BEHAVIOR OF THE EXTREMAL BOUNDS ON THE σ-IRREGULARITY

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ABSTRACT. In this paper, we establishe the extremal bounds of the topological indices —Sigma index— focusing on analyzing the sharp upper bounds and the lower bounds of the Sigma index, which is known $\sigma(G) = \sum_{uv \in E(G)} (d_G(u) - d_G(v))^2$. We establish precise lower and upper bounds for the Sigma index, leveraging a non-increasing degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$, A fundamental challenge in the study of topological indices lies in establishing precise bounds, as such findings illuminate intrinsic relationships among diverse indices.

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1. INTRODUCTION

Throughout this paper. Let $G = (V, E)$ be a simple, connected graph, where $n = |V(G)|$, $m = |E(G)|$. Let $\mathscr{D} = (d_1, d_2, \ldots, d_{n-1}, d_n)$ be a degree sequence and consider $\mathscr{D}$ is non-increasing. S. L. Hakimi [31] had provided the concept of realizability as a set of integers with degrees of the vertices of a graph. Among [13] had presented a study of degree sequence index strategy.

In [37, 12] had presented the methodology for solving the inverse problem of topological indexes. One of this topological indexes called the *Albertson index* was first introduced in 1997 by M. O. Albertson [10]. I. Gutman [24] had presented topological indices and irregularity measures where many equivalent formulas for Albertson index considered as the concept of *irregularity* were presented in [1, 3, 5, 7, 8, 11]. Generally, Albertson index is defined as

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

Z. Che and Z. Chen [15] had established new mathematical lower and upper bounds for the *forgotten topological index* $F(G)$ where the forgotten topological index had provided by Furtula and Gutman [21] and defined of a molecular graph G as

$$F(G) = \sum_{uv \in E(G)} \left(d_G(u)^2 + d_G(v)^2 \right).$$

In [19, 34, 38, 39] had established that the *harmonic topological index* $H(G)$. It inherently prioritizes edges linking vertices of lower bound, as the ratio attains greater magnitude when the aggregate degree sum is minimal. Z. Lingping [33] defined $H(G)$ as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(v)}.$$

The rational extension of the quantum harmonic oscillator and exceptional Hermite polynomials had presented in [23]. Topological indices study of molecular structure [22] such that one of the topological indices which was associated with irregularity [2] in the graph theory called *Sigma*

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index, denoted by σ. Relationships between other topological indices had presented through [17] and Sigma index introduced by [25, 5, 42, 9] , which is defined as

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

There are many studies that have examined the bounds on the Albertson index, some of which have been related to the sigma index, such as [3, 1, 4, 10, 24, 11, 16]. Through [9] provided a study of Sigma index and forgotten index. In [14] had discussed specific issues of Sigma called *sigma chromatic number*. The σ_t-*irregularity* (or sigma total index) of a graph G is defined [32, 18] as

$$\sigma_t(G) = \sum_{\{u,v\} \subseteq V(G)} (d_G(u) - d_G(v))^2,$$

some results on σ_t-irregularity had given through [20]. This index has been studied in the context of extremal graph theory, yielding bounds and characterizations of graphs maximizing σ_t-irregularity.

Let $\sigma \bigodot (T)$ be the average of Sigma index for the case $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, and the case $d_n \geqslant \cdots \geqslant d_1$. The *reduced Sigma index* defined as

$$(1) \qquad \sigma_{red}(T) = \sum_{uv \in E(T)} \left[(d_T(u) - 1)^2 + (d_T(v) - 1)^2 \right].$$

This particular expression resembles modified Zagreb-type indices (see Definition 1), which are degree-based or related indices for trees, emphasizing the degrees decreased by one rather than the degrees themselves. The *increase Sigma index* $\sigma_{inc}(T)$ of a tree T defined as

$$(2) \qquad \sigma_{inc}(T) = \sum_{uv \in E(T)} \left[(d_T(u) + 1)^2 + (d_T(v) + 1)^2 \right].$$

The *modified Sigma index* $\sigma^*(T)$ of a tree T defined as

$$(3) \qquad \sigma^*(T) = \sum_{uv \in E(T)} \left[\frac{1}{(d_T(u) + 1)^2 + (d_T(v) + 1)^2} \right].$$

A fundamental challenge in the study of topological indices lies in establishing precise bounds, as such findings illuminate intrinsic relationships among diverse indices. Given that topological indices serve as mathematical descriptors closely linked to the chemical attributes of compounds, pinpointing the compound exhibiting extremal behavior for a particular property is tantamount to the problem of optimizing a strongly correlated topological index within the designated class of graphs.

The main goal of this paper is to study the optimal behavior of the Sigma index by evaluating its upper and lower bounds along with some elicited topological indices. Since many important studies have been derived from the Albertson index and the Sigma index, we see it as important to determine the closest bounds for these indices. Also, in this paper lies in examining the upper and lower bounds of the Sigma index to determine the strictest bound. According to upper or lower bounds it smells like studying the behavior of the Sigma index, which effectively influences the behavior of other topological indices. There are fundamental challenges that to find the sharp and strictly upper and lower bound of Sigma index. The paper also aims to present a new topological indices derived from the Sigma index that will lay the foundation for future studies to overcome major challenges in the optimal improvement of topological indices.

This paper is organized as follows. In Section 3, we presented the upper bound of Sigma index for a degree sequence $\mathscr{D}$ order such that $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. Section 4 discussed the lower bounds of Sigma index among degree sequence. In Section 5, we presented the effects of this bounds.

2. Preliminaries

In this section, we introduce several essential concepts to ensure the reader fully comprehends the results presented in this paper. Several studies have introduced the concept of bounds on topological indices [35, 36]. Therefore, we will review some bounds on topological indices that contribute to strengthening our study regarding extremal bounds. Through this paper, we point out that all the trees included in the study are caterpillar trees, we consider caterpillar trees denoted by $\mathscr{C}(n, m)$, where n is the number of backbone (or path) vertices and m is the number of pendant vertices attached to each.

Definition 1 (Zagreb Indices [27, 26, 40, 41]). *Let $G = (V, E)$ be a graph. The first and second Zagreb indices are given by*

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2, \quad M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v).$$

In the following Theorem 2.1, we provide the relationship with the second Zagreb index, the forgotten indx and Sigma index.

Theorem 2.1 ([9]). *For any connected graph G we have $\sigma(G) = F(G) - 2M_2(G)$.*

During our study of the Sigma index through this paper, we will not use the traditional definition but will instead use the relation obtained from Theorem 2.2, which is associated with degree sequence $\mathscr{D}$.

Theorem 2.2 ([28, 29]). *Let T be a tree of order n, and let $\mathscr{D} = (d_1, \ldots, d_n)$ be a degree sequence such that $d_n \geqslant \cdots \geqslant d_1$. Then, the Sigma index of the tree T is given by:*

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

For a duplicate star graph $\mathcal{S}_{r,k}$, Theorem 2.3 provide us the relationship of Sigma index with special terms.

Theorem 2.3 ([25]). *Let $\mathcal{S}_{r,k}$ be a duplicate star graph where $\deg_{\mathcal{S}_{r,k}}(u) = k$ and $d_{\mathcal{S}_{r,k}}(v) = r$. Then,*

$$\sigma(\mathcal{S}_{r,k}) = (k - 1)^3 + (r - 1)^3 + (k - r)^2.$$

Proposition 2.1. *Let T be a tree, $\mathscr{D}(d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. Then, Sigma index satisfy*

$$(4) \qquad \frac{1}{3} < \left\lfloor \frac{2n^2 - 1}{2} \right\rfloor \frac{1}{\sigma(T) + d_1^3 + (d_1 - d_2)^3 - (d_{n-1} - d_n)^3} < \frac{1}{10}.$$

Proof. Assume $\mathscr{D}(d_1, d_2, \ldots, d_n)$ is a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ and the maximum degree $\Delta > 3$. Since $n > \Delta$ and $2n^3 + m > 4\Delta$, the term $(2n^3 + m/(4\Delta)$ yields the Sigma index that satisfies the relationship (5), where $\Delta \geqslant d_1$,

$$(5) \qquad \sigma(T) \geqslant \left\lfloor \frac{2n^3 + m}{4\Delta} \right\rfloor.$$

Let $k > 0$ be an integer. Then, according to the required relationship (4), we observe that $k \leqslant n^2 - \frac{1}{2} \leqslant k + 1$. For $j \geqslant k$, according to (5), we find that $4\Delta j + 4\Delta \leqslant 2n^3 + m \leqslant 4\Delta j$. Thus, according to relationship (5) we observe that

$$(6) \qquad \left\lfloor \frac{2n^3 + m}{4\Delta} \right\rfloor - \left\lfloor \frac{2n^2 - 1}{2} \right\rfloor \leqslant 4\Delta(k - j).$$

Therefore, the Sigma index satisfies $\sigma(T) > d_1^3 + (d_1 - d_2)^3$. Next, for the term $d_1^3 + (d_1 - d_2)^3$, we observe that

$$(d_{n-1} - d_n)^3 < d_1^3 + (d_1 - d_2)^3 < \sum_{i=1}^{n} d_i^3,$$

which implies $\sigma(T) \geqslant d_1^3 + (d_1 - d_2)^3 - (d_{n-1} - d_n)^3$. Thus, according to (6), it holds that

$$(7) \qquad \sigma(T) \geqslant \frac{d_1^3 + (d_1 - d_2)^3 - (d_{n-1} - d_n)^3}{4\Delta(k - j)}.$$

Therefore,

$$(8) \qquad 1 \leqslant \frac{d_1^3 + (d_1 - d_2)^3 - (d_{n-1} - d_n)^3}{4\Delta(k - j)} \leqslant 3.$$

Thus, from (7) and (8), by adding the value of the Sigma index in relation (8), we conclude that (4) holds. $\qquad\square$

Through Figure 1, we present some different values for each of the two topological indices — the Sigma index and the Albertson index — using a connected graph. It is worth noting in this case that we observe different values for the indices when the graph is closed, which differ significantly from those when the graphs are trees; therefore, it is necessary to highlight this through the figure.
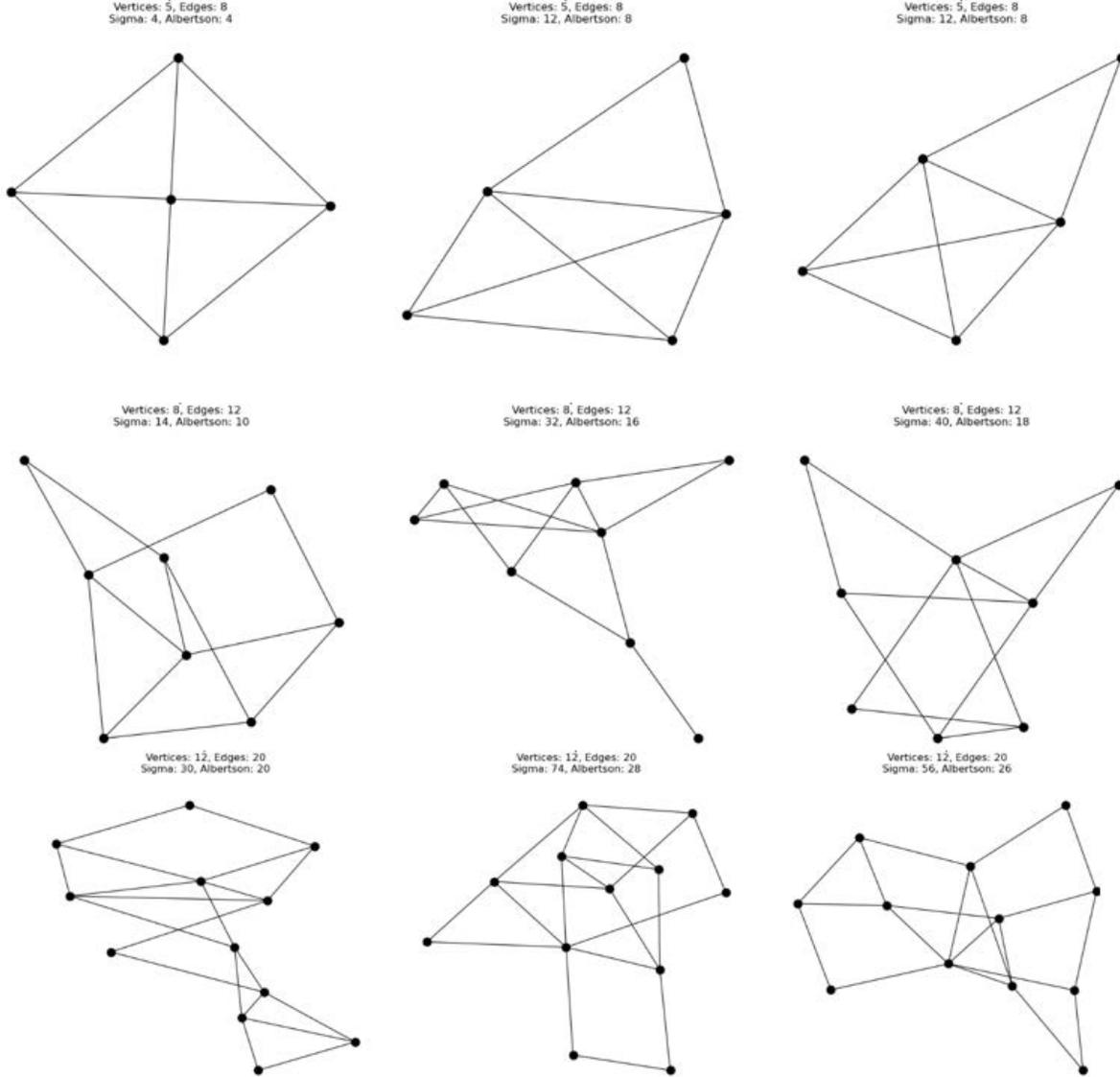
Figure 1. Compare value of the Sigma index and the Albertson index.

3. Upper Bound of Sigma Index

In this section, the upper bound of the Sigma index is characterized by encompassing several bounds. We observe through Proposition 2.1 a confinement of the Sigma index within the interval $[\frac{1}{3}, \frac{1}{10}]$ by considering the term $2n^2 - 1$. Lemma 3.1 presented the constant upper bound related to $n^3 + m^2$.

Lemma 3.1. *Let T be a tree and $\mathscr{D}(d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ with the maximum degree Δ. Then,*

$$(9) \qquad 0 < \frac{1}{m-1}\left(\frac{2n^3 + m^2}{\Delta(\Delta - 1)^2} + \left\lfloor \frac{3nm}{7} \right\rfloor - \left\lceil \frac{3nm}{7} \right\rceil \right) < 3,$$

if and only if $\sqrt{\sigma(T)} > n$.

