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Extremal Topological Indices with Prescribed Degree Sequences

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Abstract. This paper explores the extremal properties and bounds of two significant topological indices in graph theory: the Albertson and Sigma indices, with an emphasis on trees and bipartite graphs. We identify the unique trees that maximize and minimize the Albertson index, including stars and paths, and extend this characterization to bipartite graphs. In this paper, we investigate the sharp upper and lower bounds of topological indices for a given degree sequence $\mathcal{D} = (d_1, d_2, \dots, d_n)$. We derive exact lower and upper bounds for the Albertson index and Sigma index based on a non-increasing degree sequence $\mathcal{D} = (d_1, d_2, \dots, d_n)$. Establishing such bounds is a fundamental challenge in the study of topological indices, as these results reveal inherent relationships among various indices. For generating bipartite graphs and tournaments with prescribed degree sequences, analyzing their mixing times and convergence properties. The sharp upper and lower bounds for the Sigma index based on degree sequences, providing a deeper understanding of its behavior in trees. Our findings offer novel insights into graph irregularity measures, supported by rigorous proofs and computational algorithms for evaluating these indices in random trees and forests. These results contribute to the understanding of extremal properties and combinatorial structures in graph theory, with applications in chemical graph theory and network analysis.

Key words: Trees, Degree sequence, Bipartite graph, Topological indices, Extremal, Irregularity.

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Экстремальные топологические индексы с заданными последовательностями степеней

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Аннотация. Данная статья исследует экстремальные свойства и оценки двух значимых топологических индексов в теории графов: индексов Альбертсона и Сигма, с акцентом на деревья и двудольные графы. Мы идентифицируем уникальные деревья, которые максимизируют и минимизируют индекс Альбертсона, включая звёзды и пути, и расширяем эту характеристику на двудольные графы. В этой работе мы изучаем точные верхние и нижние оценки топологических индексов для заданной последовательности степеней $\mathcal{D} = (d_1, d_2, \dots, d_n)$. Мы выводим точные нижние и верхние оценки для индексов Альбертсона и Сигма на основе неубывающей последовательности степеней $\mathcal{D} = (d_1, d_2, \dots, d_n)$. Установление таких оценок является фундаментальной задачей в изучении топологических индексов, поскольку эти результаты выявляют внутренние взаимосвязи различных индексов. Для генерации двудольных графов и турниров с заданными последовательностями степеней проводится анализ времени смешивания и свойств сходимости. Точные верхние и нижние оценки индекса Сигма на основе последовательностей степеней обеспечивают более глубокое понимание его поведения в деревьях. Наши результаты предлагают новые взгляды на меры структурной нерегулярности графов, подкреплённые строгими доказательствами и вычислительными алгоритмами для оценки этих индексов в случайных деревьях и лесах. Эти результаты способствуют пониманию экстремальных свойств и комбинаторных структур в теории графов с приложениями в химической теории графов и анализе сетей.

Ключевые слова: деревья, последовательность степеней, двудольный граф, топологические индексы, экстремальность, нерегулярность.

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1 Introduction

Throughout this paper. Let $G = (V, E)$ be a simple, connected graph, where $n = |V(G)|$, $m = |E(G)|$. The *degree* of a vertex w in G, denoted by $d_G(w)$, is the number of vertices adjacent to w. One of the earliest and most influential measures of graph irregularity is the *Albertson index*, introduced in [2], and defined for a simple graph $G = (V, E)$ as:

$$\operatorname{irr}(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|. \tag{1}$$

where $d_G(u)$ denotes the degree of vertex u. This index captures local disparities between adjacent vertex degrees and has inspired numerous variants and generalizations [1, 3].

Parallel foundational contributions by Harary [7] and Chen [13] provided combinatorial frameworks that laid the groundwork for modern graph descriptors. To further enrich the understanding of irregularity, global measures such as the *total irregularity* $\operatorname{irr}_T(G)$ have been proposed [1], satisfying inequalities that relate them to local measures (e.g., $\operatorname{irr}_T(G) \le (n-2)\operatorname{irr}(G)$ for trees [8]). More recently, the *Sigma index* was introduced as a quadratic analogue of the Albertson index [15], defined by:

$$\sigma(G) = \sum_{uv \in E(G)} (d_G(u) - d_G(v))^2 = F(G) - 2M_2(G),$$

where $F(G)$ is the sum of squared degrees over all edges, and $M_2(G)$ is the second Zagreb index. This formulation amplifies large degree differences and provides a more sensitive measure of irregularity. Beyond general graphs, significant research has concentrated on trees with specified degree sequences. Molloy and Reed [17] and Broutin and Marckert [9] investigated the asymptotic properties of such trees, while Zhang et al. [18] studied their realizability and enumeration under degree constraints. These findings have been crucial in the analysis of extremal irregularity measures within structured families of trees.

Let $\mathcal{D} = (d_1, d_2, \dots, d_{n-1}, d_n)$ be a degree sequence where $d_n \geqslant d_{n-1} \geqslant \cdots \geqslant d_2 \geqslant d_1$, and $\mathcal{A} = (a_1, a_2, \dots, a_r)$ be a degree sequence from $\mathcal{D}$ where $a_1 = (d_2 + d_1)/2, a_2 = (d_3 + d_2)/2, \dots, a_r = (d_n + d_{n-1})/2$. Among these, *caterpillar trees*—distinguished by a linear spine with pendant vertices attached—are prominent in chemical graph theory owing to their manageable structure, which facilitates explicit analytical formulations.

This paper is organized as follows. In Section 2, we review the important concepts relevant to our work, including a literature survey of the most related papers. Section 3 had presented the Albertson index among extremal trees. Section 4 had presented Sigma index among extremal trees. Section 5 had provide the effect of topological indices on each other in order to determine the behaviour of these indices.

2 Preliminaries

In this section, we review the most important basic concepts that we will use in establishing this research. Yang and Deng [19] had presented the terms $1 \le p \le n-3$

for caterpillar tree, then, $\Delta(G) = n-1$. Through [16] consider for any connected simple graph G has not satisfied with the null graphs and path graphs, the Albertson index satisfy $\mathrm{irr}(G^*) = \mathrm{irr}(G) + 2$. For Caterpillar tree [11] with path vertices and degrees $d_1, d_2, \ldots, d_n$, the Albertson index satisfy

$$\mathrm{irr}(G) = (d_n - 1)^2 + (d_1 - 1)^2 + \sum_{i=2}^{n-1} (d_i - 1)(d_i - 2) + \sum_{i=1}^{n-1} |d_i - d_{i+1}|. \quad (2)$$

According to (1), we consider the Albertson index had given by (2), where the graph G be a regular graph. Equivalent to the basic definition in (1), Proposition 2.1 illustrates this relationship through both vertices and edges.

