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STUDY OF THE IMPACT OF BOUNDS ON TOPOLOGICAL INDICES WITH SELECTED MODEL OF THE ALBERTSON INDEX AND THE SIGMA INDEX

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Abstract. *In this paper, we present a study on the impact of bounds on selected topological indices, utilizing the extreme values of each topological index. In this study, we choose the Albertson index and the Sigma index as selected models. The Sigma index is defined by the following relationship:*

$$\sigma(G) = \sum_{uv \in E(G)} (d_u(G) - d_v(G))^2 .$$

Additionally, we derive bounds for the minimum and maximum Albertson indices ($\mathrm{irr}_{\min}$ *and* $\mathrm{irr}_{\max}$*) across various tree structures. We also provide upper and lower bounds, incorporating parameters such as the maximum degree* Δ *and the minimum degree* δ*.*

Keywords: Trees, Degree Sequence, Bounds, Zagreb, Topological, Isomorphic.

1. Introduction

Throughout this paper, let $G = (V, E)$ be a simple, connected graph, where $|V(G)| = n$, $|E(G)| = m$, the minimum and the maximum degree of G are denoted by δ, Δ, where $1 \leqslant \delta < \Delta \leq n-1$. Let $\mathcal{P}_n$ be a path of order n and $\mathcal{S}_n$ the star tree of order n, typically denoted by $K_{1,n-1}$. Let $e = uv \in E(G)$ be an edge; then the imbalance of e, known as $|d_G(u) - d_G(v)|$, is employed in the "Albertson index". In 1997, Albertson in [1] denoted the imbalance of an edge uv by $\mathrm{imb}(uv)$, where a graph G is considered regular if all of its vertices have the same degree. The irregularity measure is defined in [1,2,3,4] as:

$$\mathrm{irr}(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|. \tag{1.1}$$

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Denote by $\mathrm{irr}_{\max}$ the maximum of the Albertson index and $\mathrm{irr}_{\min}$ the minimum of the Albertson index. Furthermore, there are studies related to the Albertson index and irregularity; see [1,5,6,7,8,9,10]. Two graphs G and H are deemed identical if their vertex sets are equal, $V(G) = V(H)$, and their edge sets are equal, $E(G) = E(H)$, or equivalently, if $G \subseteq H$ and $H \subseteq G$. The graphs G and H are said to be isomorphic [11], denoted $G \cong H$, if there exists a bijection $\psi : V(G) \to V(H)$ such that an edge $uv \in E(G)$ exists if and only if the edge $\psi(u)\psi(v) \in E(H)$. A subset $S \subseteq V$ of vertices in a graph $G = (V, E)$ is termed a dominating set [11] if every vertex $v \in V$ either belongs to S or is adjacent to at least one vertex in S.

Let $\mathscr{D}(G) = (d_1, d_2, \cdots, d_i)$ be a degree sequence [6,12,13,14,15] of G where $d_1 \geq d_2 \geq \cdots \geq d_n$. Let $\mathscr{D} = (d_1, d_2, \cdots, d_n)$ be a non-increasing degree sequence with $n \geq 2$. There is a graph G_1 with $V(G_1) = \{v_2, v_3, \cdots, v_n\}$; then the degrees of the vertices [17] are:

$$d_{G_1} v_i = \begin{cases} d_i - 1 & \text{if } 2 \leq i \leq d_1 + 1, \\ d_i & \text{if } d_1 + 2 \leq i \leq n. \end{cases} \tag{1.2}$$

We assemble a graph G from G_1 by adding a new vertex v_1 and the e_1 edges $v_1 v_i$ for $2 \leq i \leq d_1 + 1$. By considering $\deg_G v_i = d_i$ for $1 \leq i \leq n$, if $d_1 \geq 1$, this is graphical if and only if the sequence $\mathscr{B} = (d_2 - 1, d_3 - 1, \cdots, d_{e_1+1} - 1, d_{e_1+2}, \cdots, d_n)$ is graphical. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$, respectively, are defined in [21,22,1] as:

$$M_1(G) = \sum_{i=1}^{n} d_i^2, \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) \cdot d_G(v).$$

The recently introduced $\sigma(G)$ irregularity index is a simple diversification of the previously established Albertson irregularity index, where $\sigma_{\max}$ denotes the maximum Sigma index and $\sigma_{\min}$ the minimum Sigma index. The Sigma index is defined in [16,20] as:

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

where $F(G)$ is the sum of squared degrees over all edges, and $M_2(G)$ is the second Zagreb index. This formulation amplifies large degree differences and provides a more sensitive measure of irregularity.

Our goal in this paper is to conduct a study of the bounds related to the selected topological indices, specifically the Albertson index and the Sigma index, particularly when examining the maximum and minimum values of each index and linking these values with the first Zagreb index, the second Zagreb index, and the forgotten index.

This paper is organized as follows. In Section 1, we observe the important concepts for our work, including a literature review of the most related papers. In Section 2, we provide preliminaries on some of the important theories and properties we utilize in understanding the work. In Section 3, we introduce the main results in Subsection 3.1, for some bounds on the Albertson index, and in Subsection 3.2, for some bounds on the Sigma index.