Proof. Consider $\mathscr{D}(d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ with the maximum degree Δ where $4\Delta \leqslant n$. Since $m = n - 1$ and $2n^3 + m^2 = 2n^3 + n^2 - 2n + 1$, we find that

$2n^3 + n^2 - 2n + 1 > \Delta(\Delta - 1)^2$. For a certain term of Δ, the lower bound of Sigma index satisfy:

$$(10) \qquad \sigma(T) \geqslant \frac{2n^3 + n^2 - 2n + 1}{\Delta(\Delta - 1)^2} + 2n.$$

Thus, from (10) we noticed that $\sigma(T) > 2n$ and $\sqrt{\sigma(T)} > n$. Therefore, we must prove under the assumption that the condition related to the Sigma index is satisfied according to equation (9). Here, let us discuss both the bounds and their relation to the Sigma index until we obtain the relation of these bounds through equation (9) with the Sigma index. Thus, we have:

$$(11) \qquad \sigma(T) \leqslant \left\lfloor \frac{3nm}{7} \right\rfloor + \left\lceil \frac{3nm}{7} \right\rceil + 2n^2 + 2,$$

where $2n^2 + 2$ is the constant term. Since $\sigma(T) > 2n^2 + 2$ implies that $\sigma(T) > \left\lfloor \frac{3nm}{7} \right\rfloor + \left\lceil \frac{3nm}{7} \right\rceil$. In this case, let $3 < k < n/2$ and $k \in \mathbb{N}$. Then, according to (11) the lower bound of Sigma index satisfy

$$(12) \qquad \sigma(T) \geqslant \left\lfloor \frac{knm}{k+4} \right\rfloor + \left\lceil \frac{knm}{k+4} \right\rceil.$$

Thus, according to both lower bounds (11) and (12) we find that

$$\begin{aligned} \sigma(T) &\geqslant \left\lfloor \frac{knm}{k+4} \right\rfloor + \left\lceil \frac{knm}{k+4} \right\rceil \\ &\geqslant \frac{1}{m-1} \left(\left\lfloor \frac{knm}{k+4} \right\rfloor + \left\lceil \frac{knm}{k+4} \right\rceil \right) \\ &\geqslant \frac{1}{m-1} \left(\left\lfloor \frac{knm}{k+4} \right\rfloor + \left\lceil \frac{knm}{k+4} \right\rceil + 2n^2 + 2 \right). \end{aligned}$$

Therefore, the lower bounds of Sigma index had discussed among (12) and (10). Thus, according to Proposition 2.1 we find that $\sigma(T) \geqslant \left\lfloor \frac{2n^3 + m}{4\Delta} \right\rfloor$. Thus, it holds

$$(13) \qquad n < \frac{1}{m-1} \left(\left\lfloor \frac{knm}{k+4} \right\rfloor + \left\lceil \frac{knm}{k+4} \right\rceil + 2n^2 + 2 \right) < n\Delta$$

Since $2n^2 + 2$ is the constant term and $\sigma(T) > 2n^2 + 2$ according to (13) noticed that

$$(14) \qquad 2n < \frac{2n^3 + n^2 - 2n + 1}{\Delta(\Delta - 1)^2} < n\Delta.$$

Thus, when $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, we have $2n/(m-1) \approx 2$ and $n\Delta/(m-1) \leqslant n^2/\Delta$. Thus,

$$(15) \qquad 0 < \frac{1}{m-1} \left(\frac{2n^3 + n^2 - 2n + 1}{\Delta(\Delta - 1)^2} \right) < 3.$$

Finally, according to (11) and (12) we find that the difference $\left\lfloor \frac{3nm}{7} \right\rfloor - \left\lceil \frac{3nm}{7} \right\rceil$ holds $\sigma(T) > \left\lceil \frac{3nm}{7} \right\rceil - \left\lfloor \frac{3nm}{7} \right\rfloor$. Then, by combining this results with (13), (14) and (15) we find that (9) holds. As desire. $\qquad \square$

The sharp upper bound of Sigma index had disccused among Lemma 3.2, where we assume $d_T(v_2) = d_T(v_3) = \cdots = d_T(v_{n-1}) = k$. Sigma index satisfying $\sigma(T) = d_1(d_1 - k)^2 + d_n(k - d_n)^2$. Defining the sharp bounds, whether upper or lower, in the topological indices provides a clear indication of the extent to which these bounds approximate the actual values of the indicators, which is the objective we aim to achieve.

Lemma 3.2. *Let T be a tree, let $\mathscr{D}(d_1, d_2, \ldots, d_n)$ 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*

$$(16) \qquad \sigma(T) \leqslant \left\lfloor \frac{3n}{5} \right\rfloor \left\lceil \frac{2n}{5} \right\rceil \frac{2nm}{\Delta(\Delta-1)^2} + \delta \sqrt{\frac{nm}{2\Delta(\Delta-1)}} + \frac{1}{2}(n^2 + m^2) + n(m - \Delta)^2.$$

Proof. Assume $\mathscr{D}(d_1, d_2, \ldots, d_n)$ 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

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

Then, we notice that $\beta \geqslant \alpha + \gamma$. Thus, α satisfies the bound $\alpha \leqslant n\Delta + m$ and β satisfies the bound $\beta \geqslant (m-1)^2 + 3n$. On the other hand, we observe that the bound according to 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 $\mathscr{D}$ satisfies the order $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, for any path in the tree, we observe that each of the vertices $V(T) = \{v_1, v_2, \ldots, v_n\}$ satisfies $d_T(v_1) > d_T(v_2) \geqslant d_T(v_3) \geqslant \cdots \geqslant d_T(v_{n-1}) > d_T(v_n)$. Hence, assume $d_T(v_2) = d_T(v_3) = \cdots = d_T(v_{n-1}) = k$. Then, the Sigma index satisfies

$$(17) \qquad \sigma(T) = \sum_{v_i \in N(v_1)} (d_T(v_1) - k)^2 + \sum_{v_i \in N(v_n)} (k - d_T(v_n))^2,$$

noting that all neighbors of v_1 and v_n have degree k. Then, the Sigma index is $\sigma(T) = d_T(v_1)(d_T(v_1) - k)^2 + d_T(v_n)(k - d_T(v_n))^2$. Actually, since $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ in $\mathscr{D}$, we find that

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

Thus,

$$(18) \qquad \sigma(T) \leqslant \alpha \sum_{v_i \in N(v_1)} (d_T(v_1) - k)^2 + \gamma \sum_{v_i \in N(v_n)} (k - d_T(v_n))^2.$$

Then, to determine the lower bound of the Sigma index according to parameters α, β, and γ, and by considering equations (17) and (18), we find

$$(19) \qquad \sigma(T) \geqslant \left\lfloor \frac{3n}{5} \right\rfloor \left\lceil \frac{2n}{5} \right\rceil \frac{2nm}{\Delta(\Delta-1)^2} + \sum_{v_i \in N(v_1)} (d_T(v_1) - \alpha)^2 + \sum_{v_i \in N(v_n)} (\gamma - d_T(v_n))^2.$$

Thus, these relations ultimately lead, according to the conditions we obtained in

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

to the Sigma index satisfying relation (20), which represents the lower bound we want to achieve for the required relation (16) as:

$$(20) \qquad \sigma(T) \leqslant \left\lfloor \frac{3n}{5} \right\rfloor \left\lceil \frac{2n}{5} \right\rceil \frac{2nm}{\Delta(\Delta-1)^2} + \frac{(n^2 + m^2)\sqrt{\frac{nm}{2\Delta(\Delta-1)}}}{2}.$$

Therefore, the term $n(m - \Delta)$ grows rapidly and according to (20), by combining it with $n(m - \Delta)$, the Sigma index satisfies the sharp upper bound. $\square$

Throughout Theorem 3.3, we determine the relationship of the harmonic topological index and Sigma index according to Lemma 3.2.

Theorem 3.3. *Let T be tree of order n, $H(G)$ be the harmonic topological index and let η be an integer, $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ be non-decreasing degree sequence with $\lambda_{\mathscr{D}}$ the average of elements $\mathscr{D}$. Then, the upper bound of Sigma index satisfy*

$$(21) \qquad \sigma(T) \leqslant \left\lfloor \frac{2n^2}{3\lambda_{\mathscr{D}}} \right\rfloor + \frac{2^\eta (m - \Delta)^2}{5(n-1)^3} + (n-1)H(G).$$

From the proof of Lemma 3.2, we would like to point out that the satisfied condition $3 < \sqrt{nm/2\Delta(\Delta - 1)} < 4$ and $0 < 2nm/\Delta(\Delta - 1)^2 < 2$ is also fulfilled for degree sequence $\mathscr{D}$ where $d_1 \leqslant d_2 \leqslant \cdots \leqslant d_n$; hence, these bounds are considered to be confined by one or more increases.

Theorem 3.4 establishes the initial upper bounds by analyzing the sum of the squared differences between the degrees of $\mathscr{D}$, while considering the influence of the average relative to these degrees.

Theorem 3.4. *Let T be a tree, and let $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, with maximum degree Δ, minimum degree $\delta \geqslant 2$, and let $\lambda_{\mathscr{D}}$ be the average of $\mathscr{D}$. Then, the upper bound of the Sigma index satisfies*

$$(22) \qquad \sigma(T) \leqslant \sum_{i=1}^{n-1} \lambda_{\mathscr{D}} (d_i - d_{i+1})^3 + 2(n^2 + m^2) + 3m + n + 2.$$

Proof. Assume $\mathscr{D}(d_1, d_2, \ldots, d_n)$ is a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ with the maximum degree Δ, the minimum degree $\delta \geqslant 2$, and $\lambda_{\mathscr{D}}$ the average of $\mathscr{D}$. It is clear that n satisfies $n > \sum_{i=1}^{n-1} (d_i - d_{i+1})^2$ and $2n > \sum_{i=1}^{n-1} (d_i - d_{i+1})^3$. Both terms involving n are essentially established for the lower bound with respect to the Sigma index. Thus, the lower bound of the Sigma index is

$$(23) \qquad \sigma(T) \geqslant \sum_{i=1}^{n-1} \lambda_{\mathscr{D}} (d_i - d_{i+1})^3 + 2n^2 + 2.$$

According to Lemma 3.1, we compare the term $2n^3 + n^2 - 2n + 1$ with the term $\Delta(\Delta - 1)^2$ by considering the value of $m - 1$,

$$0 < \frac{1}{m-1} \left(\frac{2n^3 + n^2 - 2n + 1}{\Delta(\Delta - 1)^2} \right) < 3.$$

Based on this reduction, the lower bound (23) is difficult to determine within a certain bound. Thus, we have

$$\Delta(n - \Delta)^2 - \Delta(m - \Delta)^2 \geqslant \sum_{i=1}^{n-1} \lambda_{\mathscr{D}} (d_i - d_{i+1})^3,$$

and for the term $\Delta(\Delta - 1)^2$ compared with the term $(2m^2 + 2m + n)/2(n + m)$, considering that $\sigma(T) < 2m^2 + 2m + n$ holds, we obtain

$$(d_1 - d_n)^2 \geqslant \frac{1}{\Delta(\Delta - 1)^2} \left(\frac{2m^4 + 2m + n}{2(n + m)} \right).$$

The sharp lower bound of the Sigma index satisfies the inequality by considering (23) and the value of the term $(d_1 - d_n)^2$,

$$(24) \qquad \sigma(T) > \frac{1}{\Delta(\Delta - 1)^2} \left(\frac{2m^4 + 2m + n}{2(n + m)} + 2nm + (d_1 - d_n)^2 \right).$$

Thus, relationship (24) implies that $\Delta(2n - m)^2$ satisfies the lower bound according to the value of $\lambda_{\mathscr{D}}$ and the upper bound according to the value d_i^2. Hence,

$$(25) \quad \sum_{i=1}^{n-1} \lambda_{\mathscr{D}} (d_i - d_{i+1})^3 \leqslant \frac{1}{4} \left(\frac{2m^4 + 2m + n}{2\Delta(n + m)(2n - m)^2} + 2nm + (d_1 - d_n)^2 \right) \leqslant 3 \sum_{i=1}^{n} d_i^2 - (n + m),$$

where

$$2 \leqslant \frac{1}{4}\left(\frac{2m^4 + 2m + n}{2\Delta(n+m)(2n-m)^2}\right) \leqslant 3.$$

Therefore, from (24) and (25), the relationship with (23) implies (22). □

Actually, according to (23), (24) and (25) we obtain from discussing these bounds, we obtain the equivalent upper bound to the upper bound given in Theorem 3.4. This bound, which we obtain through Theorem 3.5, is a direct result of the discussion carried out through the relationships (23), (24) and (25).

Theorem 3.5. *For any tree T with degree sequence $\mathscr{D}(d_1, d_2, \ldots, d_n)$ where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ and $\lambda_{\mathscr{D}}$ the average of $\mathscr{D}$. Then, according to Theorem 3.4 the upper bound of Sigma index satisfy*

$$(26) \qquad \sigma(T) \leqslant \sum_{i=1}^{n} d_i^3 + \frac{2\lambda_{\mathscr{D}}(n^2 + m^2)}{3(n+m)}.$$

The following result is similarly achieved for the upper bound of the Sigma index, making it a sharply distinct and clear extreme value. Therefore, the approximate study to determine a specific sharp value for the Sigma index may not be consistent.

Corollary 3.6. *For any tree T of order n. The upper bound of Sigma index satisfy*

$$(27) \qquad \sigma(T) \leqslant \sum_{i=1}^{n-1} \lambda_{\mathscr{D}}(d_i - d_{i+1})^3 + 2m^2 + 2m + n.$$

Corollary 3.7. *For any tree T of order n. The upper bound of Sigma index satisfy*

$$(28) \qquad \sigma(T) \leqslant \sum_{i=1}^{n-1} \lambda_{\mathscr{D}}(d_i - d_{i+1})^3 + 2n^2 + 2.$$

Corollary 3.8. *For any tree T of order n. Let $F(G)$ be the forgotten topological index. Then, the upper bound of Sigma index satisfy*

$$(29) \qquad \sigma(T) \leqslant 2F(G) + 2n^2 + 2.$$

Proof. According to the relationship of the forgotten topological index $F(G)$ and according to Theorem 2.1, we noticed that $\sigma(T) = F(G) + \sum_{uv \in E(G)} 2d_G(u)d_G(v)$. Therefore,

$$\sum_{uv \in E(G)} (d_G(u)^2 + d_G(v)^2) > \sum_{uv \in E(G)} (d_G(u) - d_G(v))^2.$$

Thus, $\sigma(T) \leqslant 2F(G)$ and the term $2n^2 + 2$ is confirmed of the upper bound of Sigma index. □

Through the following table, we noticed that the degree sequences with corresponding values for Theorem 3.4, parameters α, β and γ, and values from Lemma 3.1.