Proposition 2.1 ([6]): Let G be a simple graph with vertices set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Then, the Albertson index satisfy

$$\mathrm{irr}(G) = \sum_{\{u,v\}\subseteq V(G)} |d_G(u) - d_G(v)|, \quad \mathrm{irr}(G) = n\sum_{i=1}^{n} d_G(v_i)^2 - 4m^2. \quad (3)$$

By computing constraints on all degree sequences of n-vertex graphs, the degree sequence that maximizes in (4) by considering (3) this bound corresponds to a graph G with a maximum irregularity. Using variance, Mandal et al. in [16] showed:

$$\mathrm{irr}(G) \leq \sqrt{m\left(\sum_{i=1}^{n} d_i^2\right) - 4m^2}, \quad (4)$$

For a vertices set $V(T) = \{v_0, v_1, \ldots, v_n\}$ where the degree of center vertex v_0 satisfy $d_T(v_0) = d_T(v_i)_{i>0} + 1$. Furthermore, by Lemma 2.2, we established Albertson index with certain terms included for (1).

Lemma 2.2 ([11, 12]): Let be T tree of order $n \geqslant 5$, a degree sequence $d = (d_1, d_2, d_3, d_4, d_5)$ where $d_5 \geqslant d_4 \geqslant d_3 \geqslant d_2 \geqslant d_1$, then Albertson index among tree T is:

$$\mathrm{irr}(T) = d_1^2 + d_n^2 + \sum_{i=2}^{n-1} |d_i - d_{i+1}| + \sum_{i=2}^{4} (d_i + 2)(d_i - 1) - 2. \quad (5)$$

During our study of the Sigma index through this paper, we will not use the traditional definition but will instead use the relation obtained for extremal tree from Theorem 2.3, which is associated with degree sequence $\mathcal{D}$.

Theorem 2.3 ([11]): Let T be a tree of order n, and let $\mathcal{D} = (d_1, \ldots, d_n)$ be a degree sequence such that $d_n \geqslant \cdots \geqslant d_1$. Then, the Sigma index of the tree T is given by:

$$\sigma(T) = \sum_{i\in\{1,n\}} (d_i + 1)(d_i - 1)^2 + \sum_{i=2}^{n-1} (d_i + 2)(d_i - 1)^2 + \sum_{i=2}^{n-1} (d_i - d_{i+1})^2 + 2n - 2.$$

3 Extremal Value of Albertson Index

In this section, a *spider* is a tree containing at most one vertex of degree greater than 2, called *the center* [4]. If no vertex exceeds degree 2, any vertex with degree 2 may serve as the center, as in the case of *a path*. A *leg* of the spider is defined as the path from the center to a pendant vertex. This leg is termed short if its length is 1; otherwise, it is called long. Let $\mathcal{G}$ be a class of graphs, we define the maximum and minimum value of Albertson index as

$$\begin{cases} \mathrm{irr}_{\max} = \{\max \mathrm{irr}(G) \mid G \in \mathcal{G}\}, \\ \mathrm{irr}_{\min} = \{\min \mathrm{irr}(G) \mid G \in \mathcal{G}\}. \end{cases} \tag{6}$$

Maximum and minimum Albertson index for trees had provide among Proposition 3.1 for the unique maximizer and the unique minimizer.

Proposition 3.1: Let $\mathcal{T}_n$ denote the set of all trees with $n \geq 2$ vertices. Then,

$$\mathrm{irr}_{\max}(\mathcal{T}_n) = (n-1)(n-2),$$

$$\mathrm{irr}_{\min}(\mathcal{T}_n) = \begin{cases} 0 & \text{if } n = 2, 3, \\ 2\left\lfloor \frac{n}{2} \right\rfloor - 2 & \text{if } n \geq 4. \end{cases}$$

The unique maximizer is the *star* S_n, while for $n \geq 4$, the unique minimizer is the *path* P_n.

Proof. Assume $\mathcal{T}_n$ denote the set of all trees with $n \geq 2$ vertices. Then, for determine $\mathrm{irr}_{\max}(\mathcal{T}_n)$ and $\mathrm{irr}_{\min}(\mathcal{T}_n)$ should be divided into the following cases:

Case 1: Maximum. Since a tree on n vertices has exactly $n-1$ edges, each edge uv contributes at most $n-2$ to $\mathrm{irr}(T)$ because $\left|d(u) - d(v)\right| \leqslant n-2$. Equality holds if and only if $\{d(u), d(v)\} = \{1, n-1\}$. The star S_n has one vertex of degree $n-1$ and $n-1$ leaves each of degree 1, so every edge contributes exactly $\left|d(u) - d(v)\right| = n-2$. Hence, according to (6) it satisfies

$$\mathrm{irr}(S_n) = (n-1)(n-2). \tag{7}$$

Actually, no other tree can exceed this since no edge can contribute more than $n-2$ (furthermore, see Table 1).

Case 2: Minimum. In this case, for $n = 2$, the unique tree K_2 is regular with degree 1, so $\mathrm{irr} = 0$. For $n = 3$, the only tree is P_3 with degrees $(1, 2, 1)$ and $\mathrm{irr}(P_3) = 2$, which is minimal. For $n \geq 4$, it is established that the path P_n uniquely attains the minimum Albertson index.

In P_n, exactly two vertices have degree 1 (the leaves), and all others have degree 2. Two edges incident to leaves contribute 1 each. The remaining $n-3$ edges connect two degree-2 vertices, contributing 0 each. Thus,

$$\mathrm{irr}(P_n) = 2\left\lfloor \frac{n}{2} \right\rfloor - 2, \quad \text{for } n \geq 4, \tag{8}$$

which accounts for the linear growth of degree differences along the path. Therefore, the bound according to (7) and (8) is sharp and uniquely attained by P_n. □

One of the most important challenges in examining topological indices lies in determining the extremal values for each of the topological indices. This requires us to compare the numerical effects according to the values of the topological indices. According to (7), we observe that among the Table 1 to determine explicit calculations for small values of n.

Table 1

Calculations for small values of n

n	Star S_n	Degrees	Number of edges	Contribution per edge	$irr(S_n)$
2	$K_{1,1}$	$\{1,1\}$	1	$1-1=0$	$1\cdot 0=0$
3	$K_{1,2}$	$\{2,1,1\}$	2	$2-1=1$	$2\cdot 1=2$
4	$K_{1,3}$	$\{3,1,1,1\}$	3	$3-1=2$	$3\cdot 2=6$
5	$K_{1,4}$	$\{4,1,1,1,1\}$	4	$4-1=3$	$4\cdot 3=12$
6	$K_{1,5}$	$\{5,1,1,1,1,1\}$	5	$5-1=4$	$5\cdot 4=20$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
n	S_n	$\{n-1,\ 1^{n-1}\}$	$n-1$	$n-2$	$(n-1)(n-2)$

3.1 Minimum Value of Albertson Index

Let Δ be the maximum value of a spider tree T where $T \in \mathcal{T}_{n,\Delta}$. Then, the minimum value of Albertson index bounded by (0,1) through Proposition 3.2 and 3.3.

Proposition 3.2: Let $T \in \mathcal{T}_{n,\Delta}$. Then, the Albertson index satisfy $irr(T) = (\Delta^2 + p^2) - (\Delta + p)$, where p denotes number of short legs.