2. Preliminaries

In this section, we explore important concepts and recent advancements in graph irregularity indices, with a particular emphasis on trees. Let $\mathcal{S}$ be a class of graphs. Then we have the maximum and minimum Albertson indices of a graph G, where:

$$\operatorname{irr}_{\max}(\mathcal{S}) = \max\{\operatorname{irr}(G) \mid G \in \mathcal{S}\},$$
$$\operatorname{irr}_{\min}(\mathcal{S}) = \min\{\operatorname{irr}(G) \mid G \in \mathcal{S}\}.$$

In [8], total irregularity is mentioned when $\sum_{i\geq 1} n_i = |V(G)|$, where $|V(G)|$ is the number of vertices of degree i in graph G; it is known as $\operatorname{irr}_T(G) = \sum_{1\leq i<j\leq n-1} n_i n_j (j-i)$. Thus, [8] proved $\operatorname{irr}_T(G) \leq \frac{n^2}{4} \operatorname{irr}(G)$. In this case, if G is a tree, then $\operatorname{irr}_T(G) \leq (n-2) \operatorname{irr}(G)$. Lina, Z., et al. [13] defined the "general Albertson irregularity index" of a graph such that for any number $p > 0$:

$$\operatorname{irr}_p(G) = \left(\sum_{uv \in E(G)} |d(u) - d(v)|^p \right)^{\frac{1}{p}}.$$

According to [13,18], if $p \geq 1$ and $0 \leq d \leq n-1$, then for a degree sequence $\mathscr{D}$ satisfying:

$$\left(\sum_{i=1}^{n} d_i^p \right)^{\frac{1}{p}} \leq (n-1)^{1-\frac{1}{p}} \sum_{i=1}^{n} d_i^{\frac{1}{p}}. \tag{2.1}$$

We present the concept of a *caterpillar tree* in Definition 2.1.

Definition 2.1. *A tree T of order $n \geq 3$ is a caterpillar tree if the graph obtained from T by deleting all its pendant vertices is a path, called the spine of T. We write $T = \mathcal{T}(n, m)$ for a caterpillar tree with n vertices and m pendant vertices, where $2 \leq m \leq n-1$. The spine of $\mathcal{T}(n, m)$ has $k = n - m$ vertices, and $m = n - 1$ if and only if $T \cong \mathcal{S}_n$.*

Let T be the caterpillar tree whose spine is $v_1 v_2 \cdots v_n$ and in which exactly three pendant vertices are attached to each v_i, as illustrated in Figure 1. The degree of v_i is denoted by d_i, for $1 \leq i \leq n$.

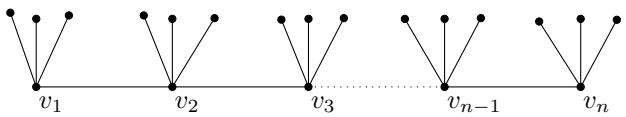


Figure. 1. Caterpillar tree with three pendant vertices at each spine vertex.

Theorem 2.2. *[13] Let G be a connected graph. If $\frac{1}{p} + \frac{1}{q} = 1$, then:*

$$\operatorname{irr}_p(G) \operatorname{irr}_q(G) \geq F - 2M_2,$$

with equality if and only if $p = 2$, or G is a regular graph.

Proposition 2.3 (Upper Bound Sigma index [16]). *For any connected graph G with n vertices, minimum degree δ, maximum degree Δ, and maximal σ irregularity, the upper bound of σ is:*

$$\sigma(G) > \frac{\delta}{\Delta+1}(\Delta-\delta)^3 n, \quad \sigma(G) > \frac{1}{\Delta+1}(\Delta-1)^3 n. \tag{2.2}$$

Yang and Deng [25] provided $1 \leq p \leq n-3$. Then $\Delta(G) = n-1$. According to [23], with path vertices of degrees $d_1, d_2, \cdots, d_n$, we have:

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

Theorem 2.4. *[5] Let T be a tree of order $n \geq 4$. The total Albertson index of T satisfies:*

$$\mathrm{irr}_t(G) = \begin{cases} \mathrm{irr}_{t_{\max}}(G) = (n-1)(n-2), \\ \mathrm{irr}_{t_{\min}}(G) = 2(n-2). \end{cases}$$

3. Main Result

In this section, we present some bounds on the Albertson index in Subsection 3.1, starting with Proposition 3.1 on the Fibonacci number of the Albertson index.

3.1. *Some Bounds of Albertson Index*

In this subsection, we present a study of some bounds on the Albertson index and specify certain bounds between $\mathrm{irr}_{\max}$ and $\mathrm{irr}_{\min}$. In Proposition 3.2, we provide the lower bound of $\mathrm{irr}_{\min}$ and the upper bound of $\mathrm{irr}_{\max}$.

Proposition 3.1. *Let $F_1 = F_2 = 1$, $F_{i+1} = F_i + F_{i-1}$, and let $\mathcal{T}_m$ be the caterpillar where $m \geq 4$ with spine degrees $(F_3, F_4, \cdots, F_m)$. Then*

$$\mathrm{irr}(\mathcal{T}_m) = F_m F_{m+1} - 3F_{m+2} + 2F_m + 2m + 1. \tag{3.1}$$

Proof. According to [23], $\mathrm{irr} = \sum_{i=3}^{m}(F_i-1)(F_i-2) - 2 + 2F_m$. Since $\sum_{i=1}^{m} F_i^2 = F_m F_{m+1}$ and $\sum_{i=1}^{m} F_i = F_{m+2} - 1$ we find that: for $i = 1, 2$,

$$\sum_{i=3}^{m} F_i^2 = F_m F_{m+1} - 2, \quad \sum_{i=3}^{m} F_i = F_{m+2} - 3 \tag{3.2}$$

Then,

$$\sum_{i=3}^{m}(F_i^2 - 3F_i + 2) = F_m F_{m+1} - 2 - 3F_{m+2} + 9 + 2(m-2). \tag{3.3}$$

Hence, from (3.2) and (3.3) and by adding $-2 + 2F_m$ gives (3.1). □

Proposition 3.2. *Let T be a caterpillar tree of order n, let $\mathscr{D} = (d_1, d_2, \cdots, d_n)$ be an increasing degree sequence, let* $\mathrm{irr}_{\max}$ *be the maximum Albertson index, let* $\mathrm{irr}_{\min}$

be the minimum Albertson index, and let Δ *be the maximum degree of vertices and* δ *the minimum degree of vertices. Then:*

$$\mathrm{irr}_{\min}(T) < 2n\delta \frac{2(nm)^3 + 2m\Delta^2}{8n^4\Delta + 8m^3\delta\Delta + \Delta^2(\Delta - 1)} \leq \mathrm{irr}_{\max}(T). \tag{3.4}$$

Indeed, from Proposition 3.2, we present Proposition 3.3 for the upper and lower bounds of the Albertson index, and Proposition 3.4 for the lower bound.