Degree	Theorem 3.4	α	β	γ	Lemma 3.1
(20,18,16,13,10,7,3)	30191	1820	7482.5	5742	2.158060942
(23,22,20,16,12,10,5)	46550	2816	34669.5	9072	2.144822168
(26,26,24,19,14,13,7)	66437	4004	49537.5	13158	2.08831593
(29,28,28,22,16,16,9)	87470	5280	65269.5	17464	1.959715692
(32,30,29,25,18,17,11)	104816	6305	78247.5	20898	1.733419168
(35,32,30,28,20,19,13)	125141	7526	93457.5	24957	1.570714215
(38,34,32,31,22,21,15)	148805	8970	111169.5	29729	1.450753316
(41,36,34,33,24,23,17)	172850	10416	129169.5	34528	1.335001258
(44,38,36,35,26,25,19)	198695	11970	148519.5	39694	1.23630804

TABLE 1. Present value of previous discussion with Lemma 3.1 and 3.2 and Theorem 3.4.

According to Table 1, we noticed that this analytical method aligns with standard techniques for sequence data (see Figure 2), aiming to identify patterns, correlations, and structural insights to comprehend the behavior of derived indices or parameters for specific degree sequences.
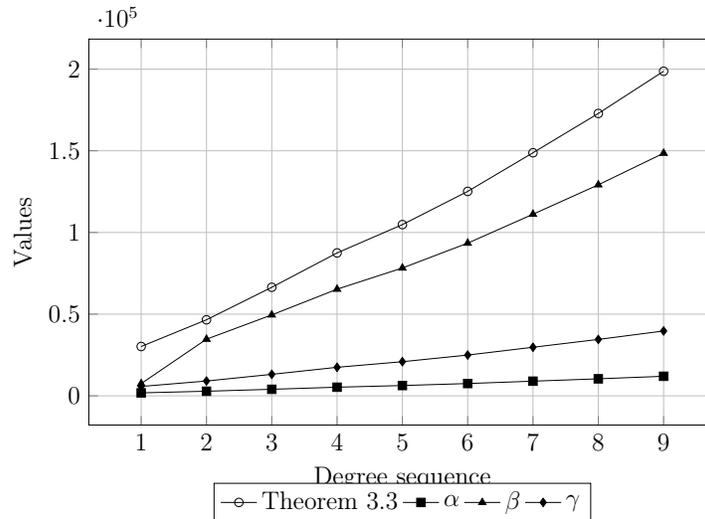

FIGURE 2. Explain the value among Table 1.

4. LOWER BOUNDS OF SIGMA INDEX

In this section, The discussion previously presented in section 3 is continued, focusing on the analysis of the lower bound of the Sigma index. Both extreme values play a pivotal role in the behavior of the Sigma index, as illustrated in Figure 2. Through Proposition 4.1, we establish the lower bound of the Sigma index in accordance with Theorems 3.4 and 3.5, which were also employed to analyze the upper bound discussed earlier.

Proposition 4.1. *Let T be a tree, $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ and $M_1(T)$ be the first Zagreb index, and let $\lambda_{\mathscr{D}}$ be the average of $\mathscr{D}$. Then, the lower bound of the Sigma index satisfies*

$$(30) \qquad \sigma(T) \geqslant M_1(T) + \left\lfloor \frac{2(n+m)^2}{5} \right\rfloor + \frac{2\lambda_{\mathscr{D}}(n^2 + m^2)}{3(n+m)}.$$

Proof. Assume $\mathscr{D}(d_1, d_2, \ldots, d_n)$ is a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ with the maximum degree Δ and $\lambda_{\mathscr{D}}$ is the average of $\mathscr{D}$. Since $2\lambda_{\mathscr{D}}(n^2 + m^2) > 3(n + m)$ and $\Delta < \frac{2\lambda_{\mathscr{D}}(n^2 + m^2)}{3(n+m)} \leqslant 3\Delta$, according to Theorem 3.5 we find the upper bound of the Sigma index given as

$$\sigma(T) \leqslant \sum_{i=1}^{n} d_i^3 + \frac{2\lambda_{\mathscr{D}}(n^2 + m^2)}{3(n + m)}.$$

Thus, let us consider the term $\Delta(\Delta - 1)^2$ satisfies $\Delta(\Delta - 1)^2 < 2(m + n)^2$. Then, we find that $\Delta(\Delta - 1)^3 \leqslant 2\lambda_{\mathscr{D}}(n^2 + m^2)$. Thus, the lower bound of the Sigma index satisfies

$$(31) \qquad \sigma(T) \geqslant \Delta(\Delta - 1)^2 + \frac{2\lambda_{\mathscr{D}}(n^2 + m^2)}{3(n + m)}.$$

Therefore, from (31) we observe that this bound approaches the Sigma index very closely, due to the values of Δ that come from the condition we imposed on $\mathscr{D}$ where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. In this case, we note that the term $2(n + m)^2$ satisfies the relation $2(n + m)^2 < \lambda_{\mathscr{D}}(n^2 + m^2)$. Therefore, we obtain the lower bound of the Sigma index as:

$$(32) \qquad \sigma(T) \geqslant \left\lfloor \frac{2(n + m)^2}{5} \right\rfloor + \frac{2\lambda_{\mathscr{D}}(n^2 + m^2)}{3(n + m)}.$$

Hence, for the last term in (30) we notice that $\sum_{i=1}^{n} d_i^2 < \Delta(\Delta - 1)^2$. Thus, according to the lower bounds (31) and (32), the relationship (30) clearly holds. As desired. $\square$

We observe from Proposition 4.1 that it directly leads to Corollary 4.1. Also, we notice through Equation (33) and by directly relying with the term $\sum_{i=1}^{n} d_i^2 < \Delta(\Delta - 1)^2$, that it gives us the lower bound of Sigma index.

Corollary 4.1. *For any tree T of order n. The lower bound of Sigma index satisfy*

$$(33) \qquad \sigma(T) \geqslant \sum_{i=1}^{n-1} \lambda_{\mathscr{D}}(d_i - d_{i+1})^2 + \left\lfloor \frac{2(n + m)^2}{5} \right\rfloor + \frac{2\lambda_{\mathscr{D}}(n^2 + m^2)}{3(n + m)}.$$

Based on Conjecture 4.2 which establishes Proposition 4.2, this conjecture is employed to refine the optimal terms that play a crucial role in enhancing the optimal behavior of the Sigma index.

Conjecture 4.2. *For any tree T with n vertices and m edges. Let k be an integer where $0 < k < 5$. Then,*

$$(34) \qquad 0 \leqslant \frac{2^k(n + m)^2}{2(k + 1)\Delta(\Delta - 1)^2} \leqslant 2k.$$

Proof. Let k be an integer where $0 < k < 5$, and assume $m = n - 1$ in a tree T. Then the term 2^k with $(n + m)^2$ holds the bound $2^k < (n + m)^2$. Thus, clearly we find that:

$$(35) \qquad \frac{2^k(n + m)^2}{2(k + 1)} > 0$$

Therefore, through relationship (35), the left-hand side of inequality (34) is satisfied when considering the term $\Delta(\Delta - 1)^2$, which make (34) approach zero closely. Thus, for the right-hand side of the inequality (34), we find that $(n + m)^2/\Delta(\Delta - 1)^2 < 2k$. Thus, for the term $2^k(n + m)^2$ is growing up. The right-hand side of inequality (34) is satisfied. $\square$

Proposition 4.2. *Let T be a tree and $\mathscr{D}(d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. Then, the lower bound of the Sigma index satisfies*

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

Proof. Assume $\mathscr{D}(d_1, d_2, \ldots, d_n)$ is a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, and according to Conjecture 4.2, we noticed that $0 < (n+m)^2/\Delta(\Delta-1)^2 \leqslant 2$. Thus, we find that $d_n^3 + d_1^3 < \Delta(\Delta-1)^2$ and $\sigma(T) \leqslant d_n^3 + d_1^3 + \Delta(\Delta-1)^2$. Then,

$$(37) \qquad \sigma(T) \geqslant d_n^3 + d_1^3 + \Delta(\Delta-1)^2 - \left\lfloor \frac{n^2}{2} \right\rfloor.$$

Thus, for d_i and d_{i+1} we noticed that $1 \leqslant d_i/d_{i+1} \leqslant 2$. Then,

$$\frac{(n+m)^2}{\Delta(\Delta-1)^2} \leqslant \sum_{i=1}^{n-1} \frac{d_i}{d_{i+1}} \leqslant 2n+2,$$

considering the fact that $0 < (n+m)^2/\Delta(\Delta-1)^2 \leqslant 2$. Thus, according to (37) we find that

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

Therefore, the relationship (38) establishes the lower bound by comparing the terms as

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

$$\geqslant d_n^3 + d_1^3 + \Delta(\Delta-1)^2 + \sum_{i=1}^{n-1} \frac{d_i}{d_{i+1}} - 2n - 2$$

$$\geqslant d_n^3 + d_1^3 + \sum_{i=1}^{n-1} \frac{d_i}{d_{i+1}} + \left\lfloor \frac{n^2}{2} \right\rfloor.$$

Thus, as we know, the value $2n+2$ is close to $2n$. Hence, we find that (36) holds. $\square$

Furthermore, we observed that according to $\mathscr{D}$ where we optimize the terms $(d_i - d_{i+1})^3$ and $(d_i - d_{i+1})^2$. In fact, these terms significantly improve the determination of the lower bounds of the Sigma index, especially when studying the differences according to the given conditions in $\mathscr{D}$.

Lemma 4.3. *Let T be a tree with n vertices and m edges. Let $\mathscr{D}(d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. The lower bound of Sigma index satisfies*

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

Proof. Assume $\mathscr{D}(d_1, d_2, \ldots, d_n)$ is a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. To determine the lower bound of the Sigma index given in equation (39), we will use mathematical induction. Consequently, we prove the validity of equation (39) for specific values of n, namely $n = 4, 5, 6$.

For $n = 4$, we have

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

For $n = 5$ we observe that

$$(41) \qquad \sigma(T) \geqslant \sum_{i=1}^{n-1} (d_i - d_{i+1})^3 + \sum_{i=2}^{n-2} (d_i - d_{i+1})^2 + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m)^2}{5} \right\rfloor - 2n.$$

Similarly, for $n = 6$ we find

$$(42) \qquad \sigma(T) \geqslant \sum_{i=1}^{n-1}(d_i - d_{i+1})^3 + \sum_{i=2}^{n-2}(d_i - d_{i+1})^2 + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m)^2}{5} \right\rfloor - 3n.$$

From (40), (41), and (42), considering the term with respect to n (since $m = n - 1$), the relationship (39) holds true for $n = 4, 5, 6$.

Assume the relationship is true for n; we must prove it for $n + 1$. Therefore,

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

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

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

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

Note that the constant term is $\left\lfloor \frac{2(n+m)^2}{5} \right\rfloor$ and since $(d_i - d_{i+1})^3$ is positive due to the non-increasing order $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, we have

$$(43) \qquad \sigma(T) \geqslant n(d_i - d_{i+1})_{i \geqslant 1}^3 + n(d_i - d_{i+1})_{i \geqslant 2}^2 + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m-i)_{i \leqslant m}^2}{5} \right\rfloor.$$

Finally, from (42) and (43), we conclude that the lower bound of the Sigma index holds true for all $n + 1$ and $n + 2$. Thus, equation (39) is established. $\qquad \square$

Similarly, according to Lemma 4.3 we obtained the following result such that we optimized the constant term $2(n+m-i)_{i \geqslant 2}^2$ with $n(d_i - d_{i+1})_{i \geqslant 1}^3$ and $n(d_i - d_{i+1})_{i \geqslant 2}^2$.

Corollary 4.4. *For any tree T with $\mathscr{D}(d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. The lower bound of Sigma index satisfy*

$$(44) \qquad \sigma(T) \geqslant \sum_{i=1}^{n-1}(d_i - d_{i+1})^4 + \sum_{i=2}^{n-2}(d_i - d_{i+1})^3 + d_1^2 + d_n^2 + \left\lfloor \frac{2(n+m-2)^2}{5} \right\rfloor.$$

Throughout Corollary 4.4, discusses a clear case derived from Lemma 4.3. In this case, through both these results, we observed that among Theorem 4.5 which establishes an improvement in the lower bound for the Sigma index to be sufficiently close to Sigma index, and identifying it as a sharp and explicit value with respect to $\mathscr{D}$.

Theorem 4.5. *Let T be a tree with n vertices, m edges, and the maximum degree Δ. Let $\mathscr{D}(d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. The lower bound of the Sigma index satisfies*

$$(45) \qquad \sigma(T) \geqslant \sum_{i=1}^{n-1}(d_i - d_{i+1})^4 + \sum_{i=2}^{n-2}(d_i - d_{i+1})^3 + \sum_{i=1}^{n} d_i^2 + d_1^3 + d_n^3 + 2(d_1 - d_n) - n\Delta.$$

Proof. Let T be a tree with maximum degree Δ and $\mathscr{D}(d_1, d_2, \ldots, d_n)$ is a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. According to Lemma 4.3 we find that the lower bound of Sigma index satisfy

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

Then, we obtain from Corollary 4.4 another lower bound by considering the increase of the terms $(d_i - d_{i+1})^3$ and $(d_i - d_{i+1})^2$. Thus,

$$(46) \qquad \sigma(T) \geqslant \sum_{i=1}^{n-1}(d_i - d_{i+1})^4 + \sum_{i=2}^{n-2}(d_i - d_{i+1})^3.$$

For that reason, by returning to the discussion we presented in Lemma 4.3, we confirm that the relation (45) holds for $n = 2, 3, 4$. Now, let us assume its validity for n and prove that it also holds for $n + 1$.

