically quantify aspects of these graphs for multiple purposes, such as sparseness, regularity, and centrality. In addition, the first and second Zagreb indices appeared for the first time in \( \text{(Gutman and Trinajstić 1972)} \), then it is defined in \( \text{(Randić 1975)} \) the Randić index. These indices are mostly historical and well-known indices which have been widely used to predict the properties of compounds; since have been proved to have a wide range of functions as topological variables supported by chemical experiment data. In \( \text{(Gutman 2021)} \), a novel topological index was introduced via a geometric approach, named Sombor index defined as

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\[ SO(G) = \sum_{uv \in E(G)} \sqrt{(d_u)^2 + (d_v)^2}, \]

where \( d_v \) is the degree of a vertex \( v \). Nowadays, several graph invariants related to the Sombor index have been presented. For example, in [Kulli 2021], Kulli introduced the Nirmala index of a graph \( G \) as follows

\[ N(G) = \sum_{uv \in E(G)} \sqrt{d_u + d_v}. \]

Recent work on the Nirmala index can be consulted in [Kulli, Chaluvaraju, and Asha 2021] and [Gutman, Kulli, and Redzepovic 2021]. In general, topological indices that can be constructed for static and random graphs represent a major part of the current research in mathematical chemistry and chemical graph theory.

On the other hand, the martingale theory is a very powerful and deep mathematical tool. The concept was introduced by Paul Lévy in 1934, and was given its name in 1939 by J. André Ville. The development of a whole theory around martingales is due to Joseph L. Doob. Nowadays, the concept of martingales is well-known. In particular, there are martingale central limit theorems, which give conditions under which the whole process is approximately normally distributed. Actually, in [Feng and Hu 2015] and [Kazemi 2021] the authors used a martingale approach to study topological indices, such as the Zagreb, Gordon-Scantlebury and Platt indices.

In [Li, Shi, and Gao 2021], [Raza and Imran 2021], [Raza 2021], [Fang, You, and Liu 2021], [Jahanbani 2020], [Wei, Ke, and Hao 2018], [Raza 2020], [Deng 2012] and [Zhang, You, Liu, and Huang 2021] the authors studied topological indices in random chains. In particular, spiro compounds are an important class of cycloalkanes in organic chemistry. The derivatives of spiros are fairly often seen chemicals, which may be utilized in organic synthesis, drug synthesis, heat exchanger, etc. Motivated for the above information, we make researches on topological indices in random spiro chains. In this paper, our goal is to associate a martingale to the topological index, so that, the properties that can be deduced from the martingale are useful to show those of the topological index. We first establish exact formulas for the expected value, variance and the exact distribution of topological indices in random spiro chains. Moreover, we find a general result for the asymptotic distribution via this approach. Finally, as applications, using the Nirmala, Sombor, Randić and Zagreb index, the results are given for random spiro chains (see in Definition 1).

**Definition 1.** The random spiro chain \( \text{RSC}_n = \text{RSC}(n, p_1, p_2, p_3) \) with \( n \) hexagons is constructed by the following way:

- \( \text{RSC}_1 \) is a hexagon and \( \text{RSC}_2 \) contains two hexagons, see Figure 1.
• For every \( n > 2 \), \( RSC_n \) is constructed by attaching one hexagon to \( RSC_{n-1} \) in three ways, resulted in \( RSC_1, RSC_2, RSC_3 \) with probability \( p_1, p_2 \) and \( p_3 \) respectively, where \( 0 < p_i < 1 \) and \( p_1 + p_2 + p_3 = 1 \), see Figure 2.

\[
\begin{align*}
\text{Figure 1: The graphs of } RSC_1 \text{ and } RSC_2.
\end{align*}
\]

\[
\begin{align*}
\text{Figure 2: The three link ways for } RSC_n (n > 2).
\end{align*}
\]

2 Topological indices in random spiro chains.

Let \( G = (V(G), E(G)) \), many important topological indices can be defined as

\[
TI(G) = \sum_{v \in V(G)} h(d_v)^a,
\]

or

\[
TI(G) = \sum_{vu \in E(G)} f(d_v, d_u)^a,
\]

where \( a \in \mathbb{R} \), \( h : \{1, 2, \ldots\} \to (0, \infty) \) and \( f : \{1, 2, \ldots\} \times \{1, 2, \ldots\} \to (0, \infty) \) is any symmetric function. The main topological indices of the form (2) and (3) are:

• If \( h(t) = t \) and \( a = 2 \) then \( TI(G) \) is the first Zagreb index.
• If \( h(t) = t \) and \( a = -1 \) then \( TI(G) \) is the inverse degree index.
• If \( h(t) = t \) and \( a = 3 \) then \( TI(G) \) is the forgotten index.
• If \( h(t) = t \) and \( a \in \mathbb{R} \) then \( TI(G) \) is the variable first Zagreb index.
• If \( f(x, y) = xy \) and \( a = 1 \) then \( TI(G) \) is the second Zagreb index.
• If \( f(x, y) = xy \) and \( a = -1/2 \) then \( TI(G) \) is the usual Randić index.
• If \( f(x, y) = x + y \) and \( a = -1 \) then \( 2TI(G) \) is the harmonic index.
• If \( f(x, y) = x + y \) and \( a \in \mathbb{R} \) then \( TI(G) \) is the variable sum-connectivity index.

Remark 1. Note that the Nirmala index \([7]\) is the reverse version of the sum-connectivity index. In addition, the Nirmala index is the variable sum-connectivity index, for \( a = 1/2 \).

Theorem 1. Let \( RSC_n = RSC(n, p_1, p_2, p_3) \) with \( n \geq 2 \) be a random spiro chain. Then

\[
\mathbb{E}(TI_n) = T1_2 + \alpha(n - 2), \\
V(TI_n) = (\beta - \alpha^2)(n - 2),
\]

where \( i = 1, 2, 3 \), \( TI_n = TI(RSC_n) \), \( T1_{n,i} = TI(RSC_{n,i}) \), \( \alpha_i = TI_{3,i} - TI_2 \),
\( \alpha = \sum_{i=1}^{3} \alpha_i p_i \) and \( \beta = \sum_{i=1}^{3} \alpha_i^2 p_i \).

Proof. Let \( n \geq 3 \) and \( L_n \) denote a random variable with range \( \{1, 2, 3\} \) and let \( p_i = P(L_n = i) \) and \( L_2 \) denote the initial link, i.e., \( L_n \) denote the link selected at time \( n \). Note that, at time \( n - 1 \) we have

\[
\underbrace{HL_2H L_3HL_4HL_5 \ldots L_{n-1}H}_{RSC_2} \underbrace{RSC_{n-1}}_{RSC_n}.
\]

Then, at time \( n \), we obtain

\[
\underbrace{HL_2H L_3HL_4HL_5 \ldots L_{n-1}H L_nH}_{RSC_2} \underbrace{RSC_{n-1}}_{RSC_n}.
\]
Therefore, we must pay attention to the change in the calculation of the topological index by joining $H$ with $H$ via $L_n$. Let $n \geq 3$ and $i = 1, 2, 3$, then based on this approach, by the definition of a random spiro chain and $TI(G)$ in Equation (2) and (3), we obtain the following almost-sure recursive relation between $TI_{n-1}$ and $TI_n$, conditional on the event that at time $n$ the link $i$ is selected and $F_{n-1}$

$$TI_{n,i} - TI_{n-1} = TI_{3,i} - TI_2,$$

where $F_{n-1}$ denotes the $\sigma$-field generated by the history of the growth of the random spiro chain in the first $n - 1$ stages. Now, we take the expectation with respect to $L_n$ to get,

$$\mathbb{E}(TI_n | F_{n-1}) = \sum_{i=1}^{3} (TI_{n-1} + \alpha_i)p_i$$

$$= TI_{n-1} + \sum_{i=1}^{3} \alpha_ip_i,$$

where, $\alpha_i = TI_{3,i} - TI_2$. Then, taking expectation, we obtain a recurrence relationship for $\mathbb{E}(TI_n)$,

$$\mathbb{E}(TI_n) = \mathbb{E}(TI_{n-1}) + \sum_{i=1}^{3} \alpha_ip_i.$$  

(4)