Proposition 3.3. *Let* $\mathcal{T}_{n,\Delta}$ *be the class of trees of order* n *and maximum degree* Δ*, where* $2 \leq \Delta \leq n-1$*. Then,*

$$\mathrm{irr}_{\min}(\mathcal{T}_{n,\Delta}) = \Delta(\Delta - 1), \tag{3.5}$$

and consequently,

$$\mathrm{irr}_{\min}(\mathcal{T}_{n,\Delta}) \geq \frac{(\Delta - 2)^3}{n\Delta - \delta}, \tag{3.6}$$

$$\mathrm{irr}_{\min}(\mathcal{T}_{n,\Delta}) \leq \frac{\delta}{\Delta + 1}\, n\Delta^2 + \frac{\Delta^2(\Delta - \delta)}{6\delta(\Delta - 1)}. \tag{3.7}$$

Proof. Since every tree has a leaf, $\delta = 1$, and all degrees lie in $[1, \Delta]$. Let $T \in \mathcal{T}_{n,\Delta}$ and let v be a vertex with $\deg v = \Delta \geq 2$. The forest $T - v$ has exactly Δ components $C_1, \cdots, C_\Delta$, and each C_i is joined to v by exactly one edge vw_i with $w_i \in C_i$. We claim that each C_i contains a leaf ℓ_i of T. If $C_i = \{w_i\}$, then $\deg w_i = 1$ in T, and we put $\ell_i = w_i$. Otherwise C_i is a tree with at least two vertices, hence with at least two leaves, and we choose a leaf ℓ_i of C_i with $\ell_i \neq w_i$. The only edge joining C_i to the rest of T is vw_i, so ℓ_i has degree 1 in T.

Let $\mathcal{P}_i$ be the path from v to ℓ_i in the subgraph induced by $C_i \cup \{v\}$. The sets $C_1, \cdots, C_\Delta$ are pairwise disjoint, so the paths $\mathcal{P}_1, \cdots, \mathcal{P}_\Delta$ share only the vertex v, and therefore they are pairwise edge-disjoint.

Lower bound. Along $\mathcal{P}_i$, the triangle inequality gives

$$\sum_{uw \in E(\mathcal{P}_i)} |d_u - d_w| \;\geq\; |\deg v - \deg \ell_i| = \Delta - 1. \tag{3.8}$$

Summing over the edge-disjoint paths and dropping the non-negative contribution of the remaining edges,

$$\mathrm{irr}(T) \;\geq\; \sum_{i=1}^{\Delta} \sum_{uw \in E(\mathcal{P}_i)} |d_u - d_w| \;\geq\; \Delta(\Delta - 1). \tag{3.9}$$

Since $n - 1 \geq \Delta$, we can choose integers $a_1, \cdots, a_\Delta \geq 1$ with $\sum_{i=1}^{\Delta} a_i = n - 1$. Let S be the spider with centre v of degree Δ and legs of lengths $a_1, \cdots, a_\Delta$. Then $S \in \mathcal{T}_{n,\Delta}$. A leg of length 1 is a leaf adjacent to v and contributes $\Delta - 1$. A leg of length at least 2 has degrees $\Delta, 2, \cdots, 2, 1$ and contributes $(\Delta - 2) + 0 + 1 = \Delta - 1$. Hence,

$$\mathrm{irr}(S) = \Delta(\Delta - 1). \tag{3.10}$$

Inequality (3.9) holds for every $T \in \mathcal{T}_{n,\Delta}$, and (3.10) shows that it is attained.

Since $n \geq \Delta + 1$ and $\delta = 1$, we have $n\Delta - \delta \geq \Delta^2 + \Delta - 1 \geq \Delta^2$. Then, for $\Delta \geq 2$,

$$\frac{(\Delta-2)^3}{n\Delta-\delta} \;\leq\; \frac{(\Delta-2)^3}{\Delta^2} \;\leq\; \Delta - 2 \;\leq\; \Delta(\Delta-1) \;=\; \mathrm{irr}_{\min}(\mathcal{T}_{n,\Delta}), \tag{3.11}$$

which gives (3.6).

Upper bound. With $\delta = 1$ the right-hand side of (3.7) equals:

$$\frac{n\Delta^2}{\Delta+1} + \frac{\Delta^2}{6}. \tag{3.12}$$

Since $n \geq \Delta + 1$, we have $\frac{n\Delta^2}{\Delta+1} \geq \Delta^2$, and therefore:

$$\frac{n\Delta^2}{\Delta+1} + \frac{\Delta^2}{6} \;\geq\; \Delta^2 \;\geq\; \Delta(\Delta-1) \;=\; \mathrm{irr}_{\min}(\mathcal{T}_{n,\Delta}), \tag{3.13}$$

which gives (3.7). □

Proposition 3.4. *Let T be a caterpillar tree, where $n = |V|$ and $m = |E|$, with maximum degree Δ and minimum degree δ. Then the upper bound of the minimum Albertson index* $\mathrm{irr}_{\min}$ *is:*

$$\mathrm{irr}_{\min} \geq \lceil \log_2(n+1) - 1 \rceil + 2\Delta(T) - 1. \tag{3.14}$$

Lemma 3.6 considers a pair of caterpillar trees, T_1 and T_2, with distinct degree sequences: T_1 possesses a degree sequence dominated by vertices of degree 2, resembling a path graph, while T_2 is characterized by a degree sequence comprising prime numbers. Lemma 3.7 focuses on a single tree with general degree properties, introducing a parameterized lower bound that accounts for the maximum and minimum degrees, modulated by a scaling factor α.

The next result gives sharp bounds for arbitrary trees.