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

$$\geqslant \sum_{i=1}^{n-2}(d_i - d_{i+1})^4 + \sum_{i=1}^{n-3}(d_i - d_{i+1})^3 + \sum_{i=1}^{n} d_i^2 + d_1^3 + d_{n-1}^3 + 2(d_1 - d_{n-1}) - 2(n-1)\Delta$$

$$\geqslant \sum_{i=2}^{n}(d_i - d_{i+1})^4 + \sum_{i=3}^{n-1}(d_i - d_{i+1})^3 + \sum_{i=2}^{n+1} d_i^2 + d_1^3 + d_n^3 - d_{n-1}^3 + 2(d_1 - d_n) + d_{n-1} - (n+1)\Delta$$

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

Then, it holds the following relationship (47) by considering that the term $d_i - d_{i+1}$ satisfies $d_i - d_{i+1} \leqslant \Delta$, with the constant term $2(d_1 - d_n)$.

$$(47) \quad \sigma(T) \geqslant (n-1)\Delta^4 - (n-3)\Delta^3 + \sum_{i=3}^{n+2}(d_1 + (i-1)\Delta)^2 + \sum_{i=1}^{n} d_i^3 - \left(\frac{3}{2}(d_1 + d_n) + (n+2)\Delta \right).$$

Thus, for the term $d_1^3 + d_n^3$ we find that $d_1^3 + d_n^3 - d_{n-2}^3 - d_{n-1}^3 \leqslant \lfloor 2(n+m)^2/9 \rfloor$. Then, for the constant term $2n - 2$ where $2n - 2 > 2(d_1 - d_n)$ we noticed that

$$(48) \qquad \sigma(T) \geqslant \sum_{i=1}^{n-1} d_i(d_i - d_{i+1})^4 + \sum_{i=2}^{n-2} d_i(d_i - d_{i+1})^3 + 2n - 2.$$

Hence, from (48) for the term $d_1^3 + d_n^3 - d_{n-2}^3 - d_{n-1}^3 + 2(d_1 - d_n) - (n+2)\Delta$, we noticed that

$$(49) \qquad \sigma(T) \geqslant \sum_{i=1}^{n-1} d_i(d_i - d_{i+1})^4 + \sum_{i=2}^{n-2} d_i(d_i - d_{i+1})^3 + (d_1 - 1)^3 + (d_n - 1)^3 - (n+2)\Delta.$$

Finally, from (46)–(49) we find that the relationship (45) is true for $n + 1$ and $n + 2$. Thus, the lower bound of Sigma index (45) holds. $\qquad \square$

The constant term has many cases to optimize the behavior of Sigma index such that in Theorem 4.6. Therefore, we consider the constant term had given as $\lfloor \frac{2n-1}{2} \rfloor \lceil \frac{3n-2}{3} \rceil$ by considering the value of n and Δ.

Theorem 4.6. *Let T be a tree with n vertices, m edges, and the maximum degree Δ. Let $\mathscr{D}(d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. The lower bound of the Sigma index satisfies*

$$(50) \qquad \sigma(T) \geqslant d_1^3 + d_n^3 + \sum_{i=2}^{n-1}(d_i - d_{i+1})^4 + \left\lfloor \frac{2n-1}{2} \right\rfloor \left\lceil \frac{3n-2}{3} \right\rceil + \frac{1}{2}n\Delta.$$

Proof. Assume $\mathscr{D}(d_1, d_2, \ldots, d_n)$ is a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. Then, according to Theorem 4.5, 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,

$$(51) \qquad \sigma(T) \geqslant d_1^3 + d_n^3 + \sum_{i=2}^{n-1}(d_i - d_{i+1})^4.$$

Therefore, the lower bound discussed in Theorem 4.5 and Lemma 4.3 establishes the required lower bound in (50). Thus,

$$(52) \qquad \sigma(T) \geqslant \sum_{i=1}^{n-1}(d_i - d_{i+1})^3 + \sum_{i=2}^{n-2}(d_i - d_{i+1})^2 + d_1^3 + d_n^3.$$

Hence, from (51) and (52), we find that, for the value of n,

$$(53) \qquad \sigma(T) \geqslant d_1^3 + d_n^3 + \left\lfloor \frac{2n-1}{2} \right\rfloor \left\lceil \frac{3n-2}{3} \right\rceil + \frac{1}{2}n\Delta.$$

Here, through relations (51), (52), and (53), relation (50) 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 (50) holds:

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

$$\geqslant d_1^3 + d_2^3 + d_{n-1}^3 + \sum_{i=1}^{n-2}(d_i - d_{i+1})^4 + \left\lfloor \frac{n-2}{2} \right\rfloor \left\lceil \frac{n-3}{3} \right\rceil + \frac{1}{2}n\Delta$$

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

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

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

$$(54) \qquad \sigma(T) \geqslant \sqrt{\sum_{i=1}^{n} d_i^3 - \sum_{i=2}^{n-1} d_i^2} + \left\lfloor \frac{2n-1}{2} \right\rfloor \left\lceil \frac{3n-2}{3} \right\rceil + \frac{1}{2}n\Delta.$$

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 (50) is valid for $n+1$ and $n+2$. Therefore, as the final result among all lower bounds (51)–(54), we find that (50) holds.

$\square$

5. Discussion The Effects of Bounds

From the results studied in Sections 3 and 4, we emphasize that the optimal behavior study of the Sigma index is conducted by evaluating the upper and lower bounds of the index along with some selected topological indices. According to Lemma 3.2, we find that we presented the upper bound of the Sigma index as

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

Also, we presented upper bound of the Sigma index through Theorem 3.4 as

$$\sigma(T) \leqslant \sum_{i=1}^{n-1} \lambda_{\mathscr{D}}(d_i - d_{i+1})^3 + 2(n^2 + m^2) + 3m + n + 2.$$

Hence, we observe that the difference making the upper bound sufficiently close is $n^2 + m^2$ and $n(m - \Delta)$. Thus, we presented among Theorem 3.5, the relationship of the sharp upper bound of Sigma index with it collories as

$$\sigma(T) \leqslant \sum_{i=1}^{n} d_i^3 + \frac{2\lambda_{\mathscr{D}}(n^2 + m^2)}{3(n + m)}.$$

Thus, let k be an integer where $2 \leqslant k < m - 1$. Then, the upper bound of Sigma index associated with the terms $n^2 + m^2$ and $n(m - \Delta)$. Therefore, the closest upper bound of Sigma index satisfy

(55) $$\sigma(T) \leqslant k(n^2 + m^2) + n(km - \Delta).$$

From another perspective, based on PropositionS 4.1, 4.2 and Lemma 4.3, the fixed constant in each that ensures the lower bound closely approximates the Sigma index related to the term $\lfloor (2(n + m)^2)/5 \rfloor$. Consequently, by considering relation (55) and employing a similar reasoning, we derive the value that most accurately approaches the Sigma index through the tightest possible lower bound as:

(56) $$\sigma(T) \geqslant \frac{1}{k}(n^2 + m^2) + \frac{1}{m - k}n(m - \Delta) + \left\lfloor \frac{2(n + m)^2}{5k} \right\rfloor.$$

Furthermore, from (55) and (56) we noticed that the difference between both bounds

$$k(n^2 + m^2) + n(km - \Delta) - \left(\frac{1}{k}(n^2 + m^2) + \frac{1}{m - k}n(m - \Delta) + \left\lfloor \frac{2(n + m)^2}{5k} \right\rfloor \right)$$

yield to

$$\frac{k^2 - 1}{k}(n^2 + m^2) + n\left(km - \Delta - \frac{m - \Delta}{m - k} \right) - \left\lfloor \frac{2(n + m)^2}{5k} \right\rfloor$$

Therefore, the difference provides the upper bound of Sigma index which we noticed that:

$$\sigma(T) < \frac{k^2 - 1}{k}(n^2 + m^2) + n\left(km - \Delta - \frac{m - \Delta}{m - k} \right) - \left\lfloor \frac{2(n + m)^2}{5k} \right\rfloor.$$

Enhancing the previous discussion, through Table 2 we demonstrate a comparison between the behavior of these extreme bounds.

Proposition 5.1. *Let T be a tree with degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. Then, the lower bound of $\sigma(T)$ satisfies*

$$(57) \qquad \sigma(T) \geqslant \left\lceil \frac{2(n+m)^2}{3} \right\rceil - 2 \left(n \sum_{i=1}^{n-1} (d_i - d_{i+1})^2 + \sqrt{m\eta(n)} \right).$$

Proof. Assume the degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, and let $\sigma \odot (T)$ be the average Sigma index for the cases $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ and $d_n \geqslant \cdots \geqslant d_1$. Then, according to Convention 6.1, we find that $2m < \sqrt{m\eta(n)} < m^2$. Thus, we have

$$(58) \qquad \sigma(T) \geqslant \left\lceil \frac{2(n+m)^2}{3} \right\rceil - \sigma \odot (T) + 2\sqrt{m\eta(n)}.$$

Therefore, let $a, b \in \mathbb{N}$ with $a < b$, satisfying $a < \sigma(T) < b$ and $a < \sigma \odot (T) + 2\sqrt{m\eta(n)} < b$. As a direct consequence, we obtain

$$\sigma(T) \geqslant \sigma \odot (T) + 2\sqrt{m\eta(n)}.$$

Then,

$$(59) \qquad \sigma(T) \geqslant 2a \left(n \sum_{i=1}^{n-1} (d_i - d_{i+1})^2 + \sqrt{m\eta(n)} \right) + \sigma \odot (T) - 2b\sqrt{m\eta(n)}.$$

Hence, from (58) and (59) we notice that

$$\sigma(T) \leqslant \left\lceil \frac{2(n+m)^2}{3} \right\rceil,$$

and this relationship establishes the lower bound of the Sigma index given by (57). $\qquad \square$

We refer to the lower bound 1 (LB1) through Lemma 4.3 and to the lower bound 2 (LB2) through Theorem 4.5. Similarly, the upper bound 1 (UB1) refers to Lemma 3.2 and the upper bound 2 (UB2) refers to Theorem 3.4. The positions labeled $n, \sigma(T)$, LB1, LB2, UB1 and UB2 correspond to the variables whose pairwise correlation coefficients are displayed in the correlation matrix as

$$M_{\mathscr{D}} = \begin{pmatrix} 1.000000 & 0.954243 & 0.985349 & 0.928820 & 0.956584 & 0.959995 \\ 0.954243 & 1.000000 & 0.991001 & 0.996741 & 0.999966 & 0.999754 \\ 0.985349 & 0.991001 & 1.000000 & 0.977349 & 0.992055 & 0.993259 \\ 0.928820 & 0.996741 & 0.977349 & 1.000000 & 0.996057 & 0.995292 \\ 0.956584 & 0.999966 & 0.992055 & 0.996057 & 1.000000 & 0.999862 \\ 0.959995 & 0.999754 & 0.993259 & 0.995292 & 0.999862 & 1.000000 \end{pmatrix}$$

Noticed that, regression coefficients $[-7.047368, -4.26834614]$, intercept 13518.783306538098, Model R^2 is 0.9999999997765274.

D	n	$\sigma(T)$	LB1	LB2	UB1	UB2
(15,13,11,10,8,6,4)	67	6318	7370	3293	179785.49	18349.43
(18,15,13,11,10,8,5)	80	10982	10553	5807	305555.00	26503.86
(21,17,15,12,12,10,7)	94	17714	14628	9543	498191.16	37144.43
(24,19,17,13,14,12,9)	108	26908	19403	14881	758415.44	50221.00
(27,21,19,14,16,14,11)	122	38972	24882	22235	1096368.79	66090.14
(30,23,21,15,18,16,13)	136	54314	31073	32091	1522259.18	85156.43
(33,25,23,16,20,18,15)	150	73342	37981	45007	2046200.62	107872.43
(36,27,25,17,22,20,17)	164	96464	45612	61613	2678413.08	134738.71
(39,29,27,18,24,22,19)	178	124088	53973	82611	3429033.56	166303.86
(42,31,29,19,26,24,21)	192	156622	63068	108775	4308189.06	203164.43

TABLE 2. Optimize of extremal bounds among Sigma index.

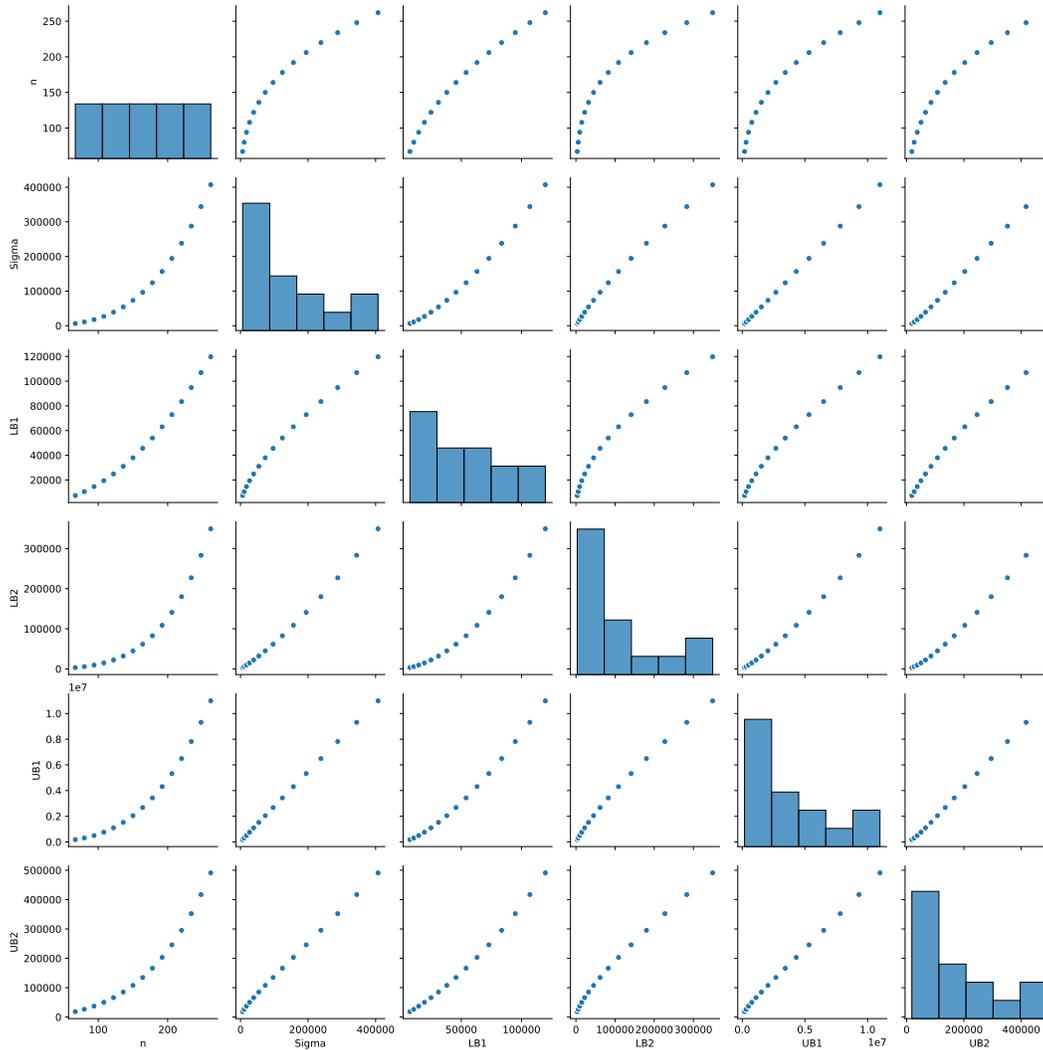Through the following Figure 3, we present analyze the data among Table 2.

