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AN ALTERNATIVE PROOF OF THE SOMBOR INDEX MINIMIZING PROPERTY OF GREEDY TREES

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ABSTRACT. Recently, Gutman defined a new graph invariant which is named the Sombor index SO(G) of a graph G and is computed via the expression

$$SO(G) = \sum_{u \sim v} \sqrt{\deg(u)^2 + \deg(v)^2},$$

where deg(u) represents the degree of the vertex u in G and the summing is performed across all the unordered pairs of adjacent vertices u and v. Damnjanović et al. have implemented an earlier result obtained by Wang in order to show that, among all the trees \mathcal{T}_D that have a specified degree sequence D, the greedy tree must attain the minimum Sombor index. Here we provide an alternative proof of this same result by constructing an auxiliary graph invariant named the pseudo-Sombor index and without relying on any other earlier results.

1. Introduction

We will consider all graphs to be undirected, finite, simple and non-null. Thus, every graph will have at least one vertex and there shall be no loops or multiple edges. For convenience we will take that each graph of order n has the vertex set $\{1, 2, 3, \ldots, n\}$.

Furthermore, for a given graph G of order n and any $u = \overline{1, n}$, we shall use the notation deg(u) to signify the degree of the vertex u, i.e., the total number of vertices adjacent to it. Taking this into consideration, it is possible to define the Sombor index SO(G) of the graph G by using the expression

$$\mathrm{SO}(G) = \sum_{u \sim v} \sqrt{\deg(u)^2 + \deg(v)^2},$$

where the summing is done across all the unordered pairs of adjacent vertices u and v, as done so by Gutman [16]. Although it was defined very recently, the

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Sombor index has already managed to attract a lot of attention from researchers — see [1-3, 7-11, 14, 15, 17-26, 28, 30, 32, 33] for a partial list of results on the Sombor index.

For a given $n \in \mathbb{N}$, let $D = (d_1, d_2, \ldots, d_n)$ be an arbitrary non-increasing sequence of n non-negative integers. We shall use \mathcal{T}_D to denote the set of all the trees of order n such that D represents their degree sequence. For convenience, we shall take into consideration only the trees such that $d_u = \deg(u)$ for each $u = \overline{1, n}$. The reason why this can be done is clear—all the other trees that adhere to the degree sequence D are surely isomorphic to at least one aforementioned tree.

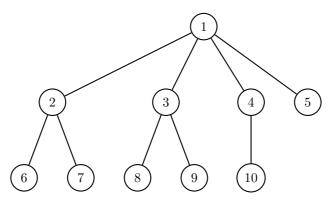


FIGURE 1. The greedy tree GT_D for D = (4, 3, 3, 2, 1, 1, 1, 1, 1, 1).

We define the greedy tree GT_D as the unique rooted tree from \mathcal{T}_D such that its breadth-first traversal yields the sequence $(1, 2, 3, \ldots, n)$. In other words, the root 1 has d_1 children $2, 3, \ldots, d_1 + 1$, its child 2 has $d_2 - 1$ children $d_1 + 2, \ldots, d_1 + d_2$, and so on. An example of a greedy tree is given in Figure 1 for the degree sequence D = (4, 3, 3, 2, 1, 1, 1, 1, 1, 1). It is known that the greedy tree must attain the minimum Sombor index among all the trees with a specified degree sequence, as shown by Damnjanović et al. [13, Corollary 2] by implementing an earlier result obtained by Wang [31]. This statement is provided in the form of the following theorem.

THEOREM 1.1. For any $n \in \mathbb{N}$ and any non-increasing degree sequence $D \in \mathbb{N}_0^n$ such that $\mathfrak{T}_D \neq \emptyset$, the greedy tree GT_D attains the minimum Sombor index in \mathfrak{T}_D .

Theorem 1.1 should not be that surprising, given the fact that the greedy tree GT_D often appears as an extremal tree in \mathcal{T}_D : for example, it minimizes the Wiener index [4], the incidence energy [4] and the sum of vertex eccentricities [29], while it maximizes the connectivity and sum-connectivity indices [31], the spectral moments [5], the spectral radius of the generalized reverse distance matrix [12], the number of pairs of vertices whose distance is at most k for arbitrary k [27] and the number of subtrees of any given order [4,6].