We solve Equation (4) with the initial value $\mathbb{E}(TI_2) = TI_2$ and we obtain the result stated in the theorem,

$$\mathbb{E}(TI_n) = TI_2 + \alpha(n-2),$$

where $\alpha = \sum_{i=1}^{3} \alpha_ip_i$. The expressions for $\mathbb{E}(TI_n^2)$ follow in a similar manner,

$$\mathbb{E}(TI_n^2 | F_{n-1}) = \sum_{i=1}^{3} (TI_{n-1} + \alpha_i)^2p_i$$

$$= \sum_{i=1}^{3} TI_{n-1}^2p_i + 2TI_{n-1}\alpha_ip_i + \alpha_i^2p_i$$

$$= TI_{n-1}^2 + 2TI_{n-1}\alpha + \beta,$$

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where $\beta = \sum_{i=1}^{3} \alpha_i^2 p_i$, thus

\[
\mathbb{E}(T_{n}^2) = \mathbb{E}(T_{n-1}^2) + 2\alpha \mathbb{E}(T_{n-1}) + \beta
\]

\[
= \mathbb{E}(T_{n-1}^2) + 2\alpha T_{n-2} + 2\alpha^2(n - 3) + \beta,
\]

with $\mathbb{E}(T_{2}^2) = T_{2}^2$, then iterating, it is obtained that

\[
\mathbb{E}(T_{n}^2) = T_{2}^2 + (2\alpha T_{2} + \beta)(n - 2) + (n - 3)(n - 2)\alpha^2.
\]

The variance of $T_{n}$ is obtained immediately by taking the difference between $\mathbb{E}(T_{n}^2)$ and $\mathbb{E}(T_{n})^2$,

\[
V(T_{n}) = \beta(n - 2) + ((n - 2)(n - 3) - (n - 2)^2)\alpha^2
\]

\[
= (\beta - \alpha^2)(n - 2),
\]

proving the theorem.

Note that $\beta - \alpha^2 = 0$ if and only if $\alpha_1 = \alpha_2 = \alpha_3$ if and only if $T_{n} = T_{2} + \alpha(n - 2)$ a.s. with $n \geq 2$ (a deterministic sequence). Now, we exploit a martingale formulation to investigate the asymptotic behavior of $T_{n}$ when $\beta - \alpha^2 > 0$. The key idea is to consider a transformation $M_{n}$ and we require that the transformed random variables form a martingale in the next proposition.

**Proposition 1.** For $n \geq 2$, $\{M_{n} = T_{n} - \alpha(n - 2)\}$ is a martingale with respect to $\mathbb{F}_{n}$.

**Proof.** Firstly, observe that $\mathbb{E}(|M_{n}|) < +\infty$. Then, by Theorem [1]

\[
\mathbb{E}(T_{n} - \alpha(n - 2) \mid \mathbb{F}_{n-1}) = \mathbb{E}(T_{n} \mid \mathbb{F}_{n-1}) - \alpha(n - 2)
\]

\[
= T_{n-1} + \alpha - \alpha(n - 2)
\]

\[
= T_{n-1} - \alpha(n - 3).
\]

The proof is completed.

We use the notation $\overset{D}{\rightarrow}$ to denote convergence in distribution and $\overset{P}{\rightarrow}$ to denote convergence in probability. The random variable $N(\mu, \sigma^2)$ appears in the following theorem for the normal distributed with mean $\mu$ and variance $\sigma^2$. 

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Theorem 2. As $n \to \infty$,

\[
\frac{T_{I_n-(n-2)\alpha}}{\sqrt{n}} \overset{D}{\to} N(0, \beta - \alpha^2).
\]

Proof. Note that, for $j \geq 3$ and $i = 1, 2, 3$, we have

\[
|\nabla M_j| = |\nabla TI_j - \alpha| \leq 2 \max_i |\alpha_i|,
\]

where $\nabla M_j = M_j - M_{j-1}$ and $\nabla TI_j = TI_j - TI_{j-1}$. Then, as $n$ goes to $\infty$

\[
\lim_{n \to \infty} \frac{|\nabla M_j|}{\sqrt{n}} = 0.
\]

That is, given $\varepsilon > 0$, there exists an $n_0(\varepsilon) > 0$ such that, the sets $\{|\nabla M_j| > \varepsilon \sqrt{n}\}$ are empty for all $n > n_0(\varepsilon)$. In what follows, we conclude that

\[
U_n := \frac{1}{n} \sum_{j=3}^{n} E \left( (\nabla M_j)^2 \mathbb{I}_{\{|\nabla M_j| > \varepsilon \sqrt{n}\}} \mid \mathcal{F}_{j-1} \right),
\]

converges to 0 almost surely, hence, $U_n \overset{P}{\to} 0$. As a result, the Lindeberg’s condition is verified. Next, the conditional variance condition is given by

\[
V_n := \frac{1}{n} \sum_{j=3}^{n} E \left( (\nabla M_j)^2 \mid \mathcal{F}_{j-1} \right) \overset{P}{\to} \beta - \alpha^2.
\]