FIGURE 3. Analysis the extremal value by Table 2.

6. Sharp Bounds on the σ-Irregularity of Trees with Given Degree Sequences

We presented the first study of topological indices — specifically the Albertson and Sigma indices — on trees through [28], and extended the research to include advanced results through [30]. Refine topological indices — specifically the Albertson and Sigma indices — on trees by findings sharply bounds to determine the optimal behavior of the Sigma index, which is crucial for establishing the tightest bounds of this index by examining its upper and lower bounds. Consequently, this research aims to anticipate and establish the bounds related to the Sigma index and to examine the influence of these bounds on both values derived according to the ordering of the included sequence.

In this section, the lower bound of $\sigma \bigodot (T)$ had presented among Proposition 6.1 for the case $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, and the case $d_n \geqslant \cdots \geqslant d_1$.

Proposition 6.1. *Let T be a tree with degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$. Then, the lower bound of $\sigma \bigodot (T)$ satisfy*

$$(60) \qquad \sigma \bigodot (T) \geqslant \sum_{i=1}^{n} d_i^3 - \sum_{i=1}^{n-1} \left\lceil \frac{d_i}{d_{i+1}} \right\rceil - \left\lfloor \frac{2n^2}{3} \right\rfloor.$$

Proof. Let us recall degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ for $\sigma \bigodot (T)$ we should be discussed with the case $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, and the case $d_n \geqslant \cdots \geqslant d_1$. Thus,

Case 1: If $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ ordered such that $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. In this case, according to Theorem 2.2, we noticed that the Sigma index satisfies $\sum_{i=1}^{n} d_i^3 \geqslant (d_n - 1)^3 + (d_1 - 1)^3$. Then,

$$(61) \qquad \sigma(T) \geqslant \sum_{i=1}^{n} d_i^3 - \left((d_n - 1)^3 + (d_1 - 1)^3 + \sum_{i=1}^{n-1} (d_i - d_{i+1})^2 \right).$$

On the other hand, let Δ be the maximum degree of vertices, since $\sum_{i=1}^{n-1} \left\lceil \frac{d_i}{d_{i+1}} \right\rceil \leqslant \Delta$ and $2n/3 \geqslant \Delta$. Thus, from (61) we have

$$(d_1 - 1)^3 < \sum_{i=1}^{n-1} \left\lceil \frac{d_i}{d_{i+1}} \right\rceil < \left\lfloor \frac{2n^2}{3} \right\rfloor$$

Therefore, in this case, we find that $\sigma(T) \geqslant \sigma \bigodot (T)$. Thus, from (61), we find that (60) is satisfied.

Case 2: If $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ ordered such that $d_n \geqslant d_{n-1} \geqslant \cdots \geqslant d_1$. Similarly, the discussion we presented in the previous case for the purpose of avoiding repetition, we find that:

$$(62) \qquad \sigma(T) \geqslant \sum_{i=1}^{n} d_i^3 - \sum_{i=2}^{n-1} (d_i + 2)(d_i - 1)^2.$$

Therefore,

$$(63) \qquad \sigma(T) \geqslant \sum_{i=1}^{n} d_i^3 - \sum_{i=2}^{n-1} d_i^2 + 2n - 2.$$

Hence, we find that $2n > \Delta$ and according to the term of degree sequence $\mathscr{D}$ we noticed that $\sigma(T) > \sum_{i=2}^{n-1} d_i^2 + 2n - 2$. Thus, we find that $\sigma(T) \leqslant \sigma \bigodot (T)$. Then, from (62) and (63) the relationship (60) holds. $\qquad \square$

Assume $\eta(n)$ be the function discussed the value of n where it defined as $\eta(n) = 2n^2 + n - 2$. Among Proposition 5.1, we observe that through Convention 6.1 for the Sigma index.

Convention 6.1. *For strictly natural numbers, we have the inequality*

$$(64) \qquad 0 < \sqrt{\eta(n)} \left(\left(\frac{1}{\sqrt{2}} \right)^n + \left(\frac{1}{\sqrt{2}} \right)^m \right) < 10.$$

Through Figure 4, we denote the Sigma index with order $d_n \geqslant d_{n-1} \geqslant \cdots \geqslant d_1$ by T_1 and that with order $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ by T_2. The figure illustrates the optimal impact of the Sigma index behavior by showing how it is directly influenced by the degree sequence when it is either increasing or decreasing. This impact is clearly reflected through $\sigma \bigodot (T)$ in Propositions 6.1 and 5.1.
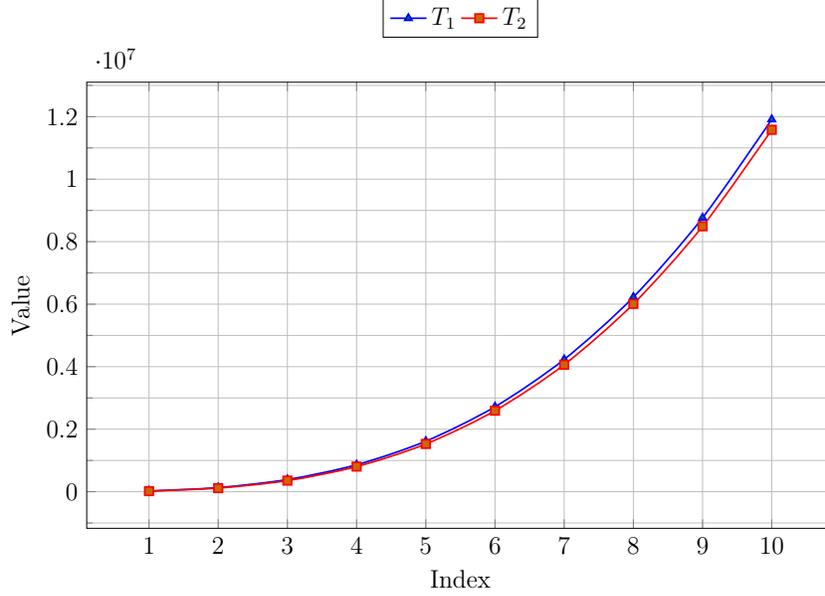

FIGURE 4. Compare $\sigma(T)$ and $\sigma \bigodot (T)$.

Study of trees in the case of paths and stars was utilized through Lemma 6.2, where we observe both the upper and lower bounds at both sides of the inequality.

Lemma 6.2. *Let T be a tree and $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. Then,*

$$(65) \qquad (n-1)\sqrt{\eta(n)} \leqslant \sigma(T) \leqslant (n-1)(2n^2 - n - 2),$$

with equality if and only if $T \cong \mathcal{P}_n$ or $T \cong \mathcal{S}_n$.

Proof. Let us consider the degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$, which we assume to be decreasing. We need to prove both sides of the inequality (65). If the path $\mathcal{P}_n$ satisfies the Sigma index condition for $n \geqslant 3$ as $\sigma(\mathcal{P}_n) = 2$, then we find that the Sigma index yields

$$\sigma(\mathcal{P}_n) > \sqrt{\eta(n)}.$$

Thus, the left-hand side of the inequality (65) holds. The Sigma index of the star tree is known as $\sigma(\mathcal{S}_n) = (n-1)(n-1)^2$. Since $\eta(n) = 2n^2 + n - 2$, we show that $\sigma(T) > \sqrt{\eta(n)}$. Then,

$$(66) \qquad \sigma(T) \leqslant 2n^2 + (n-1)(n-m)^2.$$

Therefore, we notice that

$$2n^2 + (n-1)(n-m)^2 \leqslant (n-1)(2n^2 - n - 2).$$

Then, according to (66), the right-hand side of the inequality (65) holds. $\qquad \square$

Throughout the Lemma 6.3, it involves comparing different bounds, considering how the terms behave asymptotically or approximately (e.g., $2(2n-m)^2 \sim 2m^2$) and also justifies why the degree sequence is considered in the non-increasing order $d_1 \geqslant \cdots \geqslant d_n$ based on a comparison shown in Figure 4 where one configuration T_1 is greater than another T_2.

Lemma 6.3. *Let T be a tree and $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ be a degree sequence. Then, the lower bound of Sigma index satisfying*

$$(67) \qquad \sigma(T) \geqslant \sqrt{\frac{2n}{m-2}\left(2m^2 - \sum_{i=1}^{n} d_i^2 - \left[\frac{1}{2}(d_n - 1)^3 + (d_1 - 1)^3\right]\right)}.$$

Proof. Assume $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ is a degree sequence. According to Convention 6.1, we notice that for $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ the following inequality holds:

$$(68) \qquad 2 \leqslant \frac{d_1 + d_2}{3(d_n + d_{n-1})}\sqrt{\frac{2n}{m-2}} \leqslant 4,$$

where $1 < \sqrt{\dfrac{2n}{m-2}} < 2$. Therefore, considering the relation (68), the lower bound of the Sigma index is given by

$$(69) \qquad \sigma(T) \geqslant 2m^2 + \sqrt{\frac{2n}{m-2}}.$$

Henceforth, we consider the Sigma index with $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ instead of $d_n \geqslant d_{n-1} \geqslant \cdots \geqslant d_1$ because, as shown in Figure 4, we have $T_1 > T_2$. Thus, we observe that

$$\sigma(T) \geqslant 2m^2 - \sum_{i=1}^{n} d_i^2 - \left[\frac{1}{2}(d_n - 1)^3 + (d_1 - 1)^3\right]$$

$$\geqslant 2m^2 - \sum_{i=2}^{n-1} d_i^2 - \left[\frac{1}{2}(d_{n-1} - 1)^3 + (d_2 - 1)^3\right] + 2n - 2$$

$$\geqslant 2(2n - m)^2 - \sum_{i=1}^{n+1} d_i^2 - \left[\frac{1}{2}(d_{n+1} - 1)^3 + (d_1 - 1)^3\right] + 2$$

$$\geqslant \sqrt{\frac{2n}{m-2}\left(2m^2 - \sum_{i=1}^{n} d_i^2 - \left[\frac{1}{2}(d_n - 1)^3 + (d_1 - 1)^3\right]\right)} + 2n + 2.$$

Therefore, from this last lower bound and by considering the term $2n + 2$ as a constant term and the approximation $2(2n - m)^2 \sim 2m^2$, according to (68) and (69), we conclude that (67) holds. This completes the proof. $\qquad\square$

6.1. **The Optimal Lower Bound of Sigma Index.** The findings previously discussed in relation to Properties 6.1 and 5.1, along with the theoretical framework that refined these results in Lemmas' 6.2 and 6.3, underscore the critical importance of identifying whether the sequence is increasing or decreasing, as elucidated in Figure 4. Leveraging this established foundation, we aim to present optimal results concerning the lower bound of the sigma index, which poses the primary challenge in achieving the most precise and robust outcome, both methodologically and substantively.

We presented among Theorem 6.4, basic bounds on the Sigma index $\sigma(T)$ satisfied with $\sigma(T) \geqslant 2n^2$ and $\sigma(T) < \Delta(\Delta - 1)^2$, which imply $\sigma(T) \geqslant 2n^2 + \Delta(\Delta - 1)^2$.

Theorem 6.4. *Let T be a tree with n vertices and m edges, let $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ be a degree sequence with maximum degree Δ. Then, the lower bound of Sigma index satisfying*

$$(70) \qquad \sigma(T) \geqslant \frac{2nm\sqrt{2n^2 - nm + 2}}{\Delta(\Delta - 1)^2} + \left\lfloor\frac{2(n + m)^3}{3}\right\rfloor - 2n^2 + \Delta(\Delta - 1)^2 + 2.$$

Proof. Let us consider the decreasing degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$, with n vertices, m edges, and maximum degree Δ. Clearly, $\sigma(T) \geqslant 2n^2$ and $\sigma(T) < \Delta(\Delta - 1)^2$. Thus, we observe that

$$(71) \qquad \sigma(T) \geqslant 2n^2 + \Delta(\Delta - 1)^2.$$

Assume $\mathcal{T}_{n,\Delta}$ is the class of trees where $T \in \mathcal{T}_{n,\Delta}$. Then, let $d_T(v_\ell)$ be the degree of vertex v_ℓ, with degrees ordered as $d_T(v_1) \leqslant d_T(v_2) \leqslant \cdots \leqslant d_T(v_\ell) \leqslant \cdots \leqslant d_T(v_{n-1}) \leqslant d_T(v_n)$. It follows that

$$(72) \qquad \sigma(T) \geqslant 2d_T(v_\ell)^2 + \Delta(d_T(v_n) - d_T(v_1))^2 + 2n - 2.$$

For $d_T(v_1) \geqslant 3$, we observe that

$$\sigma(T) \geqslant \left(d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 \right)^2 + 2d_T(v_\ell)^2 -$$

$$- \left(\sum_{i=2}^{n-1}(d_T(v_n) - d_T(v_2))^2 + \sum_{i=2}^{n-1}(d_T(v_{n-1}) - d_T(v_3))^2 + \cdots + (d_T(v_3) - d_T(v_2))^2 \right)$$

$$\geqslant \left(d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 \right)^2 + 2d_T(v_\ell)^2 - \sum_{i=2}^{n-1}\sum_{j=i+1}^{n} (d_T(v_j) - d_T(v_i))^2$$

$$\geqslant \left(d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 \right)^2 + 2d_T(v_\ell)^2 - \sum_{2 \leqslant i \leqslant j \leqslant n} (d_T(v_j) - d_T(v_i))^2$$

$$\geqslant \left(d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 \right)^2 + 2d_T(v_\ell)^2 - m\sum_{i=2}^{n} d_T(v_i)^2 - \left(\sum_{i=2}^{n} d_T(v_i) \right)^2.$$

Hence, from (72), it follows that $m \leqslant \sqrt{2n^2 - nm + 2} \leqslant n$. Since $\Delta(\Delta - 1)^2 < 2nm \leqslant \sigma(T)$, we deduce that

$$(73) \qquad \sigma(T) \geqslant \frac{2nm\sqrt{2n^2 - nm + 2}}{\Delta(\Delta - 1)^2} + \frac{2n^2}{m}.$$

Given that

$$2nm\sqrt{2n^2 - nm + 2} \geqslant \left\lfloor \frac{2(n + m)^3}{3} \right\rfloor,$$

we observe that the lower bound for $\sigma(T)$ from (73) satisfies

$$(74) \qquad \sigma(T) \geqslant \left\lfloor \frac{2(n + m)^3}{3} \right\rfloor - \frac{2n^3}{m}.$$

Finally, for $T \in \mathcal{T}_{n,\Delta}$ with $d_T(v_1) \geqslant 3$, we obtain that

$$(75) \qquad \sigma(T) \geqslant d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 - m\sum_{i=2}^{n} d_T(v_i)^2.$$

From (71) through (75), the inequality (70) is validated. This completes the proof. □

Corollary 6.5. *Let $\mathcal{T}_{n,\Delta}$ be the class of trees, for a tree $T \in \mathcal{T}_{n,\Delta}$ according to Theorem 6.4 satisfying*

$$(76) \qquad \sigma(T) \geqslant \left(\sum_{i=1}^{n} d_T(v_i)^3 \right)^2 + 2(d_T(v_n) + d_T(v_1))^2 - m\sum_{i=2}^{n-1} d_T(v_i)^2 - \left(\sum_{i=2}^{n-1} d_T(v_i) \right)^2.$$

The characteristic results discussed in Theorem 6.6 focus on establishing lower and upper bounds for the Sigma index $\sigma(T)$ of trees T in the class $\mathcal{T}_{n,\Delta}$. These bounds combine to explicitly characterize the strict lower bound of the Sigma index using the term in the original Theorem 6.4, equation (77).