Proposition 3.5. *Let T be a tree of order $n \geq 3$ with maximum degree Δ. Then,*

$$\mathrm{irr}(T) \leq (n-1)(\Delta-1). \tag{3.15}$$

Proof. Since T is connected and $n \geq 3$, every vertex has degree at least 1, and by the definition of Δ at most Δ. Hence for every edge $uw \in E(T)$, $1 \leq d_u,\ d_w \leq \Delta$. Then, $|d_u - d_w| \leq \Delta - 1$. The tree T has $n-1$ edges. Thus (3.15) holds. Since $n \geq 3$ we have $\Delta \geq 2$. Equality in (3.15) holds if and only if every edge has imbalance exactly $\Delta - 1$. Let u be a vertex of degree Δ. Each neighbour w of u satisfies $|d_u - d_w| = \Delta - 1$, $d_w = 1$. Thus all neighbours of u are leaves, and since T is connected, T has no other vertices. Hence $T \cong \mathcal{S}_n$. Conversely, $\mathrm{irr}(\mathcal{S}_n) = (n-1)(n-2) = (n-1)(\Delta-1)$. □

Lemma 3.6. *Let $n_1 \geq 5$ and $2 \leq \Delta_1 \leq n_1 - 3$. Let $T_1 \in \mathcal{T}_{n_1,\Delta_1}$ and $T_2 \in \mathcal{T}_{n_2,\Delta_2}$ with $n_2 = n_1 - 1$ and $\Delta_2 = \Delta_1 + 1$. Then*

$$2\Delta_1^2 \;\leq\; \mathrm{irr}(T_1) + \mathrm{irr}(T_2) \;<\; (2n_1 - 3)\Delta_1 - n_1 + 1. \tag{3.16}$$

The lower bound is attained by a pair of spiders, $\mathrm{irr}_{\min}(\mathcal{T}_{n_1,\Delta_1}) + \mathrm{irr}_{\min}(\mathcal{T}_{n_2,\Delta_2}) = 2\Delta_1^2$.

Proof. Since $\Delta_2 = \Delta_1 + 1 \leq n_1 - 2 = n_2 - 1$ and $\Delta_2 \geq 2$, the class $\mathcal{T}_{n_2,\Delta_2}$ is non-empty, and likewise $\mathcal{T}_{n_1,\Delta_1}$ is non-empty.
Lower bound. Since $\mathrm{irr}(T_i) \geq \mathrm{irr}_{\min}(\mathcal{T}_{n_i,\Delta_i}) = \Delta_i(\Delta_i - 1)$ for $i = 1, 2$. Hence,

$$\mathrm{irr}(T_1) + \mathrm{irr}(T_2) \;\geq\; \Delta_1(\Delta_1 - 1) + (\Delta_1 + 1)\Delta_1 = 2\Delta_1^2. \tag{3.17}$$

Equality holds in (3.17) whenever T_1 and T_2 are spiders with centres of degrees Δ_1 and Δ_2. Such spiders exist since $\Delta_i \leq n_i - 1$, and by (3.10) each of them has $\mathrm{irr}(T_i) = \Delta_i(\Delta_i - 1)$. Therefore,

$$\mathrm{irr}_{\min}(\mathcal{T}_{n_1,\Delta_1}) + \mathrm{irr}_{\min}(\mathcal{T}_{n_2,\Delta_2}) = 2\Delta_1^2. \tag{3.18}$$

Upper bound. Since $n_2 = n_1 - 1 \geq 4$, Proposition 3.5 applies to both trees and gives:

$$\mathrm{irr}(T_i) \;\leq\; (n_i - 1)(\Delta_i - 1), \qquad i = 1, 2, \tag{3.19}$$

with equality if and only if T_i is a star, that is, if and only if $\Delta_i = n_i - 1$. Since $\Delta_1 \leq n_1 - 3 < n_1 - 1$, the tree T_1 is not a star, so (3.19) is strict for $i = 1$ and holds for $i = 2$. Adding the two inequalities and using $n_2 = n_1 - 1$, $\Delta_2 = \Delta_1 + 1$,

$$\mathrm{irr}(T_1) + \mathrm{irr}(T_2) \;<\; (n_1 - 1)(\Delta_1 - 1) + (n_1 - 2)\Delta_1. \tag{3.20}$$

Expanding the right-hand side,

$$(n_1 - 1)(\Delta_1 - 1) + (n_1 - 2)\Delta_1 = (2n_1 - 3)\Delta_1 - n_1 + 1. \tag{3.21}$$

Inequalities (3.17), (3.20) and equation (3.21) give (3.16), and (3.18) gives the last claim of the lemma. □

Lemma 3.7. *Let T be a tree (in particular, a caterpillar tree) of order $n \geq 4$ with maximum degree Δ, minimum degree $\delta = 1$, and let $0 \leq \alpha \leq 1$. Then the upper bound on the Albertson index is:*

$$\mathrm{irr}(T) \leq \left\lfloor \frac{3n^2 - 10n}{2} \right\rfloor 2^{\alpha} + \Delta^2 - n\delta. \tag{3.22}$$

Proof. From (3.15), we find that $\mathrm{irr}(T) \leq (n-1)(\Delta - 1)$. Let $N = \dfrac{3n^2 - 10n}{2}$. Since $2N$ is an integer, $\lfloor N \rfloor \geq N - \frac{1}{2}$. Moreover $N \geq 4 > 0$ for $n \geq 4$. Thus, $\lfloor N \rfloor 2^{\alpha} \geq \lfloor N \rfloor$ for $0 \leq \alpha \leq 1$. Hence,

$$\left\lfloor \frac{3n^2 - 10n}{2} \right\rfloor 2^{\alpha} + \Delta^2 - n\delta \;\geq\; \frac{3n^2 - 10n - 1}{2} + \Delta^2 - n. \tag{3.23}$$