In this paper, our goal will be to provide an alternative proof of Theorem 1.1 — one that does not depend on the previous result by Wang [31] and uses a vastly

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different idea altogether. The remainder of the paper shall be structured as follows. In Section 2 we will define two auxiliary graph-related concepts: the vertex score and the pseudo-Sombor index, and prove some of their basic properties. Section 3 will combine these two concepts with edge switching in order to complete the proof of Theorem 1.1.

2. Vertex score and pseudo-Sombor index

In this and the next section, we assume that $D = (d_1, d_2, \ldots, d_n)$ is a fixed non-increasing sequence of non-negative integers for some $n \in \mathbb{N}, \ge 2$, such that $\mathcal{T}_D \neq \emptyset$. Recall that we assume $\deg(u) = d_u$ for each vertex $u \in \{1, \ldots, n\}$ of each tree in \mathcal{T}_D . Given the fact that the set \mathcal{T}_D is finite, it is clear that the set

$$Z_D = \{ \mathrm{SO}(T) \colon T \in \mathfrak{T}_D \}$$

must also be non-empty and finite. Let $z_D^{(1)} = \min Z_D$ be its smallest element. Now, we have two possibilities: either the set Z_D contains only the element $z_D^{(1)}$, or it has at least two elements, in which case we will denote its second smallest element via $z_D^{(2)} = \min (Z_D \setminus \{z_D^{(1)}\})$. By taking this into consideration, we are able to define a sufficiently small constant $q_D > 0$ via the expression

$$q_D = \begin{cases} \frac{1}{2n}, & |Z_D| = 1, \\ \min\left\{\frac{1}{2n}, \frac{z_D^{(2)} - z_D^{(1)}}{4n^3\sqrt{2}}\right\}, & |Z_D| \ge 2. \end{cases}$$

Furthermore, we will rely on q_D in order to define the vertex score scr(u) for each vertex u in the following manner:

(2.1)
$$\operatorname{scr}(u) = \operatorname{deg}(u) - u q_D.$$

We can imagine the vertex score as a property very similar to the degree, albeit slightly smaller. Unlike the degrees, the vertex scores satisfy the strict monotonicity property that we shall heavily rely on afterwards. This conclusion is disclosed in the following lemma.

LEMMA 2.1. For each tree in \mathcal{T}_D we have $\operatorname{scr}(1) > \cdots > \operatorname{scr}(n) > 0$.

PROOF. Let u and v be two distinct vertices of the given tree such that u < v. Directly from the definition of the set \mathcal{T}_D , we obtain that $\deg(u) \ge \deg(v)$. By virtue of Eq. (2.1), we see that $\operatorname{scr}(u) - \operatorname{scr}(v) = (\deg(u) - \deg(v)) + (v-u) q_D$. Given the fact that v - u > 0 and $q_D > 0$, it immediately follows that $\operatorname{scr}(u) > \operatorname{scr}(v)$.

In order to finalize the proof, it is sufficient to show that scr(n) > 0. However, since $n \ge 2$, it is clear that $deg(n) \ge 1$, as well as $q_D \le \frac{1}{2n}$, which further implies

$$\operatorname{scr}(n) = \operatorname{deg}(n) - n q_D \ge 1 - n \cdot \frac{1}{2n} = \frac{1}{2} > 0,$$

as desired.

In fact, the whole point of using vertex scores instead of their degrees is to avoid having the same value corresponding to two different vertices. By relying on a vertex score instead of its degree, we define the auxiliary pseudo-Sombor index pSO(T) of an arbitrary tree $T \in \mathcal{T}_D$ as follows:

$$pSO(T) = \sum_{u \sim v} \sqrt{\operatorname{scr}(u)^2 + \operatorname{scr}(v)^2}.$$

Due to the fact that the positive constant q_D is chosen to be fairly small, it makes sense that the difference between the pseudo-Sombor index and the Sombor index is also relatively small. We demonstrate this fact in the following lemma.