Proposition 3.3: Let T be a tree of order n with degree sequence $\mathcal{D} = (d_1, d_2, \dots, d_n)$. Then the minimum value of the Albertson index satisfies

$$0 < \frac{2\,irr_{min}}{\Delta(\Delta-1)^2} < 1. \tag{9}$$

Now, we established the value $\alpha = (d_1 + d_2)/2$ and $\beta = (d_{n-1} + d_n)/2$ for determine the behavior of the minimum value of the Albertson index.

Proposition 3.4: Let T be a tree of order n with degree sequence $\mathcal{D} = (d_1, d_2, \dots, d_n)$ and integers α and β. Then

$$\frac{\beta m(m+1)}{\alpha} + \alpha\, irr_{min}(T) \geqslant \sum_{i=1}^{n} d_i^3. \tag{10}$$

Proof. Assume a degree sequence $\mathcal{D} = (d_1, d_2, \dots, d_n)$ ordered such that $d_n \geqslant d_{n-1} \geqslant \cdots \geqslant d_2 \geqslant d_1$. Consider a connected graph T with n vertices and m edges satisfying $irr_{min} < m(m+1)$. By (6), the minimum Albertson index satisfies $2^{\alpha} m(m+1) \leqslant \alpha^4\, irr_{min}(T)$, which implies

$$\alpha\, irr_{min}(T) \geqslant \sum_{i=1}^{n} d_i^2. \tag{11}$$

Since $\beta < 2^\alpha$ and $\operatorname{irr}_{\min} < m(m+1)$, relation (11) yields $\operatorname{irr}_{\min} \leqslant n(2m-n+\Delta)$, where $0 < \operatorname{irr}_{\min}/2^\alpha < n$. This condition restricts α to satisfy Equation (10).

This restriction directly influences Equation (12), paving the way to the desired result:

$$\frac{\beta m(m+1)}{\alpha} \geqslant \sum_{i=1}^{n} d_i^2, \quad \frac{\beta m(m+1)}{\alpha} + 2^\alpha m(m+1) \geqslant \alpha^4 \operatorname{irr}(T). \tag{12}$$

From (12), and using $2^{-\alpha}\operatorname{irr}_{\min} < n$ (which ensures $2^\alpha m(m+1) > \alpha \operatorname{irr}_{\min}(T)$), we obtain

$$\frac{\beta m(m+1)}{\alpha} + 2^\alpha m(m+1) \geqslant \sum_{i=1}^{n} d_i^3. \tag{13}$$

Combining (13) with (12) and (11) confirms that Equation (10) holds. □

3.2 The Optimal Behavior of Albertson Index Among Set of Trees

In this subsection, we extended the discussion among subsection 3.1. Thus, we emphasize that the optimal behavior [10] of Albertson index satisfy

- Caterpillar $\mathcal{C}(n,m)$ (m pendants): $\operatorname{irr} = m(m+1)n - 2m + 2$
- Identity with Zagreb index: $\operatorname{irr}(T) = \sum(d_u + d_v) - 2M_1(T) = 2(n-1) - 2M_1(T)$

Among trees with degree sequence $\mathcal{D}$, maximum irr is achieved by the "greedy caterpillar" (attach leaves to highest-degree vertices possible), minimum by the most balanced tree. Through Lemma 3.5 we presented the upper bound of Albertson index.

Lemma 3.5: Let T be a tree with $n = |V(T)|, m = |E(T)$ with the maximum degree Δ and the minimum degree $\delta \geqslant 1$ and $0 \leq \alpha \leq 1$. Then, the upper bound of Albertson index is

$$\operatorname{irr}(T) \leq \left\lfloor \frac{3n^2 - 10n}{2} \right\rfloor 2^\alpha + \Delta^2 - n\delta.$$

Proof. Let T be a tree with maximum degree $\Delta \geqslant 3$. Then, by considering $\Delta > \delta$, we find that $\operatorname{irr}(T) \leq 3(\Delta^2 - n)$. The upper bound is given by:

$$\operatorname{irr}(T) \leq \left\lfloor \frac{3n^2}{\Delta} \right\rfloor. \tag{14}$$

If T is a star tree $\mathcal{S}_n$, then we know $\operatorname{irr}(\mathcal{S}_n) = (n-1)(n-2)$. In this case, by considering $0 \leq \alpha \leq 1$, where each edge of the star is adjacent to every other edge at the central vertex, we have

$$\alpha \geq \log_2 \left(\frac{(n-1)(n-2) - \Delta^2 + n}{\left\lfloor \frac{3n^2 - 10n}{2} \right\rfloor} \right).$$

Evaluating inequality (14), it holds across the range of α as

$$\operatorname{irr}(\mathcal{S}_n) \leq \left\lfloor \frac{3n^2 - 10n}{2} \right\rfloor 2^\alpha + \Delta^2 - n. \tag{15}$$

Now, if T is a path $\mathcal{P}_n$, each end vertex is connected to a vertex of degree 2, contributing all pairs of adjacent vertices. We have $\mathrm{irr}(\mathcal{P}_n) = 2$. To provide a bound for all vertices, from (14) we get

$$\mathrm{irr}(\mathcal{P}_n) \leq \left\lfloor \frac{3n^2 - 10n + \Delta^2}{\Delta} \right\rfloor. \tag{16}$$

Let $\alpha = n/(\Delta^2 - 1)$. Then, the term 2^n describes the growth of the bounds (14) and (16). For this case, the term $1 \leq 2^{n/(\Delta^2-1)} \leq 2$ governs the growth of the Albertson index bounds. Since Δ is typically positive and $\Delta > \delta$, we need to prove the bound

$$\mathrm{irr}(\mathcal{P}_n) \leq \left\lfloor \frac{3n^2 - 10n}{2} \right\rfloor 2^{\alpha} + \Delta^2 - n. \tag{17}$$

In this case, we need to determine if

$$\left\lfloor \frac{3n^2}{\Delta} \right\rfloor - \left\lfloor \frac{3n^2 - 10n + \Delta^2}{\Delta} \right\rfloor \tag{18}$$

satisfies the required relationship. Let us define $a = 3n^2/\Delta$, $b = 10n/\Delta$, and $c = \Delta$. Then, we have $a = \lfloor a \rfloor + \{a\}$ where $0 \leq \{a\} < 1$. Thus,

$$\begin{aligned} \lfloor a \rfloor - \lfloor a - b + c \rfloor &= \lfloor a \rfloor - \lfloor \lfloor a \rfloor + \{a\} - b + c \rfloor \\ &= \lfloor a \rfloor - \lfloor a \rfloor - \lfloor \{a\} - b + c \rfloor \\ &= -\lfloor \{a\} - b + c \rfloor. \end{aligned}$$

Therefore, the bound (18) holds if

$$\left\lfloor \frac{3n^2}{\Delta} - \frac{10n}{\Delta} + \Delta \right\rfloor > 0. \tag{19}$$

Thus, the additional terms in the bound (17) are valid, so that the term $\Delta^2 - n$ satisfies

$$\mathrm{irr}(T) \leq \left\lfloor \frac{3n^2}{\Delta} \right\rfloor + \Delta^2 - n. \tag{20}$$

As desired. □

Furthermore, among Lemma 3.6 we provide an upper bound of T with Albertson index among T.