Therefore,

$$\frac{3n^2 - 10n - 1}{2} + \Delta^2 - n - (n-1)(\Delta - 1) = \frac{3n^2 - 10n - 3}{2} + \Delta^2 - (n-1)\Delta. \tag{3.24}$$

Since $\Delta^2 - (n-1)\Delta = \left(\Delta - \frac{n-1}{2}\right)^2 - \frac{(n-1)^2}{4}$, $\Delta^2 - (n-1)\Delta \geq -\frac{(n-1)^2}{4}$, the difference in (3.24) is at least:

$$\begin{aligned} \frac{3n^2 - 10n - 3}{2} - \frac{(n-1)^2}{4} &= \frac{5n^2 - 18n - 7}{4} \\ &= \frac{n(5n - 18) - 7}{4} > 0, \end{aligned}$$

for $n \geq 4$, because $n(5n-18) \geq 8$. Thus, from (3.23) and (3.24),

$$\mathrm{irr}(T) \leq (n-1)(\Delta-1) < \left\lfloor \frac{3n^2-10n}{2} \right\rfloor 2^{\alpha} + \Delta^2 - n\delta, \tag{3.25}$$

as desired. □

The second Zagreb index $M_2(T)$ and the forgotten index $F(T)$ were defined in [20,19] as:

$$M_2(T) = \sum_{uv \in E(T)} d_u d_v, \quad F(T) = \sum_{u \in V(G)} (d_u)^3 = \sum_{uv \in E(G)} [(d_u)^2 + (d_v)^2]. \tag{3.26}$$

Proposition 3.8. *Let G be a non-regular connected graph with m edges, minimum degree δ and maximum degree Δ. Then,*

$$\frac{F(G) - 2M_2(G)}{\Delta - \delta} \;\leq\; \mathrm{irr}(G) \;\leq\; \sqrt{m\,(F(G) - 2M_2(G))}. \tag{3.27}$$

Proof. A vertex v lies in exactly d_v edges and contributes d_v^2 to each of them, so $\sum_{uv \in E(G)} (d_u^2 + d_v^2) = \sum_{v \in V(G)} d_v \cdot d_v^2 = F(G)$. Since $\sigma(G) = F(G) - 2M_2(G)$, let $x_e = |d_u - d_v|$ for $e = uv$. Then,

$$\mathrm{irr}(G) = \sum_{e \in E(G)} x_e \leq \sqrt{m \sum_{e \in E(G)} x_e^2} = \sqrt{m\,\sigma(G)}. \tag{3.28}$$

Since $\delta \leq d_u, d_v \leq \Delta$, every edge satisfies $x_e \leq \Delta - \delta$. Hence, $x_e^2 \leq (\Delta - \delta) x_e$. Summing over the edges,

$$\sigma(G) \leq (\Delta - \delta)\,\mathrm{irr}(G). \tag{3.29}$$

As G is non-regular, $\Delta - \delta > 0$; dividing (3.29) by it and using $\sigma(G) = F(G) - 2M_2(G)$ gives the lower bound in (3.27). Equality holds iff $x_e^2 = (\Delta - \delta) x_e$ on every edge, i.e. iff $|d_u - d_v| \in \{0, \Delta - \delta\}$ for all $uv \in E(G)$. □

3.2. *Some Bounds of Sigma Index*

In this subsection, we present a study of some bounds on the Sigma index and specify certain bounds between $\sigma_{\max}$ and $\sigma_{\min}$, which we show in Proposition 3.9 and Proposition 3.10.

Let $\mathcal{T}_n$ be the class of caterpillar trees of order n, and $\sigma_{\min} = \min\{\sigma(T) : T \in \mathcal{T}_n\}$ and $\sigma_{\max} = \max\{\sigma(T) : T \in \mathcal{T}_n\}$.

Proposition 3.9. *Let $n \geq 5$, let $\mathcal{T}_n$ be the class of caterpillar trees of order n. For $T \in \mathcal{T}_n$, let $\Delta \geq 2$ and $\delta = 1$ be its maximum and minimum degrees, let $\mathscr{D} = (d_1, \cdots, d_n)$ be its degree sequence. Define:*

$$\eta(T) = n\,\frac{mn(\Delta^2 + 2\Delta) + 2m\delta\Delta}{(\Delta^2-2)(\Delta-1)^2 + 2n\Delta\sqrt{m\Delta^2}}\,(n+2)\log\frac{M_1(T)}{2n}.$$

Then $\sigma_{\min} = 2$, $\sigma_{\max} = (n-1)(n-2)^2$, and for every $T \in \mathcal{T}_n$,

$$\sigma_{\min}(T) \leq\; \eta(T) \;\leq\; \sigma_{\max}(T). \tag{3.30}$$

Proof. A tree with $n \geq 3$ has at least two leaves, each adjacent to a vertex of degree at least 2. These are two distinct edges, each with imbalance at least 1. Thus, $\sigma(T) \geq 2$, and $\sigma(\mathcal{P}_n) = 2$. Every imbalance is at most $\Delta - 1 \leq n - 2$ and there are $n - 1$ edges. Then, $\sigma(T) \leq (n-1)(n-2)^2$, with equality for the star $\mathcal{S}_n$. Both $\mathcal{P}_n$ and $\mathcal{S}_n$ are caterpillars. Hence, $\sigma_{\min}(T) = 2$ and $\sigma_{\max}(T) = (n-1)(n-2)^2$. Assume that $\eta = n(n+2)\,Q\,L$ with:

$$Q = \frac{mn\Delta(\Delta+2) + 2m\Delta}{(\Delta^2-2)(\Delta-1)^2 + 2n\Delta^2\sqrt{m}}, \qquad L = \log\frac{M_1}{2n}.$$