Note that,

\[
\frac{1}{n} \sum_{j=3}^{n} E \left( (\nabla M_j)^2 \mid \mathcal{F}_{j-1} \right) = \frac{1}{n} \sum_{j=3}^{n} E \left( (\nabla TI_j - \alpha)^2 \mid \mathcal{F}_{j-1} \right)
\]

\[
= \frac{1}{n} \sum_{j=3}^{n} \sum_{i=1}^{3} (\alpha_i - \alpha)^2 p_i
\]

\[
= \frac{n - 2}{n} \sum_{i=1}^{3} (\alpha_i - \alpha)^2 p_i.
\]

By the Martingale Central Limit Theorem [Hall and Heyde 2014], we thus obtain the stated result, since

\[
\sum_{i=1}^{3} (\alpha_i - \alpha)^2 p_i = \sum_{i=1}^{3} \alpha_i^2 p_i - 2\alpha \sum_{i=1}^{3} \alpha_i p_i + \alpha^2
\]

\[
= \beta - \alpha^2.
\]

\[\square\]
Then we may use Theorem 2 to find the following result.

**Corollary 1.** As \( n \to \infty \),

\[
\frac{T_{I_n} - E(T_{I_n})}{\sqrt{V(T_{I_n})}} \xrightarrow{D} N(0, 1).
\]

The following theorem gives further details on the distribution for topological indices in random spiro chains. Here, \( M_R(\cdot) \) denotes the moment generating function of a random variable \( R \).

**Theorem 3.** Let \( RSC_n \) with \( n \geq 2 \) be a random spiro chain. Then,

\[
T_{I_n} = T_{I_2} + a^T X,
\]

where \( a^T = (\alpha_1, \alpha_2, \alpha_3) \) and \( X = (X_1, X_2, X_3) \) is a multinomial random variable with parameters \( n - 2 \) and \( (p_1, p_2, p_3) \).

**Proof.** Let \( t \in \mathbb{R} \), note that,

\[
E\left(e^{tT_{I_n}} \mid F_{n-1}\right) = \sum_{i=1}^{3} e^{tT_{I_{n-1}} - 1} e^{t\alpha_i} p_i = e^{tT_{I_{n-1}}} \sum_{i=1}^{3} e^{t\alpha_i} p_i.
\]

Thus, we can conclude that

\[
M_{T_{I_n}}(t) = M_{T_{I_{n-1}}}(t) \sum_{i=1}^{3} e^{t\alpha_i} p_i.
\]

We may therefore write,

\[
M_{T_{I_n}}(t) = M_{T_{I_2}}(t) \left( \sum_{i=1}^{3} e^{t\alpha_i} p_i \right)^{n-2} = M_{T_{I_2}}(t) M_{X}(\alpha_1 t, \alpha_2 t, \alpha_3 t) = M_{T_{I_2}}(t) M_{a^T X}(t),
\]

which completes the proof.

It is useful to note that the approximation given in Corollary 1 is identical to the one obtained by the following method. Let \( n \geq 2 \), by Theorem 3 we have that
\[ TI_n = TI_2 + a^T X. \]

It follows from the Central Limit Theorem to the case of random vectors (Sev-\-erini et al. 2012) that \( X \) is asymptotically distributed according to a multivariate normal distribution with mean \( E(X) \) and covariance matrix \( V(X) \). Consequently, \( a^T X \) is asymptotically distributed according to a normal distribution with mean \( a^T E(X) \) and variance \( a^T V(X) a \). Then, as \( n \) goes to \( \infty \)

\[
\frac{TI_n - TI_2 - a^T E(X)}{\sqrt{a^T V(X) a}} = \frac{TI_n - E(TI_n)}{V(TI_n)} \xrightarrow{D} N(0, 1).
\]

3 Interpretation of the results and examples.

The conclusion of Section 2 can be stated as follows.

**Theorem 4.** Let \( RSC_n \) with \( n \geq 2 \) be a random spiro chain and \( a \in \mathbb{R} \). Then

\[
TI(G) = \sum_{v \in V(G)} h(d_v)^a = 2h(2)^a - h(4)^a + (4h(2)^a + h(4)^a)n,
\]

and

\[
TI(G) = \sum_{vu \in E(G)} f(d_v, d_u)^a = A + BX + Cn,
\]

\[
E(TI_n) = A + (Bp_1 + C)n - 2Bp_1,
\]

\[
V(TI_n) = B^2 p_1 (1 - p_1) (n - 2),
\]

where \( A = 4f(2, 2)^a - 4f(2, 4)^a \), \( B = f(2, 2)^a - 2f(2, 4)^a + f(4, 4)^a \), \( C = 2f(2, 2)^a + 4f(2, 4)^a \) and \( X \) has a binomial distribution with parameters \( n - 2 \) and \( p_1 \).