Lemma 3.6: Let $T \in \mathcal{T}_{n,\Delta}$ such that $T \ncong \mathcal{S}_n$. Then, $\mathrm{irr}(T) \geq \mathrm{irr}(\mathcal{P}_n)$ if and only if $T \cong \mathcal{P}_n$.

Proof. Assume $T \cong \mathcal{S}_n$, where $\mathrm{irr}(\mathcal{S}_n) = (n-1)(n-2)$. Then $\mathrm{irr}(T) \geq \mathrm{irr}(\mathcal{S}_n)$. Now, suppose $T \in \mathcal{T}_{n,\Delta} \backslash \{\mathcal{S}_n\}$ with vertex set $V(T) = \{v_0, v_1, \ldots, v_i, \ldots, v_{k-i-1}, v_{k-i}, \ldots, v_k\}$ such that there exists a vertex $v_\ell \neq v_0$ where $d_T(v_\ell) = \lambda \geqslant 3$.

If $T \cong \mathcal{P}_n$ with $n \geq 3$ vertices, it has two endpoints of degree 1, and $n-2$ internal vertices of degree 2. Then, we have $\mathrm{irr}(T) \geq \mathrm{irr}(\mathcal{P}_n)$. Consider a tree T' with vertex set $V(T') = \{v_1, \ldots, v_i, \ldots, v_{k-i-1}, v_{k-i}, \ldots, v_k\}$, a subset of $V(T)$. Then,

$$\begin{aligned}
\mathrm{irr}(T)-\mathrm{irr}(T') &= \sum_{uv\in E(T)} |d_T(u)-d_T(v)| - \sum_{uv\in E(T')} |d_{T'}(u)-d_{T'}(v)| \\
&= \sum_{i=0}^{k/2} |d(v_i)-d(v_{k-i})| - \sum_{i=1}^{(k+1)/2} |d(v_i)-d(v_{k-i+2})| \\
&= |d_T(v_0)-d_T(v_1)| + \cdots + |d_T(v_i)-d_T(v_{k-i-1})| + \cdots + \\
&+ |d_T(v_{k-1})-d_T(v_k)| - \big(|d_{T'}(v_1)-d_{T'}(v_2)| + \cdots + \\
&+ |d_{T'}(v_i)-d_{T'}(v_{k-i-1})| + \cdots + +|d_T(v_{k-1})-d_{T'}(v_k)|\big) + \\
&+ (d_T(v_0)+1)|d_T(v_0)-1| + \sum_{i=1}^{k-1}(d_T(v_i)+2)|d_T(v_i)-1| \\
&\quad + (d_T(v_k)+1)|d_T(v_k)-1| \\
&\quad - \Big((d_{T'}(v_1)+1)|d_{T'}(v_1)-1| + \sum_{i=2}^{k-1}(d_{T'}(v_i)+2)|d_{T'}(v_i)-1| \\
&\quad + (d_{T'}(v_k)+1)|d_{T'}(v_k)-1|\Big) \\
&= |d_T(v_0)-d_T(v_1)| + (d_T(v_0)+1)|d_T(v_0)-1| \\
&= \lambda^2+\lambda-1 \\
&> 0.
\end{aligned}$$

Suppose that $N_T(v_i)=\{v_{i-1},v_{i+1},v_{i1},\dots,v_{ik}\}$. Then, for the path $v_iv_{i1},v_iv_{i2},\dots,v_iv_{ik}$, we notice that $\mathrm{irr}(T)-\mathrm{irr}(T')>\lambda>0$.

A path $\mathcal{P}_n$ has degrees $d(v_1)=d_T(v_k)=1$ and $d(v_2)=\cdots=d_T(v_{k-1})=2$. Then, we have $\mathrm{irr}(\mathcal{P}_n)=2$. Thus, by considering $T\in\mathcal{T}_{n,\Delta}$, we obtain $\mathrm{irr}(T)\geq\mathrm{irr}(\mathcal{P}_n)$ if and only if $T\cong\mathcal{P}_n$. This completes the proof. □

Lemma 3.7: Let $T\in\mathcal{T}_{n,\Delta}$. Then, consider $v_0\in V(T)$ be a vertex with maximum degree Δ. For any vertex v_ℓ in T, different from v_0, where $d(v_\ell)\geqslant 3$ satisfy

$$2^\lambda \leq \mathrm{irr}(T) \leq (n-1)(n-2)^\lambda.$$

The lower bound holds if and only if $T\cong\mathcal{P}_n$. The upper bound holds if and only if $T\cong S_n$.

Now, the maximum value and minimum value of Albertson index among bipartite graph had presented by Theorem 3.8. It is depended on terms of both partition in G.

Theorem 3.8: Let G be a bipartite graph where $n_1\leq 2n_2$. Let $\lambda>0$ be given as:

$$\lambda=\frac{4}{3}n_1-\sqrt{\frac{28}{9}n_1^2-\frac{8}{3}n_2n_1}, \tag{21}$$

where the Albertson index is given by:

$$\mathrm{irr}_{\{n_1,n_2\}}(G)=\frac{3}{4}\lambda^3+\frac{n_2}{2^{n_2}}\lambda^{n_2}+\frac{\lambda n_2^2}{2}. \tag{22}$$

Then, the maximum and minimum values of the Albertson index are:

$$\mathrm{irr}(G) = \begin{cases} \mathrm{irr}_{\max}(G) = \frac{1}{108}\left(4n_1 - \sqrt{28n_1^2 - 24n_1n_2}\right)^3 + \alpha n_1^2 - \alpha^2 n_1, \\ \mathrm{irr}_{\min}(G) = \frac{4}{3}n_1 - \sqrt{\frac{28}{9}n_1^2 - \frac{8}{3}n_2n_1}, \end{cases} \tag{23}$$

where $\alpha = n_2 - \frac{4}{3}n_1 + \frac{1}{3}\sqrt{28n_1^2 - 24n_1n_2}$.