Since $\sum_{i=1} d_i = 2m$ and $\delta = 1$, we have $4n - 6 \leq M_1(T) \leq \Delta\sum_{i=1} d_i = 2m\Delta$, the lower bound attained by the path. Hence, for $n \geq 5$, $\ln(2 - 3/n) \leq L < \ln\frac{\Delta(n-1)}{n} < \ln n$, and in particular $L \geq \ln 1.4 > 0.33$.
Lower bound. Since $(\Delta^2-2)(\Delta-1)^2 \leq \Delta^2(n-1)^2$, the numerator of Q is at least $mn\Delta^2$. The denominator is at most $\Delta^2\big((n-1)^2 + 2n\sqrt{m}\big)$. Thus, by considering $\sqrt{n-1} \geq 2$,

$$Q \geq \frac{n}{(n-1) + 2n/\sqrt{n-1}} \geq \frac{n}{2n-1} > \frac{1}{2} \tag{3.31}$$

Then, from (3.31) gives $\eta > \sigma_{\min}(T)$.
Upper bound. Dropping $(\Delta^2-2)(\Delta-1)^2 \geq 0$ from the denominator gives:

$$Q \leq \frac{\sqrt{m}}{2}\Big(1 + \frac{2}{\Delta} + \frac{2}{n\Delta}\Big) \leq \sqrt{m}\Big(1 + \frac{1}{2n}\Big) \leq 1.1\sqrt{m}.$$

Hence, $\eta \leq 1.1\,n(n+2)\sqrt{n-1}\,\ln n$. Thus,

$$0 < \frac{\eta}{\sigma_{\max}(T)} < 1 \tag{3.32}$$

For $6 \leq n \leq 399$ we evaluate the bound $n(n+2)Q\ln\big(\min\{2m\Delta,\, n(n-1)\}/2n\big)$ over all $2 \leq \Delta \leq n-1$. For $n = 5$ there are three caterpillars ($\mathcal{P}_5$, the spider, $\mathcal{S}_5$). Thus, from (3.32), direct computation gives $\eta < \sigma_{\max}(T)$, which (3.30) yields. □

Proposition 3.10. *Let $n \geq 3$ and $2 \leq \Delta \leq n-1$. Let $\mathcal{T}_{n,\Delta}$ be the class of trees of order n with maximum degree Δ, so that $\delta = 1$, and let $\sigma_{\min}(\mathcal{T}_{n,\Delta}) = \min\{\sigma(T) : T \in \mathcal{T}_{n,\Delta}\}$. Then,*

$$\sigma_{\min}(\mathcal{T}_{n,\Delta}) \;\geq\; \frac{\Delta^2(\Delta-1)^2}{n-1}, \tag{3.33}$$

$$\sigma_{\min}(\mathcal{T}_{n,\Delta}) \;\leq\; \Delta\left(\Delta^2 - 4\Delta + 5\right) + (2\Delta - 4)\max\{0,\, 2\Delta - n + 1\}. \tag{3.34}$$

Moreover, $\sigma(T) \geq \Delta^2(\Delta-1)^2/(n-1)$ holds for every $T \in \mathcal{T}_{n,\Delta}$, with equality if and only if $T \cong \mathcal{S}_n$ or T is the spider with three legs of length 2.

Proof. Lower bound. Let $T \in \mathcal{T}_{n,\Delta}$ and let v be a vertex with $\deg v = \Delta$. The forest $T - v$ has exactly Δ components, and each of them contains a leaf ℓ_i of T. Let $\mathcal{P}_i$ be the path from v to ℓ_i and let $L_i \geq 1$ be its length, for $1 \leq i \leq \Delta$. These paths

share only the vertex v, hence they are pairwise edge-disjoint, and $\sum_{i=1}^{\Delta} L_i \leq n-1$. Let $a_1, \cdots, a_{L_i}$ be the imbalances of the edges of $\mathcal{P}_i$. By the triangle inequality,

$$\sum_{j=1}^{L_i} a_j \;\geq\; \deg v - \deg \ell_i = \Delta - 1. \tag{3.35}$$

Then, from (3.35)

$$\sum_{j=1}^{L_i} a_j^2 \;\geq\; \frac{1}{L_i}\Big(\sum_{j=1}^{L_i} a_j\Big)^2 \;\geq\; \frac{(\Delta-1)^2}{L_i}. \tag{3.36}$$

Hence, by summing (3.36) over the edge-disjoint paths and dropping the non-negative contribution of all other edges gives:

$$\begin{aligned}\sigma(T) &\geq\; (\Delta-1)^2 \sum_{i=1}^{\Delta} \frac{1}{L_i} \\ &\geq \frac{\Delta^2\,(\Delta-1)^2}{\sum_{i=1}^{\Delta} L_i} \\ &\geq \frac{\Delta^2(\Delta-1)^2}{n-1},\end{aligned}$$

which proves (3.33). Hence the paths $\mathcal{P}_i$ contain all $n-1$ edges of T. Thus, T is a spider with centre v and every other vertex of degree at most 2. It also forces $L_1 = \cdots = L_\Delta = L$ and, in (3.36), that all imbalances along each leg are equal. For $L = 1$ this gives $T \cong \mathcal{S}_n$. For $L \geq 2$ the degrees along a leg are $\Delta, 2, \cdots, 2, 1$ and the imbalances are $\Delta-2, 0, \cdots, 0, 1$. These are equal only if $L = 2$ and $\Delta - 2 = 1$, that is $\Delta = 3$ and $n = 7$.