**Proof.** As can be seen from the results obtained in Section 2 we need to find \( TI_2 \) and \( \alpha_i \) with \( i = 1, 2, 3 \). By the definition of \( TI_n \) in Equation (2), \( RSC_2 \) and \( RSC_3 \), we have that,

\[
TI_2 = 10h(2)^a + h(4)^a,
\]

\[
T_{3,1} = T_{3,2} = T_{3,3} = 14h(2)^a + 2h(4)^a.
\]

Then,

\[
\alpha_1 = \alpha_2 = \alpha_3 = 4h(2)^a + h(4)^a.
\]

On the other hand, by the definition of \( TI_n \) in Equation (3), it follows that,
\[ TI_2 = 8f(2,2)^a + 4f(2,4)^a, \]
\[ T_{3,1} = T_{3,2} = 10f(2,2)^a + 8f(2,4)^a, \]
\[ T_{3,3} = 11f(2,2)^a + 6f(2,4)^a + f(4,4)^a. \]

Then,
\[ \alpha_1 = \alpha_2 = 2f(2,2)^a + 4f(2,4)^a, \]
\[ \alpha_3 = 3f(2,2)^a + 2f(2,4)^a + f(4,4)^a. \]

In each case, applying Theorem 1, 2 and 3, we verify the results.

Remark 2. Note that if \( TI(G) = \sum_{v \in V(G)} h(d_v)^a \) then \( TI_n \) is a deterministic sequence and if \( TI(G) = \sum_{vu \in E(G)} f(d_v, d_u)^a \), we have that \( TI_n = TI_2 + \alpha_1(n - 2) \) with \( n \geq 2 \) (a deterministic sequence) if and only if \( f(2,2)^a + f(4,4)^a = 2f(2,4)^a \). In particular, if \( a = 1 \) then taking \( f(x,y) = x^\theta + y^\theta \) with \( \theta \in \mathbb{R} \), it is verified that \( f(2,2) + f(4,4) = 2f(2,4) \); which make sense, since \( TI(G) = \sum_{vu \in E(G)} d_v^\theta + d_u^\theta = \sum_{v \in E(G)} d_v^{\theta+1} \).

Now, in order to apply Theorem 4, we present the following corollaries.

Corollary 2. Let \( RSC_n = RSC(n,p_1,p_2,p_3) \) be a random spiro chain and \( N_n \) be the Nirmala index of a \( RSC_n \), with \( n \geq 2 \). Then
\[ N_n = 8 - 4\sqrt{6} + (2 - 2\sqrt{6} + 2\sqrt{2})X + (4 + 4\sqrt{6})n, \]
\[ E(N_n) = 8 - 4\sqrt{6} + (2 - 2\sqrt{6} + 2\sqrt{2})p_1 + 4 + 4\sqrt{6} - 2(2 - 2\sqrt{6} + 2\sqrt{2})p_2, \]
\[ V(N_n) = (2 - 2\sqrt{6} + 2\sqrt{2})^2p_1 (1 - p_1) (n - 2), \]
\[ \frac{N_n - E(N_n)}{\sqrt{V(N_n)}} \xrightarrow{D} N(0,1), \]
where \( X \) has a binomial distribution with parameters \( n - 2 \) and \( p_1 \).

Corollary 3. Let \( RSC_n = RSC(n,p_1,p_2,p_3) \) be a random spiro chain and \( M_{1,n} \) be the first Zagreb index of a \( RSC_n \), with \( n \geq 2 \). Then
\[ M_{1,n} = 32n - 8. \]
Corollary 4. Let $RSC_n = RSC(n, p_1, p_2, p_3)$ be a random spiro chain and $R_n$ be the Randić index of a $RSC_n$, with $n \geq 2$. Then

$$R_n = 2 - \sqrt{2} + (3/4 - \sqrt{2}/2)X + (1 + \sqrt{2})n,$$

$$\mathbb{E}(R_n) = 2 - \sqrt{2} + \left((3/4 - \sqrt{2}/2)p_1 + 1 + \sqrt{2}\right)n + (\sqrt{2} - 3/2)p_1,$$

$$V(R_n) = (3/4 - \sqrt{2}/2)^2 p_1 (1 - p_1) (n - 2),$$

$$\frac{R_n - \mathbb{E}(R_n)}{\sqrt{V(R_n)}} \xrightarrow{D} N(0,1),$$

where $X$ has a binomial distribution with parameters $n - 2$ and $p_1$.