LEMMA 2.2. If $|Z_D| \ge 2$, then for any tree $T \in \mathfrak{T}_D$ we have $SO(T) - \frac{1}{2} (z_D^{(2)} - z_D^{(1)}) < pSO(T) < SO(T).$

PROOF. Given the fact that all the vertex scores are positive and smaller than the corresponding degrees, the inequality pSO(T) < SO(T) is obvious. Hence, we only need to prove that $SO(T) - pSO(T) < \frac{1}{2}(z_D^{(2)} - z_D^{(1)})$. To start, it is easy to see that for any vertex $u = \overline{1, n}$, we necessarily have

$$\deg(u) - \operatorname{scr}(u) = u \, q_D \leqslant n \, \frac{z_D^{(2)} - z_D^{(1)}}{4n^3 \sqrt{2}} \leqslant \frac{z_D^{(2)} - z_D^{(1)}}{4n^2 \sqrt{2}},$$

as well as $\deg(u) + \operatorname{scr}(u) \leq 2 \deg(u) < 2n$, which immediately gives

(2.2)
$$\deg(u)^2 - \operatorname{scr}(u)^2 = (\deg(u) - \operatorname{scr}(u))(\deg(u) + \operatorname{scr}(u)) < \frac{z_D^{(2)} - z_D^{(1)}}{2n\sqrt{2}}.$$

Furthermore, for any two vertices u and v, we quickly obtain

(2.3)
$$\sqrt{\deg(u)^2 + \deg(v)^2} + \sqrt{\operatorname{scr}(u)^2 + \operatorname{scr}(v)^2} > \sqrt{\deg(u)^2 + \deg(v)^2} \\ \ge \sqrt{2},$$

given the fact that no vertex degree can be less than one.

Now, for any two adjacent vertices $u \sim v$, we conclude that

$$\begin{split} \sqrt{\deg(u)^2 + \deg(v)^2} &- \sqrt{\operatorname{scr}(u)^2 + \operatorname{scr}(v)^2} = \\ &= \frac{(\deg(u)^2 + \deg(v)^2) - (\operatorname{scr}(u)^2 + \operatorname{scr}(v)^2)}{\sqrt{\deg(u)^2 + \deg(v)^2} + \sqrt{\operatorname{scr}(u)^2 + \operatorname{scr}(v)^2}} \\ &= \frac{(\deg(u)^2 - \operatorname{scr}(u)^2) + (\deg(v)^2 - \operatorname{scr}(v)^2)}{\sqrt{\deg(u)^2 + \deg(v)^2} + \sqrt{\operatorname{scr}(u)^2 + \operatorname{scr}(v)^2}}. \end{split}$$

By implementing both Eq. (2.2) and Eq. (2.3), we promptly reach

$$\sqrt{\deg(u)^2 + \deg(v)^2} - \sqrt{\operatorname{scr}(u)^2 + \operatorname{scr}(v)^2} < \frac{\frac{z_D^{(2)} - z_D^{(1)}}{2n\sqrt{2}} + \frac{z_D^{(2)} - z_D^{(1)}}{2n\sqrt{2}}}{\sqrt{2}} = \frac{z_D^{(2)} - z_D^{(1)}}{2n}.$$

Finally, we get

$$SO(T) - pSO(T) = \sum_{u \sim v} \left(\sqrt{\deg(u)^2 + \deg(v)^2} - \sqrt{\operatorname{scr}(u)^2 + \operatorname{scr}(v)^2} \right)$$
$$< \sum_{u \sim v} \frac{z_D^{(2)} - z_D^{(1)}}{2n} = \frac{z_D^{(2)} - z_D^{(1)}}{2n} (n-1) < \frac{z_D^{(2)} - z_D^{(1)}}{2}. \quad \Box$$

The approximation obtained in Lemma 2.2 can now be used to show a key property of the pseudo-Sombor index that plays a central role in the proof of Theorem 1.1. This property is given in the next lemma.

LEMMA 2.3. If a tree T has the minimum pseudo-Sombor index in T_D , then T also has the minimum Sombor index in T_D .