Theorem 6.6. *Let T be a tree with n vertices and m edges, let $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ be a degree sequence with maximum degree Δ. Then, the lower bound of Sigma index satisfying*

$$(77) \quad \sigma(T) \geqslant \left(d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 \right)^2 + \sqrt{\frac{5(n+m)^4}{\Delta(\Delta-1)^2}} - \sum_{i=1}^{n} \left(\frac{d_T(v_1)^2 + 3n!}{2^n(m-1)!} \right) - \Delta(\Delta - n)^2.$$

Proof. Recall some information from Theorem 6.4. Let $\mathcal{T}_{n,\Delta}$ be the class of trees such that $T \in \mathcal{T}_{n,\Delta}$. Let $d_T(v_\ell) \geqslant 3$ be the degree of vertex v_ℓ, where $d_T(v_1) \leqslant d_T(v_2) \leqslant \cdots \leqslant d_T(v_\ell) \leqslant \cdots \leqslant d_T(v_{n-1}) \leqslant d_T(v_n)$. Assume the decreasing degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$, with n vertices, m edges, and maximum degree Δ. Then,

$$(78) \quad \sigma(T) \geqslant \left(d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 \right)^2 - m\sqrt{\frac{5(n+m)^4}{\Delta(\Delta-1)^2}} - \left(\sum_{i=2}^{n} d_T(v_i) \right)^2 + 2d_T(v_\ell),$$

by considering the term

$$\sqrt{\frac{5(n+m)^4}{\Delta(\Delta-1)^2}} \leqslant \sum_{i=2}^{n} d_T(v_i)^2 - 2d_T(v_\ell)^2.$$

Therefore, from (78), the Sigma index satisfies $\sigma(T) \leqslant \Delta(\Delta - n)^2$ and $nm \leqslant \Delta(4\Delta - n)^2$. We notice that

$$(79) \quad \sigma(T) \geqslant \left(d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 \right)^2 - \left(\frac{2nm}{3} + \Delta(4\Delta - n)^2 \right).$$

From another perspective, since the condition $d_n \geqslant d_{n-1} \geqslant \cdots \geqslant d_1$, which also holds for the reverse order $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, we observe that the optimal improvement of the lower bound of the Sigma index must achieve an optimal improvement of these lower bounds. From this, it follows that $5(n+m)^4 \geqslant \Delta(4\Delta - n)^2$ and

$$(80) \quad m\sum_{i=2}^{n} d_T(v_i)^2 + \left(\sum_{i=2}^{n} d_T(v_i) \right)^2 \leqslant d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 + 2d_T(v_\ell)^2.$$

Hence, from (79) and (80), we find that

$$(81) \quad \sigma(T) \leqslant \left(d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 \right)^2 + \sqrt{\frac{5(n+m)^4}{\Delta(\Delta-1)^2}}.$$

Thus, we need to prove the lower bound of the Sigma index given in (77). According to other terms in (77), we notice that

$$(82) \quad \sum_{i=1}^{n} \frac{d_T(v_1)^2 + 2n!}{2^n(m-1)!} \leqslant nd_T(v_1)^2 + \frac{2nm^2 + d_T(v_1)^2}{2^n}.$$

Therefore, we have

$$(83) \quad \sigma(T) \geqslant \left(d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 \right)^2 - nd_T(v_1)^2 + \frac{2nm^2 + d_T(v_1)^2}{2^n}.$$

Thus, these convergent bounds of the Sigma index contribute to strictly obtaining the lower bound. Then, we have

$$(84) \qquad \sigma(T) \geqslant \left(d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 \right)^2 - \left(\sum_{i=1} \left(\frac{d_T(v_1)^2 + 3n!}{2^n(m-1)!} \right) + \Delta(\Delta - n)^2 \right).$$

Finally, according to (83) and (84), we notice that the lower bound of the Sigma index strictly holds from the term (77). □

6.2. **Behavior Lower Bound of Sigma Index.** The study of the behavior of any topological index is considered highly important due to several factors, including determining the bounds that are closest to this index. From this perspective, we review through Theorems 6.7 and 6.8 the optimal behavior of the Sigma index according to the given minimum bound. Through Properties 4 and 5, we attempted to present the optimal minimum bound for the Sigma index, which effectively contributes to determining the innovative behavior of the minimum bound of the Sigma index. This is considered the real challenge in understanding the direction of this index and its impact.

Theorem 6.7. *Let T be a tree with n vertices and m edges, let $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ be a degree sequence with maximum degree Δ. Then, according to Theorem 6.6 the lower bound of the Sigma index satisfies*

$$(85) \qquad \sigma(T) \geqslant \sqrt{\sum_{i=1}^{n} d_i^3 - \sum_{i=2}^{n-1} d_i^2 + \left\lfloor \frac{2n-1}{2} \right\rfloor \left\lceil \frac{3n-2}{3} \right\rceil} + \frac{1}{2}n\Delta.$$

Theorem 6.8. *Let T be a tree with n vertices and m edges, let $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ be a degree sequence with maximum degree Δ. Then, the lower bound of the Sigma index satisfies*

$$(86) \qquad \sigma(T) \geqslant \frac{1}{2}\eta(T) + \frac{2n^4 + n^3 - (m-1)^2 + n - 2}{3m^2 - 2n + 2} + \sqrt{\left\lfloor \frac{2n-1}{2} \right\rfloor \left\lceil \frac{3n-2}{3} \right\rceil}.$$

Proof. Let $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ be a degree sequence with maximum degree Δ. Then, among the functions $\eta(T)$, we find that $\sigma(T) \geqslant \eta(T)$. Thus, the inequality is valid for $\sigma(T) > \eta(T)/2$. The Sigma index satisfies $\sigma(T) \leqslant 2n^4 + n^3 - (m-1)^2 + n - 2$ and $\sigma(T) \leqslant 3m^2 - 2n + 2$. Thus,

$$(87) \qquad \sigma(T) \geqslant \frac{2n^4 + n^3 - (m-1)^2 + n - 2}{3m^2 - 2n + 2},$$

where this relationship satisfies

$$\frac{2n^4 + n^3 - (m-1)^2 + n - 2}{3m^2 - 2n + 2} \ll \frac{1}{2}\eta(T).$$

Therefore, according to Theorem (6.7), we notice that

$$(88) \qquad \left\lfloor \frac{2n-1}{2} \right\rfloor \left\lceil \frac{3n-2}{3} \right\rceil \leqslant n(n-\Delta)^2 + 2n + 2.$$

Thus, from (87) and (88) we find that

$$(89) \qquad \sigma(T) \geqslant nm + \sqrt{n(n-\Delta)^2 + 2n + 2}.$$

Hence, from (89) we establish that $\sigma(T) \leqslant \frac{1}{2}\eta(T) + nm$, which implies that $nm + \sqrt{n(n-\Delta)^2 + 2n + 2} \geqslant \eta(T)/2$, and the lower bound of the Sigma index yields

$$(90) \qquad \sigma(T) \geqslant \frac{1}{2}\eta(T) + nm - \frac{2n^4 + n^3 - (m-1)^2 + n - 2}{3m^2 - 2n + 2} + \sqrt{\left\lfloor \frac{2n-1}{2} \right\rfloor \left\lceil \frac{3n-2}{3} \right\rceil}.$$

Actually, according to (90), we find that for (86) the equivalent relation for the term related to the square root achieves $3m^2 - 2n + 2 \leqslant \sqrt{n(n-1)}$, and here we notice that

$$(91) \qquad \sigma(T) \geqslant \frac{1}{2}\eta(T) + \frac{2n^4 + n^3 - (m-1)^2 + n - 2}{3m^2 - 2n + 2} + \sqrt{n(n-1)}.$$

Finally, according to (87)–(91), we find that the lower bound of the Sigma index satisfies $\sigma(T) \geqslant \sqrt{n(n-1)}$. Thus, the relation (86) holds. $\qquad\square$

The following corollaries provide lower bounds for the Sigma index $\sigma(T)$ of a tree T, building upon the main results established in Theorems 6.7 and 6.8.

Corollary 6.9. *For any tree T according to Theorems 6.7 and 6.8 the lower bound of Sigma index satisfy*

$$(92) \qquad \sigma(T) \geqslant d_1^3 + d_n^3 + \sqrt{n(m-1) + \eta(T)} + \frac{1}{2}n\Delta.$$

This result refines the lower bound for $\sigma(T)$ by directly incorporating boundary degree terms $d_1^3 + d_n^3$, which reflect the influence of extremal degrees on $\sigma(T)$.

Corollary 6.10. *According to Theorems 6.7, 6.8 and Corollary 6.9, the lower bound of Sigma index satisfy*

$$(93) \qquad \sigma(T) \geqslant \frac{2n^4 + n^3}{3m^2 - 2n + 2} + \sqrt{n(m-1) + \eta(T)} + \frac{1}{2}n\Delta.$$

6.3. **The Efficiency of Upper Bound.** In this section, Lemma 6.11 gives us the sharp upper bound for the Sigma index, which significantly $2n(m-1)^2 \sim 2n^3$.

Lemma 6.11. *Let T be a tree, and $\mathscr{D} = (d_1, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. Then, the upper bound of Sigma index is $\sigma(T) \leqslant 2n(m-1)^2$.*

Proof. Assume $\mathscr{D} = (d_1, \ldots, d_n)$ be a degree sequence where $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$ with the maximum degree Δ of T. Then, according to Theorem 6.8 the Sigma index satisfy $\sigma(T) \leqslant 2n^4 + n^3 - (m-1)^2 + n - 2$ and $\sigma(T) \leqslant 3m^2 - 2n + 2$. Thus, the sharp upper bound of Sigma index satisfied with the term $2(n+m)^2$. Therefore, let $k \geqslant 2$ and $k \in \mathbb{N}$, we need to show that $\sigma(T) \leqslant 2nk + (km-1)^2$. In this case, clearly $\sigma(T) > 2nk$ where we consider $2 \leqslant k \leqslant n - \Delta$. On the other hand, we notice that

$$(94) \qquad \sigma(T) \leqslant \sqrt{2k + n^2} + (km-1)^2.$$

Thus, the equation (94) established that $\sqrt{2k + n^2} \ll (km-1)^2$. Thus, the upper bound of Sigma index is $\sigma(T) \leqslant (km-1)^2$. $\qquad\square$

Let $\mathscr{D} = (d_1, \ldots, d_n)$ be a degree sequence satisfying $d_1 \leqslant d_2 \leqslant \cdots \leqslant d_n$ had employed for Lemma 6.12. According to Lemma 6.11, if the degrees satisfy the reverse ordering $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, then the $\sigma(T)$ of the tree T is bounded in Lemma 6.11 by $2n(m-1)^2 \sim 2n^3$.

Lemma 6.12. *Let T be a tree, and $\mathscr{D} = (d_1, \ldots, d_n)$ be a degree sequence where $d_1 \leqslant d_2 \leqslant \cdots \leqslant d_n$. Then, the upper bound of Sigma index is*

$$(95) \qquad \sigma(T) \leqslant 2(d_n + d_1)^2 + \sum_{i=1}^{n} d_i(d_i - 1)^2 + 2(n+m)^3.$$

Proof. Assume $\mathscr{D} = (d_1, \ldots, d_n)$ is a degree sequence where $d_1 \leqslant d_2 \leqslant \cdots \leqslant d_n$. Then, according to Lemma 6.11, we find that when $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, the upper bound of the Sigma index is $\sigma(T) \leqslant 2n(m-1)^2$. Thus, we notice that

$$(96) \qquad 2(d_n + d_1)^2 + \sum_{i=1}^{n} d_i(d_i - 1)^2 \leqslant 2n(m-1)^2.$$

Then, equation (96) implies that

$$(97) \qquad \sigma(T) \leqslant 2(d_n + d_1)^2 + \sum_{i=1}^{n} d_i(d_i - 1)^2 + 2n(m - 1)^2.$$

Therefore, by considering the term $2n(m-1)^2$ satisfying $2n(m-1)^2 \ll 2(n+m)^3$, we find that

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

$$\leqslant 2(d_{n-1} + d_2)^2 + d_n^2 + d_1^2 + \sum_{i=2}^{n-1} d_i(d_i - 1)^2 + 2n(m-2)^2$$

$$\leqslant 2(d_{n+1} + d_1)^2 - (d_{n-1} + d_2)^2 + \sum_{i=2}^{n+1} d_i(d_i - 1)^2 + 2n(m+1)^2.$$

Hence, according to the term $2n(m-1)^2 \ll 2(n+m)^3$ and equation (97), the upper bound of the Sigma index satisfies

$$(98) \qquad \sigma(T) \leqslant 2(d_n + d_1)^2 + 2(n + m)^3.$$

Thus, from (98), we note that (95) holds. $\qquad\qquad\qquad\qquad\qquad\qquad\square$

Let $\mathscr{P}(n)$ be a function of vertices where $\mathscr{P}(n) = n(n + m - \Delta)^2$. Then, we noticed that $\sigma(T) \geqslant \sqrt{\mathscr{P}(n)}$, where among Theorem 6.13 had presented the upper bound of Sigma index.