Corollary 5. Let $RSC_n = RSC(n, p_1, p_2, p_3)$ be a random spiro chain and $S_n$ be the Sombor index of a $RSC_n$, with $n \geq 2$. Then

$$S_n = 8\sqrt{2} - 8\sqrt{5} + (6\sqrt{2} - 4\sqrt{5})X + (4\sqrt{2} + 8\sqrt{5})n,$$

$$\mathbb{E}(S_n) = 8\sqrt{2} - 8\sqrt{5} + \left((6\sqrt{2} - 4\sqrt{5})p_1 + 4\sqrt{2} + 8\sqrt{5}\right)n - 2(6\sqrt{2} - 4\sqrt{5})p_1,$$

$$V(S_n) = (6\sqrt{2} - 4\sqrt{5})^2 p_1 (1 - p_1) (n - 2),$$

$$\frac{S_n - \mathbb{E}(S_n)}{\sqrt{V(S_n)}} \xrightarrow{D} N(0,1),$$

where $X$ has a binomial distribution with parameters $n - 2$ and $p_1$.

Corollary 6. Let $RSC_n = RSC(n, p_1, p_2, p_3)$ be a random spiro chain and $M2_n$ be the second Zagreb index of a $RSC_n$, with $n \geq 2$. Then

$$M2_n = 4X + 40n - 16,$$

$$\mathbb{E}(M2_n) = (4p_1 + 40) n - 8p_1 - 16,$$

$$V(M2_n) = 16p_1 (1 - p_1) (n - 2),$$

$$\frac{M2_n - \mathbb{E}(M2_n)}{\sqrt{V(M2_n)}} \xrightarrow{D} N(0,1),$$

where $X$ has a binomial distribution with parameters $n - 2$ and $p_1$. 

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Remark 3. In fact, we can see that (5) and (6) are obtained in \cite{Jahanbani2020}. Also, we can see that Corollary 5 and (7) are obtained in \cite{ZhangYouLiuHuang2021} and \cite{Raza2020}, respectively.

Remark 4. For \( n \geq 2 \) and \( p_1 \in (0, 1) \), it follows from Corollary 2, 3, 4, 5 and 6 that

\[
E(R_n) \leq E(N_n) \leq E(S_n) \leq E(M_1 n) \leq E(M_2 n) \ (\text{see Figure 3}),
\]

\[
V(R_n) \leq V(N_n) \leq V(S_n) \leq V(M_2 n).
\]

Figure 3: Difference between \( E(R_n), E(N_n), E(S_n), E(M_1 n) \) and \( E(M_2 n) \).

Finally, we conduct a numerical experiment to support the asymptotic behaviors developed in Corollaries 2, 3, 4, 5 and 6. Given a fixed \( p_1 \in (0, 1) \), in each case, we independently generate 5,000 replications of a random spiro chain after \( n = 10,000 \) evolutionary steps. For each simulated random spiro chain, its topological index is computed. The histogram of the sample data with a normal approximation curve are given in Figure 4, 5, 6 and 7.
Figure 4: Histogram of the standardized Nirmala index of 5,000 independently generated random spiro chains with $n = 10,000$; the thick red curve is the estimated density of the sample.

Figure 5: Histogram of the standardized Randić index of 5,000 independently generated random spiro chains with $n = 10,000$; the thick red curve is the estimated density of the sample.

Figure 6: Histogram of the standardized Sombor index of 5,000 independently generated random spiro chains with $n = 10,000$; the thick red curve is the estimated density of the sample.
4 Concluding Remarks

In this paper, we propose a martingale approach to the study of topological indices in random spiro chains. The expected value, variance, exact distribution have been determined. Also, we formulate a martingale to characterize the asymptotic behavior of the topological indices. We show that the same analysis works here if we simply use a martingale central limit theorem instead of a classical central limit theorem. Moreover, we consider some particular topological indices, such as, Nirmala, Sombor, Randić and Zagreb index, in other words, we exploit the martingale approach.

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