Proof. Let G be a bipartite graph. The Albertson index of G, given in (22) and derived from Equation 21, satisfies the following maximum and minimum values:

$$\mathrm{irr}(G) = \begin{cases} \mathrm{irr}_{\max}(G) = \frac{1}{2}(n_2 - u_2), \\ \mathrm{irr}_{\min}(G) = n_2 - \frac{4}{3}n_1 + \sqrt{\frac{28}{9}n_1^2 - \frac{8}{3}n_1n_2}. \end{cases} \tag{24}$$

From (24) and (22), for the term $(n_2 - u_2) \neq 0$, it follows that $28n_1^2 - 24n_1n_2 > 0$. Consequently, since $u_2 = n_2 - \frac{4}{3}n_1 + \sqrt{\frac{28}{9}n_1^2 - \frac{8}{3}n_1n_2}$, we observe that $u_2n_1^2 > 0$ and $u_2^2n_1 > 0$. Thus, the Albertson index satisfies:

$$\mathrm{irr}(G) = \frac{1}{4}(n_2 - u_2)^3 + u_2n_1^2 - u_2^2n_1. \tag{25}$$

This expression is complex due to the cubic term and the square root in u_2. The Albertson index in (25) satisfies $\mathrm{irr}(G) \geqslant \min\{n_1, n_2\}$, given that $\max\{n_1, n_2\} \geqslant \min\{n_1, n_2\}$. Assume $u_2 = n_2 - \frac{4}{3}n_1 + \frac{1}{3}\sqrt{28n_1^2 - 24n_1n_2}$, where $\frac{1}{3}\sqrt{28n_1^2 - 24n_1n_2} > 0$ and $u_2 \neq 0$. Define $\alpha = u_2$. Then:

$$\alpha n_1^2 - \alpha^2 n_1 \geqslant \max\{n_1, n_2\} > 0. \tag{26}$$

Therefore, from (21) and (25), the maximum value of the Albertson index is:

$$\mathrm{irr}_{\max}(G) = \frac{1}{108}\left(4n_1 - \sqrt{28n_1^2 - 24n_1n_2}\right)^3 + \alpha n_1^2 - \alpha^2 n_1. \tag{27}$$

For the minimum value of the Albertson index, referring to (24), we have:

$$\mathrm{irr}_{\min}(G) = n_2 - \frac{4}{3}n_1 + \sqrt{\frac{28}{9}n_1^2 - \frac{8}{3}n_1n_2}.$$

When $n_1 < 2n_2$, it follows from (21) that for some parameter $\lambda > 0$:

$$\lambda \leqslant \min\{n_1, n_2\}. \tag{28}$$

Thus, from (27) and (28), Equation (24) holds as:

$$\mathrm{irr}(G) = \begin{cases} \mathrm{irr}_{\max} = \max\left\{\frac{1}{2}(n_2 - u_2)\right\}, \\ \mathrm{irr}_{\min} = \min\left\{n_2, n_2 - \frac{4}{3}n_1 + \sqrt{\frac{28}{9}n_1^2 - \frac{8}{3}n_1n_2}\right\}. \end{cases} \tag{29}$$

Finally, by determining the maximum value of the Albertson index in (27) and based on the conditions given in (24)–(29), the minimum value of the Albertson index is achieved as shown in (23), completing the proof. □

Theorem 3.9: Let T be a tree with n vertices and m edges. Then, the upper bound for the Albertson index satisfies

$$\mathrm{irr}(T) \leqslant \alpha\left\lfloor \frac{2n}{3} \right\rfloor + \beta\left\lceil \frac{2n+1}{3} \right\rceil. \tag{30}$$

Proof. Immeditaly, from Lemma 3.5, the lower bound of the Albertson index satisfy

$$\sqrt{\Delta(\Delta-1)^2} \leqslant \left\lfloor \frac{2n}{3} \right\rfloor + \left\lceil \frac{2n+1}{3} \right\rceil < \mathrm{irr}(T). \tag{31}$$

Then, from (31) satisfy

$$\left\lceil \frac{2n+1}{3} \right\rceil = \begin{cases} m+1, & \text{if } n < 1, \\ m+2, & \text{if } n \geqslant 1. \end{cases} \tag{32}$$

It holds for the sum in (31) as

$$\left\lfloor \frac{2n}{3} \right\rfloor + \left\lceil \frac{2n+1}{3} \right\rceil = m + \left\lceil \frac{2n+1}{3} \right\rceil = \begin{cases} 2m+1, & n < 1, \\ 2m+2, & n \geqslant 1. \end{cases} \tag{33}$$

Thus, from (32) and (33) we find that according to (31), it holds that $\sqrt{\Delta(\Delta-1)^2} \leqslant n+1 < \mathrm{irr}(T)$. Then,

$$\mathrm{irr}(T) \geqslant \alpha\left\lfloor \frac{2n}{3} \right\rfloor + \sqrt{\Delta(\Delta-1)^2}, \quad \mathrm{irr}(T) \geqslant \beta\left\lceil \frac{2n+1}{3} \right\rceil + \sqrt{\Delta(\Delta-1)^2}. \tag{34}$$

Finally, from (34) we conclude that (31) holds. □

4 Extremal Value of Sigma Index

In this section, we presented the study of extremal value among Sigma index. We start with Lemma 4.1 for the constant term $2\Delta(\Delta-1)$.

Lemma 4.1: Let T be a tree, let $\mathcal{D}(d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ with the maximum degree Δ and the minimum degree $\delta \geqslant 2$. Then, the upper bound of Sigma index satisfy

$$\sigma(T) \leqslant \left\lfloor \frac{3n}{5} \right\rfloor \left\lceil \frac{2n}{5} \right\rceil \frac{2nm}{\Delta(\Delta-1)^2} + \delta\sqrt{\frac{nm}{2\Delta(\Delta-1)}} + \frac{1}{2}(n^2+m^2) + n(m-\Delta)^2. \tag{35}$$

Proof. Recall $\mathcal{D}(d_1, d_2, \ldots, d_n)$ is a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ with maximum degree Δ and minimum degree $\delta \geqslant 2$. Let us have the following parameters α, β, and γ, where

$$\alpha = \left\lfloor \frac{3n}{5} \right\rfloor \left\lceil \frac{2n}{5} \right\rceil, \quad \beta = \frac{1}{2}(n^2+m^2), \quad \gamma = n(m-\Delta).$$

We observe that $\beta \geqslant \alpha + \gamma$. Thus, $\alpha \leqslant n\Delta + m$ and $\beta \geqslant (m-1)^2 + 3n$. Additionally, the bound in terms of n, m, and Δ satisfies

$$3 < \sqrt{\frac{nm}{2\Delta(\Delta-1)}} < 4, \quad \text{where} \quad 0 < \frac{2nm}{\Delta(\Delta-1)^2} < 2.$$

Since $\mathcal{D}$ is ordered as $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, the degrees in tree T satisfy $d_T(v_1) > d_T(v_2) \geqslant \cdots \geqslant d_T(v_{n-1}) > d_T(v_n)$. Assume $d_T(v_2) = \cdots = d_T(v_{n-1}) = k$. Then, the Sigma index is

$$\sigma(T) = d_1(d_1 - k)^2 + d_n(k - d_n)^2,$$

since all neighbors of v_1 and v_n have degree k. Hence,

$$\sigma(T) \leqslant \alpha \sum_{v_i \in N(v_1)} (d_T(v_1) - k)^2 + \gamma \sum_{v_i \in N(v_n)} (k - d_T(v_n))^2.$$

Considering equations (4), the lower bound for $\sigma(T)$ in terms of α, β, and γ is

$$\sigma(T) \geqslant \left\lfloor \frac{3n}{5} \right\rfloor \left\lceil \frac{2n}{5} \right\rceil \frac{2nm}{\Delta(\Delta-1)^2} + \sum_{v_i \in N(v_1)} (d_T(v_1) - \alpha)^2 + \sum_{v_i \in N(v_n)} (\gamma - d_T(v_n))^2.$$

Under the conditions

$$3 < \sqrt{\frac{nm}{2\Delta(\Delta-1)}} < 4, \quad 0 < \frac{2nm}{\Delta(\Delta-1)^2} < 2,$$

these yield the desired lower bound

$$\sigma(T) \leqslant \left\lfloor \frac{3n}{5} \right\rfloor \left\lceil \frac{2n}{5} \right\rceil \frac{2nm}{\Delta(\Delta-1)^2} + \frac{(n^2+m^2)\sqrt{\frac{nm}{2\Delta(\Delta-1)}}}{2},$$

which, combined with $n(m - \Delta)$, gives the sharp upper bound for $\sigma(T)$. □

In next theorem, we established Sigma index by Theorem 2.3. Thus, we observe that The lower bound of Sigma index among Theorem 4.2 for degree sequence ordered such that $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$.