PROOF. First of all, in case we have $|Z_D| = 1$, it can immediately be seen that all the trees in \mathcal{T}_D must have the same Sombor index, hence any tree attains the minimum Sombor index value. In the remainder of the proof, we will suppose that $|Z_D| \ge 2$.

Let T be a tree that attains the minimum pseudo-Sombor index in \mathcal{T}_D , and let T' be a tree that attains the minimum Sombor index in \mathcal{T}_D . From Lemma 2.2, we know that $pSO(T') < SO(T') = z_D^{(1)}$, which further implies that $pSO(T) \leq pSO(T') < z_D^{(1)}$. From Lemma 2.2 we also have $SO(T) - \frac{1}{2}(z_D^{(2)} - z_D^{(1)}) < pSO(T)$, which means that

$$SO(T) < z_D^{(1)} + \frac{z_D^{(2)} - z_D^{(1)}}{2} = \frac{z_D^{(2)} + z_D^{(1)}}{2} < z_D^{(2)}.$$

Since $z_D^{(1)}$ is the only possible value of Sombor index from Z_D that is smaller than $z_D^{(2)}$, we obtain that $SO(T) = z_D^{(1)}$, meaning that T has the minimum Sombor index in \mathcal{T}_D .

3. Greedy trees

As a direct consequence of Lemma 2.3, we see that in order to demonstrate that GT_D attains the minimum value of Sombor index, it is sufficient to prove that GT_D attains the minimum value of the pseudo-Sombor index. In this section we do that by showing that for any tree $T \in \mathfrak{T}_D$ with $T \ncong \operatorname{GT}_D$ there is another tree $T' \in \mathfrak{T}_D$ such that $\operatorname{pSO}(T') < \operatorname{pSO}(T)$.

For convenience, we will assume that all of the trees from \mathcal{T}_D are rooted, with the root fixed at the vertex 1. In this case, the root must have the highest score and no two vertices can have the same score, as shown in Lemma 2.1. The *level* of a vertex will denote its distance to the root 1. Bearing this in mind, we now disclose three helpful lemmas that together show that, apart from GT_D , no other tree can attain the minimum value of the pseudo-Sombor index in \mathcal{T}_D .

LEMMA 3.1. Let $T \in \mathcal{T}_D$ be a tree containing four distinct vertices u, v, w, tsuch that $u \sim v, w \sim t, u \nsim w, v \nsim t$. Suppose that the graph obtained from T by deleting the edges $\{u, v\}$ and $\{w, t\}$ and adding the edges $\{u, w\}$ and $\{v, t\}$ is a tree, and denote it by T_1 . In that case we have $T_1 \in \mathcal{T}_D$, as well as

$$pSO(T) > pSO(T_1) \iff (scr(u) - scr(t))(scr(w) - scr(v)) > 0.$$

PROOF. First of all, given the fact that T_1 is guaranteed to be a tree and T and T_1 obviously have the same degree sequence, it is clear that $T_1 \in \mathcal{T}_D$. Furthermore, pseudo-Sombor indices of these two trees will have the same summands, except for the terms that correspond to the deleted and newly added edges. With this in mind, we quickly get

$$pSO(T) - pSO(T_1) = \sqrt{scr(u)^2 + scr(v)^2} + \sqrt{scr(w)^2 + scr(t)^2} - \sqrt{scr(u)^2 + scr(w)^2} - \sqrt{scr(v)^2 + scr(t)^2}.$$

It follows that $pSO(T) > pSO(T_1)$ is equivalent to

$$\sqrt{\operatorname{scr}(u)^2 + \operatorname{scr}(v)^2} + \sqrt{\operatorname{scr}(w)^2 + \operatorname{scr}(t)^2} > > \sqrt{\operatorname{scr}(u)^2 + \operatorname{scr}(w)^2} + \sqrt{\operatorname{scr}(v)^2 + \operatorname{scr}(t)^2},$$

which, after squaring, becomes equivalent to

$$(\operatorname{scr}(u)^2 + \operatorname{scr}(v)^2)(\operatorname{scr}(w)^2 + \operatorname{scr}(t)^2) > (\operatorname{scr}(u)^2 + \operatorname{scr}(w)^2)(\operatorname{scr}(v)^2 + \operatorname{scr}(t)^2).$$