Theorem 6.13. *Let T be a tree, and $\mathscr{D} = (d_1, \ldots, d_n)$ be a degree sequence. Then, the upper bound of Sigma index is*

$$(99) \qquad \sigma(T) \leqslant 2(d_n + d_1)^2 + \sum_{i=1}^{n} d_i(d_i - 1)^2 + \frac{1}{2}\eta(T) + \sqrt{\mathscr{P}(n)}$$

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

$$(100) \qquad \sigma(T) \leqslant \frac{1}{2}\eta(T) + \sqrt{\mathscr{P}(n)} + \Delta(\Delta - 1)^2.$$

In fact, to discuss the remaining bounds, we need to specify the degree sequence in the cases when it is decreasing and when it is increasing, which we demonstrate by discussing each case separately as follows.

Case 1: If $d_1 \leqslant d_2 \leqslant \cdots \leqslant d_n$, then the Sigma index satisfies $\sigma(T) \gg 2(d_n + d_1)^2$. Thus, we find that

$$(101) \qquad \sigma(T) \leqslant 2(d_n + d_1)^2 + \sum_{i=1}^{n} d_i(d_i - 1)^2 + \Delta(\Delta - 1)^2.$$

Since $\sigma(T) \geqslant \sqrt{\mathscr{P}(n)}$, and according to (100) the upper bound of the Sigma index is $\sigma(T) \leqslant \sqrt{\mathscr{P}(n)} + 2(d_n + d_1)^3 + \Delta(\Delta - 1)^2$. Thus, we notice that

$$(102) \qquad \sigma(T) \leqslant \sqrt{\mathscr{P}(n)} + 2(d_n + d_1)^3 + \sum_{i=1}^{n} d_i(d_i - 1)^2.$$

Now, let us generate a sequence according to the terms $d_1 \leqslant d_2 \leqslant \cdots \leqslant d_n$ as $\mathscr{A}_{se} = (d_n - d_{n-1}, d_{n-1} - d_{n-2}, \ldots, d_2 - d_1)$, such that $\mathscr{A}_{se} = (a_1, a_2, \ldots, a_m)$. Then, $\sigma_{\mathscr{D}}(T) \geqslant \sigma_{\mathscr{A}_{se}}(T)$. Thus,

according to (102), we notice that

$$(103) \qquad \sigma(T) \leqslant \sigma_{\mathscr{A}_{se}}(T) + \sqrt{\mathscr{P}(n)} + 2(d_n + d_1)^3.$$

Actually, from (101) to (103), we find that when $d_1 \leqslant d_2 \leqslant \cdots \leqslant d_n$, the upper bound of the Sigma index (99) holds.

Case 2: If $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, then the Sigma index satisfies $\sigma(T) \geqslant 2(d_n + d_1)^2 + 2(d_{n-1} + d_2)^2 + d_n^2 + d_1^2$. Thus, we find that

$$(104) \qquad \sigma(T) \leqslant d_n^2 + d_1^2 + \sum_{i=n}^{2}(d_i - d_{i-1})^2 + \Delta(\Delta - 1)^2.$$

In this case, we can employ the previous discussion from Case 1 to complete this case by referring back to Figure 4, which shows the closeness of the Sigma index between both cases. Here, we note that

$$(105) \qquad \sigma(T) \leqslant \sum_{i=n}^{2}(d_i - d_{i-1})^2 + \frac{1}{2}\eta(T).$$

Thus, according to (104) and (105), the relationship of bounds among the Sigma index yields

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

Then, we notice that

$$(106) \qquad \sigma(T) \leqslant \sum_{i=1}^{n} d_i^3 + \sum_{i=n}^{2}(d_i - d_{i-1})^2 + \frac{1}{2}\eta(T).$$

Therefore, the relationship (106) establishes the upper bound of the Sigma index such that

$$(107) \qquad \sigma(T) \leqslant \sum_{i=1}^{n} d_i(d_i - 1)^2 + \frac{1}{2}\eta(T) + \sqrt{\mathscr{P}(n)} + \sum_{i=n}^{2}(d_i - d_{i-1})^2.$$

Since $\sum_{i=1}^{n} d_i^3 \geqslant 2(d_n + d_1)^2$ and $\sum_{i=1}^{n} d_i^3 \geqslant 2(d_n + d_1)^2 + 2(d_{n-1} + d_2)^2 + d_n^2 + d_1^2$, we notice that the relationship (99) holds. The inequality (99) is confirmed to hold, establishing the validity of these bounds on the Sigma index $\sigma(T)$. $\qquad \square$

6.4. **The Optimal Behavior of Upper Bound on Sigma Index.** Throughout the Theorem 6.14, it establishes upper bounds for the Sigma index $\sigma(T)$ of a tree with degree sequence $\mathscr{D}$. It shows that among equation (108) and provides refined inequalities involving parameters n, m, and k. It confirms that for $2 \leqslant k \leqslant 10$, the bounds hold and relate to the growth of $\sigma(T)$ with respect to k and (n, m).

Theorem 6.14. *Let T be a tree, and $\mathscr{D} = (d_1, \ldots, d_n)$ be a degree sequence. Then, the upper bound of Sigma index is*

$$(108) \qquad \sigma(T) \leqslant \sum_{i=n}^{i=2}(d_i - d_{i-1})^3 + \left\lfloor \frac{2(n+m)}{3} \right\rfloor + \left\lceil \frac{3m^2}{4} \right\rceil + \frac{3n^2 + nm - 2}{2(2m - 3)^2}.$$

Proof. Assume $\mathscr{D} = (d_1, \ldots, d_n)$ is a degree sequence. According to Theorem 6.13, applying equation (106) to the term $\sum_{i=n}^{i=1}(d_i - d_{i-1})^3$, we find that

$$(109) \qquad \sigma(T) \leqslant \sum_{i=n}^{i=2}(d_i - d_{i-1})^3 + \sum_{i=1}^{n} d_i^3 + \Delta(\Delta - 1)^2.$$

Now, let us discuss the remaining bounds in relation to (108), where the degree sequence is not specified as increasing or decreasing; we will handle it as required. Since $m = n - 1$, we note that $2(n + m) \leqslant \Delta(\Delta - 1)^2$ and $3m^2 \leqslant \Delta(\Delta - 1)^2$. Thus,

$$(110) \qquad \sigma(T) \leqslant \left\lfloor \frac{2(n+m)}{3} \right\rfloor + \left\lceil \frac{3m^2}{4} \right\rceil + \Delta(\Delta - 1)^2.$$

Let $k > 1$ be an integer. We emphasize the relationship in (111), where by replacing the term $\eta(T)$ with $\Delta(\Delta - 1)^2$, we need to confirm the inequality for the upper bound of the Sigma index as

$$(111) \qquad \sigma(T) \leqslant k^2 \left\lfloor \frac{2(n+m)}{3} \right\rfloor + k \left\lceil \frac{3m^2}{4} \right\rceil + 2nk - 2.$$

Thus, we observe that

$$(112) \qquad k^2 \left\lfloor \frac{2(n+m)}{3} \right\rfloor + k \left\lceil \frac{3m^2}{4} \right\rceil + 2nk - 2 \leqslant \left\lfloor \frac{2(nk)^2}{3} \right\rfloor + \left\lceil \frac{3km^2}{4} \right\rceil + 2(n+m)k.$$

Therefore, according to (112), it follows that for $2 \leqslant k \leqslant 10$, the inequality

$$(113) \qquad \sigma(T) \leqslant \left\lfloor \frac{2(nk)^2}{3} \right\rfloor + \left\lceil \frac{3km^2}{4} \right\rceil + 2(n+m)k$$

holds. Hence, from (112) and (113), we confirm that the relationship in (111) holds. Moreover, according to (109) and (110), we see that

$$(114) \qquad \sigma(T) \leqslant \sum_{i=n}^{i=2} (d_i - d_{i-1})^3 + \left\lfloor \frac{2(n+m)^2}{3} \right\rfloor + \left\lceil \frac{3m^2}{4} \right\rceil.$$

Finally, for the last term $3n^2 + nm - 2$, we have $3n^2 + nm - 2 < 2(2m - 3)^2$. Thus, from (114), we conclude that the relationship in (108) holds. $\qquad\square$

Theorem 6.15 establishes an upper bound by the relationship (115) showing the Sigma index's dependence on degree increments and structural constants.

Theorem 6.15. *Let T be a tree, and $\mathscr{D} = (d_1, \ldots, d_n)$ be a degree sequence. Then, the upper bound of Sigma index is*

$$(115) \qquad \sigma(T) \leqslant (d_1 - 1)^3 + (d_n - 1)^3 + \sum_{i=n}^{i=2} d_i(d_i - d_{i-1})^3 + 2n^2 + 3m - 2.$$

Proof. Assume $\mathscr{D} = (d_1, \ldots, d_n)$ is a degree sequence. According to Theorems 6.13 and 6.14, the lower bound of the Sigma index satisfies

$$(116) \qquad \sigma(T) \geqslant (d_1 - 1)^3 + (d_n - 1)^3 + \sum_{i=2}^{n} d_i(d_i - d_{i-1})^3.$$

Now, we need to prove that (115) holds with respect to the term $2n^2 + 3m - 2$ by considering the lower bound (116). Assume the maximum degree is Δ, where $\sigma(T) \gg \Delta(\Delta - 1)^2$. Then, clearly, $\Delta(\Delta - 1)^2 \leqslant 2n^2$. Thus,

$$(117) \qquad \sigma(T) \leqslant 2n^2 + \Delta(\Delta - 1)^2.$$

Hence, for the terms involving d_1 and d_n, we have $(d_1 - 1)^3 + (d_n - 1)^3 \leqslant \Delta(\Delta - 1)^2$ and therefore $\sigma(T) \leqslant (d_1 - 1)^3 + (d_n - 1)^3 + 2n^2 + \Delta(\Delta - 1)^2$. Thus,

$$(118) \qquad \sigma(T) \leqslant 2n^2 + \sum_{i=1}^{n} (d_i - 1)^3.$$

From (117) and (118), we observe

$$
\sigma(T) \leqslant 2n^2 + \sum_{i=1}^{n} d_i(d_i - 1)^3
$$

$$
\leqslant 2n^2 + \sum_{i=2}^{n-1} d_i(d_i - 1)^3 + d_1^3 + d_n^3
$$

$$
\leqslant (d_1 - 1)^3 + (d_n - 1)^3 + \sum_{i=2}^{n} d_i(d_i - d_{i-1})^3 + 2n^2.
$$

Accordingly, we note that the optimal behavior of the Sigma index associated with the vertices yields

$$
(119) \qquad \sigma(T) \leqslant \sum_{i=2}^{n} d_i(d_i - d_{i-1})^3 + 2n^2 + 3m - 2.
$$

Thus, according to (119) and considering the constant term $(d_1 - 1)^3 + (d_n - 1)^3$, the relationship (115) holds. $\qquad\square$

7. Novelty on Sigma Index

Through this section, we will review some novelty concepts on the Sigma index, where these concepts are represented by the *reduced Sigma index* given by (1), the *increasing Sigma index*, and the *modified Sigma index*. These indices are currently discussed on *caterpillar trees*, which we will extend to include different trees and graphs in future studies.

7.1. **On Reduced Sigma Index.** To emphasize that the *reduced Sigma index* through this subsection. For example, among Figure 5, we presented the reduced Sigma index according to (1) for the tree with degree sequence $\mathscr{D} = (4, 3, 2, 2, 2, 1, 1, 1, 1, 1)$ is 54.
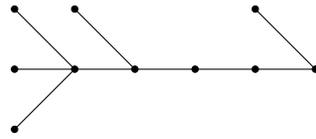

FIGURE 5. Tree with degree sequence $\mathscr{D} = (4, 3, 2, 2, 2, 1, 1, 1, 1, 1)$.

Proposition 7.1. *Let T be a tree with degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$. Then, the lower bound of $\sigma_{red}(T)$ satisfy*

$$
(120) \qquad \sigma_{red}(T) \geqslant \sum_{i=1}^{n} (d_i - 1)^3 - \sum_{i=1}^{n-1} \left\lceil \frac{2d_i}{3d_{i+1}} \right\rceil - \left\lfloor \frac{3n^2}{4} \right\rfloor.
$$

Proof. Immediately according to Proposition 6.1 by considering $\sigma_{red}(T) \geqslant \sigma \odot (T)$. $\qquad\square$

Proposition 7.2. *Let T be a tree with degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$. Then, the lower bound of $\sigma_{red}(T)$ satisfy*

$$
(121) \qquad \sigma_{red}(T) \geqslant \sum_{i=1}^{n} (d_i - 1)^4 - 2n^2 + 3m - 2.
$$

Proof. Recall the degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$ with the maximum degree Δ. Then, we noticed that $\sigma_{red}(T) \geqslant \Delta(\Delta - 1)^2$. Then, according to Theorem 6.6 we have

$$(122) \qquad \sigma_{red}(T) \geqslant \left(d_T(v_1)^2 + \sum_{i=1}^{n} d_T(v_i)^3 \right)^2 - \sum_{i=1}^{n} \left(\frac{d_T(v_1)^2 + 3n!}{2^n(m-1)!} \right) - \Delta(\Delta - n)^2.$$

Thus,

$$\sigma_{red}(T) \geqslant \sum_{i=1}^{n} (d_i - 1)^4 - \sum_{uv \in E(T)} \left[(d_T(u) - 1)^2 + (d_T(v) - 1)^2 \right]$$

$$\geqslant \sum_{i=1}^{n} (d_i - 1)^2 \left(d_i^2 - 3d_i + 1 \right) + + \Delta(\Delta - 1)^2$$

$$\geqslant \sum_{i=n}^{i=2} d_i(d_i - d_{i-1})^3 - 2n^2 + \Delta(\Delta - 1)^2$$

$$\geqslant \sum_{i=1}^{n} d_i^3 - \sum_{i=2}^{n-1} (d_i - d_{i-1})^3 + (d_1 - 1)^3 + (d_n - 1)^3 - 2n^2 + \Delta(\Delta - 1)^2$$

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

$\square$

Theorem 7.1. *Let T be a tree with degree sequence $\mathscr{D} = (d_1, d_2, \ldots, d_n)$. Then, the lower bound of $\sigma_{red}(T)$ satisfy*

$$(123) \qquad \sigma_{red}(T) \geqslant 2n^2 + \sum_{i=1}^{n} d_i(d_i - 1)^3 - \frac{2nm\sqrt{2n^2 - nm + 2}}{\Delta(\Delta - 1)^2} + \frac{2(n + m)^2}{m}.$$