Lemma 4.2: Let T be a tree with n vertices and m edges. Let $\mathcal{D}(d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. The lower bound of Sigma index satisfies

$$\sigma(T) \geqslant \sum_{i=1}^{n-1} (d_i - d_{i+1})^3 + \sum_{i=2}^{n-2} (d_i - d_{i+1})^2 + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m)^2}{5} \right\rfloor. \tag{36}$$

Proof. Assume $\mathcal{D}(d_1, d_2, \ldots, d_n)$ is a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. To establish the lower bound for the Sigma index in equation (36), we use mathematical induction. We first verify it for $n = 4, 5, 6$.

For $n = 4$,

$$\sigma(T) \geqslant \sum_{i=1}^{n-1} (d_i - d_{i+1})^3 + \sum_{i=2}^{n-2} (d_i - d_{i+1})^2 + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m)^2}{5} \right\rfloor - n. \tag{37}$$

For $n = 5$,

$$\sigma(T) \geqslant \sum_{i=1}^{n-1}(d_i - d_{i+1})^3 + \sum_{i=2}^{n-2}(d_i - d_{i+1})^2 + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m)^2}{5} \right\rfloor - 2n. \tag{38}$$

For $n = 6$,

$$\sigma(T) \geqslant \sum_{i=1}^{n-1}(d_i - d_{i+1})^3 + \sum_{i=2}^{n-2}(d_i - d_{i+1})^2 + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m)^2}{5} \right\rfloor - 3n. \tag{39}$$

Equations (37)–(39) confirm the bound for $n = 4, 5, 6$, given $m = n - 1$.
Assume the bound holds for n. To prove it for $n + 1$,

$$\begin{aligned}
\sigma(T) &\geqslant \sum_{i=1}^{n-1}(d_i - d_{i+1})^3 + \sum_{i=2}^{n-2}(d_i - d_{i+1})^2 + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m)^2}{5} \right\rfloor \\
&\geqslant \sum_{i=2}^{n-2}(d_i - d_{i+1})^3 + \sum_{i=1}^{n-3}(d_i - d_{i+1})^2 + d_1^2 + d_{n-1}^2 + d_n^2 + \left\lfloor \frac{2(n+m-2)^2}{5} \right\rfloor \\
&\geqslant \sum_{i=2}^{n}(d_i - d_{i+1})^3 + \sum_{i=3}^{n-1}(d_i - d_{i+1})^2 + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m-2)^2}{5} \right\rfloor \\
&\geqslant \sum_{i=3}^{n+1}(d_i - d_{i+1})^3 + \sum_{i=4}^{n}(d_i - d_{i+1})^2 + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m-3)^2}{5} \right\rfloor.
\end{aligned}$$

Since $(d_i - d_{i+1})^3 \geq 0$ for non-increasing $d_1 \geqslant \cdots \geqslant d_n$, the bound extends, yielding

$$\sigma(T) \geqslant n(d_i - d_{i+1})^3_{i\geqslant 1} + n(d_i - d_{i+1})^2_{i\geqslant 2} + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m-i)^2_{i\leqslant m}}{5} \right\rfloor. \tag{40}$$

Thus, equations (39) and (40) establish the bound for all $n \geq 4$. □

4.1 The Behaviour of Extremal Value Among Sigma Index

The Sigma index is a degree-based topological index in graph theory, commonly used to measure irregularity, complexity, or structural information of trees and graphs. Establishing bounds like this one is crucial for understanding extremal properties, especially in trees where degree sequences largely determine the structure. This lower bound in Theorem 4.3 aids researchers in analyzing trees' topological indices by enabling estimation or restriction of the Sigma index using easily accessible degree data and global tree parameters.

Theorem 4.3: Let T be a tree with n vertices, m edges, and the maximum degree Δ. Let $\mathcal{D} = (d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. The lower bound of the Sigma index satisfies

$$\sigma(T) \geqslant d_1^3 + d_n^3 + \sum_{i=2}^{n-1}(d_i - d_{i+1})^4 + \left\lfloor \frac{2n-1}{2} \right\rfloor \left\lceil \frac{3n-2}{3} \right\rceil + \frac{1}{2}n\Delta. \tag{41}$$

Proof. Assume $\mathcal{D}(d_1, d_2, \ldots, d_n)$ is a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. Then, according to Theorem 4.2 we find that

$$\sigma(T) \geqslant \sum_{i=1}^{n-1}(d_i - d_{i+1})^4 + \sum_{i=2}^{n-2}(d_i - d_{i+1})^3.$$

Thus,

$$\sigma(T) \geqslant d_1^3 + d_n^3 + \sum_{i=2}^{n-1}(d_i - d_{i+1})^4. \tag{42}$$

Therefore,

$$\sigma(T) \geqslant \sum_{i=1}^{n-1}(d_i - d_{i+1})^3 + \sum_{i=2}^{n-2}(d_i - d_{i+1})^2 + d_1^3 + d_n^3. \tag{43}$$

Hence, from (42) and (43), we find that, for the value of n,

$$\sigma(T) \geqslant d_1^3 + d_n^3 + \left\lfloor \frac{2n-1}{2} \right\rfloor \left\lceil \frac{3n-2}{3} \right\rceil + \frac{1}{2}n\Delta. \tag{44}$$

Here, through relations (42), (43), and (44), relation (41) is satisfied for specific values of n. Therefore, suppose it holds for all values of n, and let us prove its validity for $n+1$. In this case, we find that relation (41) holds:

$$\begin{aligned}
\sigma(T) &\geqslant d_1^3 + d_n^3 + \sum_{i=2}^{n-1}(d_i - d_{i+1})^4 + \left\lfloor \frac{2n-1}{2} \right\rfloor \left\lceil \frac{3n-2}{3} \right\rceil + \frac{1}{2}n\Delta \\
&\geqslant d_1^3 + d_2^3 + d_{n-1}^3 + \sum_{i=1}^{n-2}(d_i - d_{i+1})^4 + \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-3}{3} \right\rceil + \frac{1}{2}n\Delta \\
&\geqslant d_1^3 + d_n^3 + d_{n-1}^3 + \sum_{i=3}^{n}(d_i - d_{i+1})^4 + \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n-2}{3} \right\rceil + \frac{1}{2}n\Delta - 2(d_1 + d_n)^2 \\
&\geqslant d_1^3 + d_n^3 + d_{n-1}^3 + d_{n-2}^3 + \sum_{i=2}^{n-1}(d_i - d_{i+1})^4 + \left\lfloor \frac{2n+1}{2} \right\rfloor \left\lceil \frac{3n+1}{3} \right\rceil + \frac{1}{2}n\Delta - 2(d_1 + d_n + d_{n-1})^2.
\end{aligned}$$