Expanding the above expressions, we conclude that $pSO(T) > pSO(T_1)$ is equivalent to

$$\operatorname{scr}(u)^2 \operatorname{scr}(w)^2 + \operatorname{scr}(v)^2 \operatorname{scr}(t)^2 > \operatorname{scr}(u)^2 \operatorname{scr}(v)^2 + \operatorname{scr}(w)^2 \operatorname{scr}(t)^2,$$

which is, in turn, equivalent to $(\operatorname{scr}(u)^2 - \operatorname{scr}(t)^2)(\operatorname{scr}(w)^2 - \operatorname{scr}(v)^2) > 0$. Since all vertex scores are positive, it is trivial to see that the last expression is further equivalent to

$$(\operatorname{scr}(u) - \operatorname{scr}(t))(\operatorname{scr}(w) - \operatorname{scr}(v)) > 0.$$

We can now use the switching mechanism from Lemma 3.1 to construct a tree with a smaller pseudo-Sombor index whenever we are given a tree different from GT_D . The necessary constructions are given in the following two lemmas.

LEMMA 3.2. If a tree $T \in \mathfrak{T}_D$ contains vertices α and β such that α is at a greater level than β , but $\operatorname{scr}(\alpha) > \operatorname{scr}(\beta)$, then T cannot attain the minimum pseudo-Sombor index in \mathfrak{T}_D .

PROOF. Let j be the minimum index such that each vertex on level k, for each $0 \leq k \leq j-1$, has a higher score than any vertex belonging to a level greater than k, but such that there exists a vertex β on level j and a vertex α on a level greater than j with $\operatorname{scr}(\beta) < \operatorname{scr}(\alpha)$. Since the root 1 has the highest score, we have that $j \geq 1$, so that β has a parent, which we denote by γ . In order to make the proof more concise, we will divide it into two cases depending on whether β is the parent of α .

Case β is the parent of α . In this case, we clearly have that $\deg(\beta) \ge 2$. Since $\operatorname{scr}(\alpha) > \operatorname{scr}(\beta)$, Lemma 2.1 tells us that $\alpha < \beta$, hence $\deg(\alpha) \ge 2$ as well. (Recall that the degrees are ordered in a non-increasing order in D.) This means that the

vertex α must have at least one child, which we shall denote via δ . We now get that $\alpha \sim \delta$, $\beta \sim \gamma$, $\gamma \nsim \alpha$, $\beta \nsim \delta$. If we construct a graph T_1 from T by deleting the edges $\{\alpha, \delta\}$ and $\{\beta, \gamma\}$ and adding the new edges $\{\gamma, \alpha\}$ and $\{\beta, \delta\}$, we see that this graph must be a tree from the set \mathcal{T}_D . According to Lemma 3.1, we obtain

$$pSO(T) > pSO(T_1) \iff (scr(\alpha) - scr(\beta))(scr(\gamma) - scr(\delta)) > 0.$$

We have $\operatorname{scr}(\alpha) > \operatorname{scr}(\beta)$ by assumption, while $\operatorname{scr}(\gamma) > \operatorname{scr}(\delta)$ also holds since γ is from level j-1 and δ is from a greater level than γ . Thus, $\operatorname{pSO}(T_1) < \operatorname{pSO}(T)$, so T cannot attain the minimum pseudo-Sombor index in \mathcal{T}_D .

Case β is not the parent of α . In this case, let δ be the parent of α that is located on some level greater than j - 1. Here, it is clear that the vertices $\alpha, \beta, \gamma, \delta$ are all mutually distinct. Moreover, we have that $\alpha \sim \delta$ and $\beta \sim \gamma$, but $\gamma \nsim \alpha$. However, δ and β may or may not be adjacent. It is easy to see that these two vertices are adjacent if and only if β is the parent of δ . These two scenarios shall yield two different construction patterns for T_1 . For this reason, we shall divide the given case into two further subcases.