Upper bound. Assume that $t = \max\{0, 2\Delta - n + 1\}$. Then, $0 \leq t \leq \Delta$ and $t + 2(\Delta - t) \leq n-1$. Thus, there are integers $a_1, \cdots, a_\Delta \geq 1$ with $\sum_{i=1}^{\Delta} a_i = n-1$ such that exactly t of them equal 1 and the others are at least 2. Let S be the spider with centre of degree Δ and legs of lengths $a_1, \cdots, a_\Delta$. Then $S \in \mathcal{T}_{n,\Delta}$. A leg of length 1 contributes $(\Delta-1)^2$. A leg of length at least 2 has degrees $\Delta, 2, \cdots, 2, 1$ and contributes $(\Delta-2)^2 + 1$. Therefore

$$\sigma(S) = t(\Delta-1)^2 + (\Delta - t)\big((\Delta-2)^2+1\big) = \Delta\left(\Delta^2 - 4\Delta + 5\right) + t(2\Delta - 4). \tag{3.37}$$

Since $\sigma_{\min}(\mathcal{T}_{n,\Delta}) \leq \sigma(S)$, inequality (3.34) follows. □

Proposition 3.11. *Let T be a caterpillar tree of order $n \geq \Delta + 1$ with maximum degree $\Delta \geq 4$ and minimum degree $\delta = 1$. Then the minimum Sigma index satisfies:*

$$\sigma_{\min}(T) \;\geq\; \lceil \log_2(\Delta^2 + 1) - 1 \rceil + 2\Delta - 1, \tag{3.38}$$

that is, $\sigma(T')$ is at least this value for every caterpillar tree T' of order n with maximum degree Δ.

Proof. Let T' be such a tree and let v be a vertex with $\deg v = \Delta$. By the argument for the lower bound in Proposition 3.10, applied to the caterpillar structure of T',

we have $\sigma(T') \geq (\Delta-2)(\Delta-1)^2+2$. For $\Delta \geq 3$ we have $\Delta^2+1 \leq 2^{\Delta+1}$. Hence, $\log_2(\Delta^2+1)-1 < \Delta$ and:

$$\lceil \log_2(\Delta^2+1)-1 \rceil + 2\Delta - 1 \leq 3\Delta - 1. \tag{3.39}$$

For $\Delta \geq 4$ we have $(\Delta-2)(\Delta-1)^2+2 \geq 3\Delta-1$, since equality fails at $\Delta = 4$ where the left side is 20 and the right side is 11, and the left side grows faster. From (3.39) gives (3.38). □

Let $\mathcal{T}_n$ is the class of caterpillar trees of order n, and $n_1 \geq 8$.

Lemma 3.12. *Let T_1, T_2 be two caterpillar trees, where T_1 has $\mathscr{D} = (d_1, \cdots, d_i)$, an increasing degree sequence consisting of 2s. Tree T_2 has $\mathscr{B} = (b_1, \cdots, b_i)$, an increasing degree sequence of prime numbers. Consider $n_1 = |V(T_1)|, n_2 = |V(T_2)|$ and $m_1 = |E(T_1)|, m_2 = |E(T_2)|$. Then $n_2 = n_1 - 1$, $m_2 = m_1 - 1$, and $\Delta(T_2) = \Delta(T_1) + 1$. Then the bound on the Sigma index is given by:*

$$\sigma_{\min}(T) \leq n_1(\Delta_1-1)^2 \cdot \frac{n_1\Delta_2^3 + n_2\Delta_1^4 + m_1\Delta_2^2}{\Delta_1(\Delta_2-1)^2} \leq \sigma_{\max}(T). \tag{3.40}$$

Then, $\sigma_{\min}(T) = \sigma_{\min}(\mathcal{T}_{n_1}) + \sigma_{\min}(\mathcal{T}_{n_2})$ and $\sigma_{\max}(T) = \sigma_{\max}(\mathcal{T}_{n_1}) + \sigma_{\max}(\mathcal{T}_{n_2})$.

Proof. For a tree of order $n \geq 3$ the two leaves lie on two distinct edges, each of imbalance at least 1, so $\sigma \geq 2$, and $\sigma(\mathcal{P}_n) = 2$. Every imbalance is at most $\Delta - 1 \leq n-2$ and there are $n-1$ edges. Thus, $\sigma \leq (n-1)(n-2)^2$, with equality for $\mathcal{S}_n$. Since $\mathcal{P}_n$ and $\mathcal{S}_n$ are caterpillars,

$$\sigma_{\min}(\mathcal{T}_n) = 2, \qquad \sigma_{\max}(\mathcal{T}_n) = (n-1)(n-2)^2 \qquad (n \geq 3). \tag{3.41}$$

As $n_2 = n_1 - 1 \geq 7$, equation (3.41) applies to both n_1 and n_2. Thus,

$$\sigma_{\min}(T) = 4, \qquad \sigma_{\max}(T) = (n_1-1)(n_1-2)^2 + (n_1-2)(n_1-3)^2. \tag{3.42}$$

The degree sequence of T_1 consists of 2's, $\Delta_1 = 2$, and then $\Delta_2 = \Delta_1 + 1 = 3$. Trees satisfy $m_1 = n_1 - 1$ and $n_2 = n_1 - 1$. Hence,

$$n_1\Delta_2^3 + n_2\Delta_1^4 + m_1\Delta_2^2 = 27n_1 + 16(n_1-1) + 9(n_1-1) = 52n_1 - 25, \tag{3.43}$$

and

$$n_1(\Delta_1-1)^2 \frac{n_1\Delta_2^3 + n_2\Delta_1^4 + m_1\Delta_2^2}{\Delta_1(\Delta_2-1)^2} = \frac{n_1(52n_1-25)}{8} =: E(n_1). \tag{3.44}$$

For $n_1 \geq 8$ we have:

$$E(n_1) \geq \frac{8\cdot(52\cdot 8-25)}{8} = 391 > 4 = \sigma_{\min}(T). \tag{3.45}$$

Since $(n-1)(n-2)^2 = n^3 - 5n^2 + 8n - 4$ and $(n-2)(n-3)^2 = n^3 - 8n^2 + 21n - 18$ gives:

$$8\big(\sigma_{\max}(T) - E(n_1)\big) = 16n_1^3 - 156n_1^2 + 257n_1 - 176 =: p(n_1). \tag{3.46}$$