Therefore, by considering the term $\lfloor (2n-1)/2 \rfloor \lceil (3n-2)/3 \rceil$, we notice that the lower bound of the Sigma index satisfies

$$\sigma(T) \geqslant \sqrt{\sum_{i=1}^{n} d_i^3 - \sum_{i=2}^{n-1} d_i^2} + \left\lfloor \frac{2n-1}{2} \right\rfloor \left\lceil \frac{3n-2}{3} \right\rceil + \frac{1}{2}n\Delta. \tag{45}$$

Finally, the term $\sqrt{\sum_{i=1}^{n} d_i^3 - \sum_{i=2}^{n-1} d_i^2}$ grows the bound of the Sigma index and is closely related to the term $d_1^3 + d_n^3$. Thus, we notice that (41) is valid for $n+1$ and $n+2$. Therefore, as the final result among all lower bounds (42)–(45), we find that (41) holds. □

Let $\mathcal{P}(n)$ be a function of vertices where $\mathcal{P}(n) = n(n+m-\Delta)^2$. Then, we noticed that $\sigma(T) \geqslant \sqrt{\mathcal{P}(n)}$, where among Theorem 4.4 had presented the upper bound of Sigma index.

Theorem 4.4: Let T be a tree, and $\mathcal{D} = (d_1, \ldots, d_n)$ be a degree sequence. Then, the upper bound of Sigma index is

$$\sigma(T) \leqslant 2(d_n + d_1)^2 + \sum_{i=1}^{n} d_i(d_i - 1)^2 + \frac{1}{2}\eta(T) + \sqrt{\mathcal{P}(n)} \tag{46}$$

Proof. Assume $\mathcal{D} = (d_1, \ldots, d_n)$ is a degree sequence with maximum degree Δ. Then, $\sigma(T) \gg \frac{\eta(T)}{2}$ and $\sigma(T) \gg \sqrt{\mathcal{P}(n)}$. Thus, with $\Delta(\Delta - 1)^2$ as the constant term,

$$\sigma(T) \leqslant \frac{1}{2}\eta(T) + \sqrt{\mathcal{P}(n)} + \Delta(\Delta - 1)^2. \tag{47}$$

To derive the remaining bounds, we consider the degree sequence in decreasing and increasing orders separately.

Case 1: Increasing order $(d_1 \leqslant d_2 \leqslant \cdots \leqslant d_n)$. Here, $\sigma(T) \gg 2(d_n + d_1)^2$, so

$$\sigma(T) \leqslant 2(d_n + d_1)^2 + \sum_{i=1}^{n} d_i(d_i - 1)^2 + \Delta(\Delta - 1)^2. \tag{48}$$

Since $\sigma(T) \geqslant \sqrt{\mathcal{P}(n)}$ and, from (48), $\sigma(T) \leqslant \sqrt{\mathcal{P}(n)} + 2(d_n + d_1)^3 + \Delta(\Delta - 1)^2$, it follows that

$$\sigma(T) \leqslant \sqrt{\mathcal{P}(n)} + 2(d_n + d_1)^3 + \sum_{i=1}^{n} d_i(d_i - 1)^2. \tag{49}$$

Define the sequence $\mathcal{A}_{se} = (d_n - d_{n-1}, d_{n-1} - d_{n-2}, \ldots, d_2 - d_1) = (a_1, a_2, \ldots, a_m)$. Then, $\sigma_{\mathcal{D}}(T) \geqslant \sigma_{\mathcal{A}_{se}}(T)$, yielding

$$\sigma(T) \leqslant \sigma_{\mathcal{A}_{se}}(T) + \sqrt{\mathcal{P}(n)} + 2(d_n + d_1)^3. \tag{50}$$

Thus, (48)–(50) confirm that the upper bound (46) holds when $d_1 \leqslant d_2 \leqslant \cdots \leqslant d_n$.

Case 2: Decreasing order Assume $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. Then the Sigma index satisfies $\sigma(T) \geqslant 2(d_n + d_1)^2 + 2(d_{n-1} + d_2)^2 + d_n^2 + d_1^2$. This implies

$$\sigma(T) \leqslant d_n^2 + d_1^2 + \sum_{i=n}^{2} (d_i - d_{i-1})^2 + \Delta(\Delta - 1)^2. \tag{51}$$

The analysis from **Case 1** applies here, highlighting the similarity in Sigma index behavior across cases. In particular,

$$\sigma(T) \leqslant \sum_{i=n}^{2} (d_i - d_{i-1})^2 + \frac{1}{2}\eta(T). \tag{52}$$

Combining (51) and (52) yields

$$\sum_{i=n}^{2} (d_i - d_{i-1})^2 + \frac{1}{2}\eta(T) \geqslant 2(d_n + d_1)^2 + 2(d_{n-1} + d_2)^2 + d_n^2 + d_1^2 + \sqrt{\mathcal{P}(n)}.$$

Furthermore,

$$\sigma(T) \leqslant \sum_{i=1}^{n} d_i^3 + \sum_{i=n}^{2} (d_i - d_{i-1})^2 + \frac{1}{2}\eta(T). \quad (53)$$

Thus,

$$\sigma(T) \leqslant \sum_{i=1}^{n} d_i(d_i - 1)^2 + \frac{1}{2}\eta(T) + \sqrt{\mathcal{P}(n)} + \sum_{i=n}^{2} (d_i - d_{i-1})^2. \quad (54)$$

Since $\sum_{i=1}^{n} d_i^3 \geqslant 2(d_n + d_1)^2$ and $\sum_{i=1}^{n} d_i^3 \geqslant 2(d_n + d_1)^2 + 2(d_{n-1} + d_2)^2 + d_n^2 + d_1^2$, the bound in (46) holds, confirming the upper bounds on $\sigma(T)$. □

5 Discussed Results on Sombor Index with Random Degrees

In this section, many studies have been conducted on topological indices, and we were motivated to study the effect of these topological indices on each other in order to determine the behaviour of these indices, which is of great importance in chemical graph theory. The *Sombor index* of a graph, introduced by Ivan Gutman [14] in 2021, is a topological index defined as

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

For **trees** (connected acyclic graphs), the Sombor index has been extensively analyzed by Proposition 5.1. The star S_n uniquely attains the maximum Sombor index: $SO(S_n) = (n-1)\sqrt{n}$. The path P_n uniquely minimizes the Sombor index: $SO(P_n) = (n-3) \cdot 2\sqrt{2} + 4$.

Proposition 5.1: Let T be a tree of order n. Then, the Sombor index satisfy $SO(P_n) \leqslant SO(T) \leqslant SO(S_n)$.

In next Figure 1, we observe that the Sigma index is 180 and the Sombor index for $n = 60$ vertices is $SO(T) = 222.74$.