Proof. Since $\sigma(T) \geqslant 2n^2$ and $\sigma(T) < \Delta(\Delta - 1)^2$. Thus, we find that $\sigma(T) \geqslant \sigma_{red}(T)$ according to Theorem 6.4 the reduced Sigma index satisfies $\sigma_{red}(T) \geqslant (d_1 - 1)^3 + (d_n - 1)^3$ and Proposition 7.2,

$$(124) \qquad\qquad\qquad \sigma_{red}(T) \leqslant 2n^2 + \Delta(\Delta - 1)^2.$$

Thus, when $m \leqslant \sqrt{2n^2 - nm + 2} \leqslant n$. Then, the term holds the relationship $\Delta(\Delta - 1)^2 < 2nm \leqslant \sigma_{red}(T)$. Thus,

$$(125) \qquad\qquad\qquad \sigma_{red}(T) \geqslant \frac{2nm\sqrt{2n^2 - nm + 2}}{\Delta(\Delta - 1)^2} + \frac{2(n + m)^2}{m}.$$

Therefore, from (124) and (125) we noticed that

$$(126) \qquad\qquad\qquad \frac{2nm\sqrt{2n^2 - nm + 2}}{\Delta(\Delta - 1)^2} + \frac{2(n + m)^2}{m} \geqslant 2n^2$$

Thus, let $\theta(n)$ be the sharp bound of $\sigma_{red}(T)$ satisfied with (126), since $\Delta \to \infty$, the first term of (126) tends to zero, so the maximum is attained at small Δ. For $2nm \ll (n + m)^2$, the term $\sqrt{2n^2 - nm + 2} \sim \sqrt{n^2 + 2}$, so the first term roughly behaves such that

$$(127) \qquad\qquad\qquad \frac{2nm\sqrt{2n^2 - nm + 2}}{\Delta(\Delta - 1)^2} \sim \frac{2n^2\sqrt{n^2 + 2}}{\Delta(\Delta - 1)^2}.$$

Thus, according to (126) and (127) for large n with $2nm \ll (n+m)^2$ we noticed that the sharp bound $\theta(n)$ satisfies

$$(128) \qquad \frac{2nm\sqrt{2n^2 - nm + 2}}{\Delta(\Delta - 1)^2} + \frac{2(n+m)^2}{m} - 2n^2 \sim n^3$$

Therefore, according to (128) by considering the relationship $\sigma_{red}(T) \geqslant (d_1 - 1)^3 + (d_n - 1)^3$, we find that

$$(129) \qquad \sigma_{red}(T) \geqslant \sum_{i=1}^{n} d_i(d_i - 1)^3 - n^3.$$

Finally, from (124)–(129) we find that the relationship (123) holds. $\qquad\square$

7.2. **Novelty on Sigma Index for Future Works.** Let $\alpha > 1$, according to (2) the general increase Sigma index $\sigma_{inc}^{\alpha}(T)$ of a tree T defined as

$$(130) \qquad \sigma_{inc}^{\alpha}(T) = \sum_{uv \in E(T)} \left[(d_T(u) + 1)^{\alpha} + (d_T(v) + 1)^{\alpha} \right].$$

According to (3), the general modified Sigma index $\sigma_{\alpha}^{*}(T)$ of a tree T defined as

$$(131) \qquad \sigma_{\alpha}^{*}(T) = \sum_{uv \in E(T)} \left[\frac{1}{(d_T(u) + 1)^{\alpha} + (d_T(v) + 1)^{\alpha}} \right].$$

Parameters of Sigma index had provided among (2) and (130) holds Theorem 7.2 for all caterpillar trees.

Theorem 7.2. *Let $\mathscr{D} = (d_1, \ldots, d_n)$ be a degree sequence with $n \geq 3$, such that $d_n > d_1 > d_{n-2} > \cdots > d_3 > d_2 > d_{n-1}$. Then, the caterpillar tree with this ordering attains the maximum value of the increase Sigma index $\sigma_{inc}(T)$ among all caterpillar trees whose path vertices have the degree sequence $\mathscr{D}$.*

Also, parameters of Sigma index had provided among (3) and (131) holds Theorem 7.3 the maximum value for all caterpillar trees.

Theorem 7.3. *Let $\mathscr{D} = (d_1, \ldots, d_n)$ be a degree sequence with $n \geq 3$, such that $d_n > d_1 > d_{n-2} > \cdots > d_3 > d_2 > d_{n-1}$. Then, the caterpillar tree with this ordering attains the maximum value of the modified Sigma index $\sigma^{*}(T)$ among all caterpillar trees whose path vertices have the degree sequence $\mathscr{D}$.*

8. Conclusion

Through this paper, the study of the behavior of the effect of bounds on the Sigma index, considering the existence of many such bounds and their relation to harmonic topological indices as presented in Theorem 3.3, where we proved that the upper bound for the Sigma index is given by

$$\sigma(T) \leqslant \left\lfloor \frac{2n^2}{3\lambda_{\mathscr{D}}} \right\rfloor + \frac{2^{\eta}(m - \Delta)^2}{5(n-1)^3} + (n-1)H(G).$$

Similarly, for the forgotten topological index among Corollary 3.8, we showed that its relation with the Sigma index provides us with the upper bound for the Sigma index as follows $\sigma(T) \leqslant 2F(G) + 2n^2 + 2$. This study provides us with the behavior of extreme values that affect the Sigma index through both the upper and lower bounds.

The improvement of the upper bounds discussed through Lemma 3.1 and Lemma 3.2, and the enhancement of that discussion via Theorems 3.4 and 3.5, provide us with the strictest and most uniform bound. Through Section 4, we discussed the improvement of the lower bounds on the

Sigma index, where we reinforced this discussion using Lemma 4.3 as well as Propositions 4.1 and 4.2, and we refined these results to appear in their complete forms through Theorems 4.5 and 4.6.

The study of the Sigma index through the optimal improvement regarding the effect of extremal bounds on the behavior of the index has a genuine and clear significance concerning the importance of these bounds and their impact on topological indices in general.

Further insights into the asymptotic and minimal behavior of the Sigma index are provided by Theorems 6.7 and 6.8, underscoring key characteristics valuable for ongoing and future studies. Through section 4, Lemma 6.11 gives us the sharp upper bound for the Sigma index, which significantly $2n(m-1)^2 \sim 2n^3$. Theorem 6.15 establishes an upper bound by the relationship

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

These contributions refine previous estimates and clarify the role of extreme degree values in determining the Sigma index.

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References

[1] H. Abdo, S. Brandt, D. Dimitrov, *The total irregularity of a graph*, Discrete Mathematics & Theoretical Computer Science. 16(1) (2014), 201–206.

[2] H. Abdo, D. Dimitrov, *Non-regular graphs with minimal total irregularity*, B. Aust. Math. Soc. 92 (2015) 1–10.

[3] H. Abdo, D. Dimitrov, & I. Gutman, *Graphs with maximal σ-irregularity*, Discrete Appl. Math. 250 (2018) 57–64.

[4] H. Abdo, D. Dimitrov, I. Gutman, *Graph irregularity and its measures*, Applied Mathematics and Computation. 357 (2019), 317–324.

[5] A. Ali, A. M. Albalahi, A. M. Alanazi, A. A. Bhatti, & A. E. Hamza, *On the maximum sigma index of k-cyclic graphs*, Discrete Applied Mathematics. 325 (2023), Pages 58-62, https://doi.org/10.1016/j.dam.2022.10.009.

[6] A. Alia, D. Dimitrovb, T. Rétic, A. M. Albalahia, & A. E. Hamzaa, *Bounds and Optimal Results for the Total Irregularity Measure*, MATCH Commun. Math. Comput. Chem. 94 (2025) 5–29, doi:10.46793/match.94-1.005A.

[7] L. Alex, G. Indulal, & J. J. Mulloor, *On the inverse problem of some bond additive indices*, Communications in Combinatorics and Optimization. 2024.

[8] N. Akgüneş, Y. Nacaroğlu, *On the sigma index of the corona products of monogenic semigroup graphs*, Journal of Universal Mathematics. 2(1) (2019), 68-74.

[9] M. Ascioglu, I. N. Cangul, *Sigma index and forgotten index of the subdivision and r-subdivision graphs*, In Proceedings of the Jangjeon Mathematical Society. 21(2) (2018), pp. 1-14.

[10] M. O. Albertson, *The irregularity of a graph*, Ars Combinatoria. 46 (1997), 219–225.

[11] A. Arif, S. Hayat, & A. Khan, *On irregularity indices and main eigenvalues of graphs and their applicability*, Journal of Applied Mathematics and Computing, 69(3) (2023), 2549-2571.

[12] I. I. Baskin, E. V. Gordeeva, R. O. Devdariani, N. S. Zefirov, V. A. Palyulin, M. I. Stankevich, *Methodology for solving the inverse problem of structure-property relationships for the case of topological indexes*, Dokl. Akad. Nauk SSSR 307 (1989) 613–617.

[13] Y. Caro, R. Pepper, *Degree sequence index strategy*, Australasian Journal of Combinatorics. 59(1) (2014), 1-23.

[14] G. Chartrand, F. Okamoto, & P. Zhang, *The sigma chromatic number of a graph*, Graphs and combinatorics. 26(6) (2010), 755-773, doi:10.1007/s00373-010-0952-7.

[15] Z. Che, Z. Chen, *Lower and upper bounds of the forgotten topological index*, MATCH Commun. Math. Comput. Chem, 76(3) (2016), 635-648.

[16] X. Chen, X. Liu, *The reciprocal irregularity of a graph. Discrete Applied Mathematics*, 378, 348-357.

[17] Z. Du, A. Jahanbai, & S. M. Sheikholeslami, *Relationships between Randic index and other topological indices*, Communications in Combinatorics and Optimization. 6(1) (2021), 137-154.

[18] D. Dimitrov, D. Stevanović, *On the σ_t-irregularity and the inverse irregularity problem*, Appl. Math. Comput. 441 (2023) 127709.

[19] S. Fajtlowicz, *On conjecture sofGrati–II*, Congr.Numer.,60(1987),187–197.

[20] S. Filipovski, D. Dimitrov, M. Knor, & R. Škrekovski, *Some results on σ_t-irregularity* arXiv e-prints, arXiv-2411.

[21] B. Furtula, I. Gutman, *A forgotten topological index*, J. Math. Chem. 53 (2015) 11841190.

[22] W. Gao, W. Wang, M. R. Farahani, *Topological Indices Study of Molecular Structure in Anticancer Drugs*, Hindawi Publishing Corporation Journal of Chemistry, (2016), `http://dx.doi.org/10.1155/2016/3216327`.

[23] D. u. Gómez, Y. Grandati, & R. Milson,*Rational extensions of the quantum harmonic oscillator and exceptional Hermite polynomials*, Journal of Physics A: Mathematical and Theoretical. 47(1) (2013), 015203, doi:10.1088/1751-8113/47/1/015203.

[24] I. Gutman, *Topological indices and irregularity measures*, Bulletin of International Mathematical Virtual Institute. 8 (2018), 469-475.

[25] I. Gutman, M. Togan, A. Yurttas, A. S. Cevik, I. N. Cangul, *Inverse problem for sigma index*, MATCH Commun. Math. Comput. Chem. 79(3) (2018), 491–508.

[26] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, *Graph theory and molecular orbitals. XII. Acyclic polyenes*, The Journal of Chemical Physics. 62(9) (1975), 3399–3405.

[27] I. Gutman, N. Trinajstić, *Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons*, Chemical Physics Letters. 17(4) (1972), 535–538.

[28] J. Hamoud, D. Abdullah, *Topological Indices with Degree Sequence $\mathscr{D}$ of Tree*, `https://arxiv.org/abs/2503.12909v2`

[29] J. Hamoud, D. Abdullah, *Albertson index and Sigma index in trees given by degree sequences*, Chebyshevskii sbornik. 26(3) (2025), doi: 10.22405/2226-8383-2025-26-3-2-11.

[30] J. Hamoud, A. B. Yakovlevich, M. Almahalebi, & D. Abdullah, *Closed-Form Analysis and Extremal Bounds of Albertson and Sigma Indices in Trees with Prescribed Degree Sequences*, arXiv preprint arXiv:2510.19490, doi:10.48550/arXiv.2510.19490.

[31] S. L. Hakimi, *On the realizability of a set of integers as degrees of the vertices of a graph*, SIAM Journal on Applied Mathematics. 10 (1962), 496–506.

[32] M. Knor, R. Škrekovski, S. Filipovski, D. Dimitrov, *Extremizing antiregular graphs by modifying total σ-irregularity*, Applied Mathematics and Computation, 490 (2025), 129199, `https://doi.org/10.1016/j.amc.2024.129199`.

[33] Z. Lingping, *The harmonic index for graphs*, Applied Mathematics Letters. 25(3) (2012), PP 561-566, `https://doi.org/10.1016/j.aml.2011.09.059`.

[34] M. Matejić, I. Milovanović, & E. Milovanović, *On bounds for harmonic topological index*, Filomat, 32(1) (2018), 311-317.

[35] M. R. Oboudi, *A new lower bound for the energy of graphs*, Linear Algebra Appl. 580 (2019), 384395.

[36] P. B. Sarasija, R. Binthiya, *Bounds on the Seidel energy of strongly quotient graphs*, J. Chem. Pharm. Sci. 10 (1) (2017),p 14.

[37] D. C. Schmidt, L. E. Druffel, *A fast backtracking algorithm to test directed graphs for isomorphism using distance matrices*, Journal of the ACM (JACM), 23(3) (1976), 433-445.

[38] J. M. Sigarreta, *Mathematical properties of variable topological indices*, Symmetry, 13(1) (2020), 43.

[39] D. Vukicevic, B. Furtula, *Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges*, J. Math. Chem. 46(4) (2009), 13691376.

[40] A. Vasilyev, R. Darda, & D. Stevanović, *Trees of given order and independence number with minimal first Zagreb index*, MATCH Commun. Math. Comput. Chem. 72 (2014), 775-782.

[41] Z. Yang, M. Arockiaraj, S. Prabhu, M. Arulperumjothi, & J. B. Liu, *Second Zagreb and sigma indices of semi and total transformations of graphs*, Hindawi Complexity. 1 (2021), 6828424, `https://doi.org/10.1155/2021/6828424`.

[42] A. Jahanbanı, S. Ediz, *The sigma index of graph operations*, Sigma Journal of Engineering and Natural Sciences. 37(1) (2019), 155-162.

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