Now $p(8) = 88 > 0$ and $p(9) = 1165 > 0$. For $n_1 \geq 10$, $p(n_1) = n_1^2(16n_1 - 156) + 257n_1 - 176 > 0$ where $16n_1 - 156 > 0$. Therefore $E(n_1) < \sigma_{\max}(T)$ for all $n_1 \geq 8$. From (3.42), (3.44), (3.45) and (3.46) we obtain:

$$\sigma_{\min}(T) < E(n_1) < \sigma_{\max}(T),$$

which is (3.40). □

Lemma 3.13. *Let T be a caterpillar tree with $n = |V(T)|$, $m = |E(T)|$, with maximum degree Δ and minimum degree $\delta \geqslant 1$, and $0 \leq \alpha \leq 1$. Then the lower bound on the Sigma index is:*

$$\sigma(T) \leq \left\lfloor \frac{3n^4 - 2mn}{\Delta} \right\rfloor 2^{\alpha} + \Delta^2 - n\delta.$$

Proof. Since T is a tree with $\Delta > \delta$, we have $n \geq 3$, $\delta = 1$ and $2 \leq \Delta \leq n - 1$. Let $N = 3n^4 - 2n^2 + 2n$. Then, every edge has imbalance at most $\Delta - 1 \leq n - 2$, and T has $n - 1$ edges. Thus, $\sigma(T) \leq (n-1)(n-2)^2 < n^3$. Since $\Delta \leq n - 1$, we have $N/\Delta \geq N/(n-1)$. Moreover $N - 3n^3(n-1) = 3n^3 - 2n^2 + 2n > 0$. Then, $N/\Delta > 3n^3$. As $3n^3$ is an integer, this gives:

$$\left\lfloor \frac{N}{\Delta} \right\rfloor \geq 3n^3. \tag{3.47}$$

For $0 \leq \alpha \leq 1$ we have $2^{\alpha} \geq 1$, and the floor in (3.47) is positive,

$$\left\lfloor \frac{3n^4 - 2mn}{\Delta} \right\rfloor 2^{\alpha} \geq 3n^3. \tag{3.48}$$

Since $\Delta \geq 2$ and $\delta = 1$, we also have $\Delta^2 - n\delta \geq 4 - n$. Then, from (3.48) satisfies:

$$\left\lfloor \frac{3n^4 - 2mn}{\Delta} \right\rfloor 2^{\alpha} + \Delta^2 - n\delta \geq 3n^3 - n + 4 > n^3. \tag{3.49}$$

Combining (3.49) gives:

$$\sigma(T) < n^3 < \left\lfloor \frac{3n^4 - 2mn}{\Delta} \right\rfloor 2^{\alpha} + \Delta^2 - n\delta, \tag{3.50}$$

which proves the lemma. The inequality is strict, and it holds for every tree of order $n \geq 3$. □

Theorem 3.14. *Let $G = (V, E)$ be a connected graph of order n with a vertex $v_\ell \in V(G)$ such that $\deg_G(v_\ell) = \lambda \geqslant 3$. Let δ be the minimum degree and Δ the maximum degree. Then,*

$$\operatorname{irr}(G) \leqslant \sigma(G) \leqslant (\Delta - \delta)\operatorname{irr}(G) \leqslant \Delta(\Delta - 1)^2 \operatorname{irr}(G). \tag{3.51}$$

Proof. For an edge $e = uv$ put $\mu_e = |\deg_G(u) - \deg_G(v)|$, where Each μ_e is a non-negative integer, and since $\delta \leq \deg_G(u), \deg_G(v) \leq \Delta$, $0 \leq \mu_e \leq \Delta - \delta$. Since $\sqrt{\sigma(T)} \leq \operatorname{irr}(T) \leq \sqrt{m\,\sigma(T)}$ and $\mu_e^2 \leq (\Delta - \delta)\mu_e$, $\sigma(G) \leq (\Delta - \delta)\operatorname{irr}(G)$.

Since $\deg_G(v_\ell) = \lambda \geq 3$, we have $\Delta \geq 3$, and therefore $\Delta(\Delta - 1) \geq 1$. Together with $\delta \geq 1$ this gives $\Delta - \delta \leq \Delta - 1 \leq \Delta(\Delta - 1)^2$. Consequently,

$$\sigma(G) \leq (\Delta - \delta)\operatorname{irr}(G) \leq \Delta(\Delta - 1)^2 \operatorname{irr}(G), \tag{3.52}$$

together with (3.52) establishes (3.51). □

4. Conclusion

In this paper, we studied bounds on the Albertson index irr and the Sigma index σ for trees, expressed through the order n, the maximum degree Δ, and the classical indices M_2 and F. For the Albertson index, every tree T of order n with maximum degree Δ satisfies $\Delta(\Delta-1) \leq \operatorname{irr}(T) \leq (n-1)(\Delta-1)$. The lower bound is attained by every spider, and therefore $\operatorname{irr}_{\min}(\mathcal{T}_{n,\Delta}) = \Delta(\Delta-1)$. The upper bound is attained exactly by the star $\mathcal{S}_n$. For the Sigma index, we showed $\sigma_{\min} = 2$ and $\sigma_{\max} = (n-1)(n-2)^2$ over trees of order n. For a fixed maximum degree, every tree $T \in \mathcal{T}_{n,\Delta}$ satisfies $\frac{\Delta^2(\Delta-1)^2}{n-1} \leq \sigma(T)$, with equality exactly for the star and for the spider with three legs of length 2. In the other direction, the spiders give $\sigma_{\min}(\mathcal{T}_{n,\Delta}) \leq \Delta\left(\Delta^2-4\Delta+5\right)+(2\Delta-4)\max\{0,\, 2\Delta-n+1\}$. This upper bound equals the true minimum for $\Delta \leq 4$ in all cases we checked, but it is not sharp in general.

Several questions remain open. The exact value of $\sigma_{\min}(\mathcal{T}_{n,\Delta})$ is not known for $\Delta \geq 5$, and the bounds above are the only ones available in that range. For caterpillar trees, the minimum Sigma index behaves differently, since the spiders are not caterpillars when $\Delta \geq 3$, and the extremal caterpillars need a separate analysis.

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