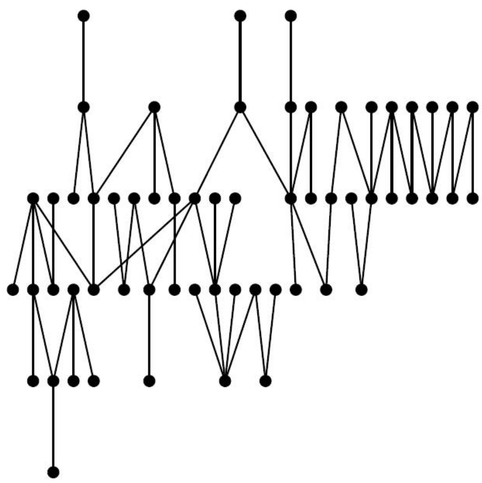

Fig. 1. Tree for $n = 60$ vertices

To begin with Algorithm 1, the initial phase involves the creation of random trees. Random trees are employed as models to represent a variety of graph topologies, facilitating the investigation of how topological indices fluctuate with structural differences. Through the generation of diverse tree configurations, researchers can better comprehend the impact of topology on these indices, thus enhancing the understanding of structural properties in complex network analysis. This approach provides the necessary flexibility to work with a variety of trees, depending on the selected number of vertices.

Algorithm 1 Generate Random Tree

```
function GenerateRandomTree(n, seed)
    if n < 1 then
        raise ValueError("Number of nodes must be at least 1")
    end if
    if n = 1 then
        return tree with a single isolated node
    end if
    Initialize random generator with seed
    Generate Prüfer sequence of length n − 2 with integers in [0, n − 1]
    Convert Prüfer sequence into tree graph
    return the tree graph
end function
```

Random trees are useful tools for investigating the extreme values of various graph indices. They help identify the boundaries and characterize the extremal structures that occur within specific categories of graphs, including those trees that attain either the maximum or minimum values for a given index. After the initial phase of random tree generation, the subsequent step in Algorithm 2 involves structuring these trees into a designated forest by applying suitable selection criteria.

Algorithm 2 Forest Specification

```
function GetUserForestSpec
    Initialize empty list nodes_per_tree
    for i = 1 to T do
        repeat
            Prompt user for number of nodes n_i for tree i
        until n_i ≥ 1
        Append n_i to nodes_per_tree
    end for
    return T, nodes_per_tree
end function
```

The Sigma index is initialized using Algorithm 3, as we apply the general definitions for both the Sigma and Sombor indices. This algorithm sets the foundation based on the conditions associated with each topological index, reflecting their clear interconnections in chemistry.

Algorithm 3 Sigma Index Computation

```
function SigmaIndex(graph)
    degrees ← degree of all nodes in graph
    total ← 0
    for each edge (u, v) in graph do
        contrib ← (degrees[u] − degrees[v])^2
        total ← total + contrib
    end for
    return total
end function
function ComputeSigmaForest(forest)
    Initialize empty list results
    total ← 0
    for each tree in forest do
        s ← SigmaIndex(tree)
        Append s to results
        total ← total + s
    end for
    Print sigma values per tree and total
    return results, total
end function
```

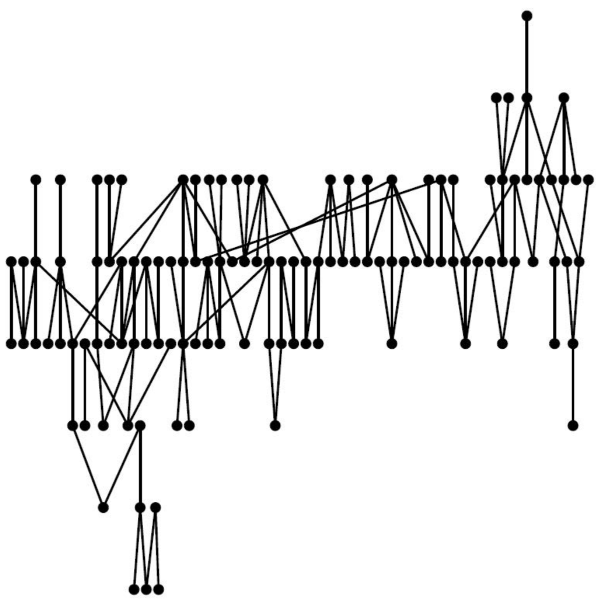

Fig. 2. Tree for $n = 120$ vertices

The link between topological indices (Lemma 5.2 ad established that.) and diverse chemical and biological properties makes random trees effective models for molecular structures. These models enable the prediction of property patterns and aid in designing molecules with desired characteristics. Corroborating what we have presented through the previous algorithms, we note, based on Figure 1, that through Figure 2, by systematically doubling the number of vertices ($SO(T) = 398$ and $\sigma(T) = 322$), we obtain values close to those obtained through Figure 1. This is because we rely on the traditional definition of both indices, which prompted us to reinforce the behaviour of both indices (55).

Lemma 5.2: Let T be a tree of order n. The Sombor index and the Sigma index satisfy the following relationship

$$SO(T) - \sigma(T) \leqslant 2n - 2. \tag{55}$$

Proof. Recall Sigma index among Theorem 2.3 and assume $\mathcal{D} = (d_1, \dots, d_n)$ be a degree sequence such that $d_n \geqslant \cdots \geqslant d_1$. Let x, y be a two vertex of $V(T)$ where $d_T(x) \neq d_T(y)$. Then, if there are a path $\mathcal{P} = xx_1 \dots y_1 y$. Then, according to [5] satisfy $d_T(x) \geqslant d_T(y)$ while $d_T(x_1) < d_T(y_1)$. Let λ_{xy} be an two edes xy_1, yx_1 and β_{xy} be an two edges xx_1 and $y_1 y$. Assume T' be the tree obtaind from T by omitted β_{xy} and add λ_{xy}. Then,

$$\sigma(T) - \sigma(T') = 2[(d_T(x) - d_T(y))(d_T(x_1) - d_T(y_1))]. \tag{56}$$

Simillarly, from (56) we find that for Sombor index

$$SO(T) - SO(T') = 2[\sqrt{(d_T(x) - d_T(y))(d_T(x_1) - d_T(y_1))}]. \tag{57}$$

Therefore, according to (56) and (57),

$$\begin{aligned} SO(T) - \sigma(T) &= \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} - \sum_{uv \in E(G)} (d_G(u) - d_G(v))^2 \\ &= \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} + 2 \sum_{uv \in E(G)} d_u \,.\, d_v - \sum_{u \in V(T)} d_u^3 \\ &\leqslant 2n - 2. \end{aligned}$$

□

6 Conclusion

Through this paper, we presented an analytical study of the extreme values of the topological indices, through which we demonstrated the significant differences between the upper and lower limits and the extreme values of the topological indices we discussed. We presented both the Albertson index and the Sigma index, and in section 5, we presented algorithms for finding topological indices to determine the effect of these topological indices on each other in order to determine the behaviour of these indices, which is of great importance in chemical graph theory.

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