Subase β is not the parent of δ . In this subcase, we get $\alpha \sim \delta$, $\beta \sim \gamma$, $\gamma \nsim \alpha$, $\beta \nsim \delta$. As in the previous case, if we construct a graph T_1 from T by deleting the edges $\{\alpha, \delta\}$ and $\{\beta, \gamma\}$ and adding the new edges $\{\gamma, \alpha\}$ and $\{\beta, \delta\}$, it can be easily seen that this graph must be a tree from the set \mathcal{T}_D . By virtue of Lemma 3.1, we have

$$pSO(T) > pSO(T_1) \iff (scr(\alpha) - scr(\beta))(scr(\gamma) - scr(\delta)) > 0.$$

As in the previous case, we have that $scr(\alpha) > scr(\beta)$, and $scr(\gamma) > scr(\delta)$ must also be true since γ is from level j - 1 and δ is from a greater level. Thus, $pSO(T_1) < pSO(T)$.

Subcase β is the parent of δ . In this subcase, we have that γ is the parent of β , which is the parent of δ , which is the parent of α . Since deg $(\beta) \geq 2$ and $\alpha < \beta$, it follows that deg $(\alpha) \geq 2$, as already observed. Thus, α must have at least one child, and we will name one of them as ε . Now, we have $\alpha \sim \varepsilon$, $\beta \sim \gamma$, $\gamma \nsim \alpha$, $\beta \nsim \varepsilon$. If we construct a graph T_1 from T by deleting the edges $\{\alpha, \varepsilon\}$ and $\{\beta, \gamma\}$ and adding the new edges $\{\gamma, \alpha\}$ and $\{\beta, \varepsilon\}$, it can be quickly noticed that this graph must be a tree from the set \mathcal{T}_D . Furthermore, Lemma 3.1 gives us

$$pSO(T) > pSO(T_1) \iff (scr(\alpha) - scr(\beta))(scr(\gamma) - scr(\varepsilon)) > 0.$$

Now, it is clear that $scr(\gamma) > scr(\varepsilon)$, since γ is from level j - 1 and ε is from a greater level, which again implies that $pSO(T_1) < pSO(T)$.

As a direct consequence of Lemma 3.2, we see that a tree $T \in \mathcal{T}_D$ with the minimum value of the pseudo-Sombor index satisfies the property that whenever a vertex α is at a greater level than a vertex β , then $\operatorname{scr}(\alpha) < \operatorname{scr}(\beta)$. We will now show that the scores of vertices at the same level are aligned according to the scores of their parents.

LEMMA 3.3. If a tree $T \in \mathfrak{T}_D$ contains two vertices α and β on the same level with $\operatorname{scr}(\alpha) > \operatorname{scr}(\beta)$, such that α has a child γ and β has a child δ with $\operatorname{scr}(\gamma) < \operatorname{scr}(\delta)$, then T cannot attain the minimum pseudo-Sombor index in \mathfrak{T}_D .

PROOF. It is clear that $\alpha \sim \gamma$, $\beta \sim \delta$, $\alpha \nsim \delta$, $\beta \nsim \gamma$. If T_1 is obtained from T by deleting the edges $\{\alpha, \gamma\}$ and $\{\beta, \delta\}$ and adding the new edges $\{\alpha, \delta\}$ and $\{\beta, \gamma\}$, then it is easy to see that T_1 is a tree from \mathcal{T}_D as well. From Lemma 3.1

$$pSO(T) > pSO(T_1) \iff (scr(\alpha) - scr(\beta))(scr(\delta) - scr(\gamma)) > 0,$$

which by the above assumptions implies that $pSO(T_1) < pSO(T)$. Hence T does not attain the minimum pseudo-Sombor index in \mathcal{T}_D .

Taking into consideration both Lemma 3.2 and Lemma 3.3, we see that the only way for a tree $T \in \mathcal{T}_D$ to attain the minimum pseudo-Sombor index is if the children of the root have the highest possible scores, then the children of the highest-scored child have the highest possible scores, etc. In other words, if we select the children in such a way that the ones with the higher scores go first, the tree T must be such that its breadth-first traversal yields a strictly decreasing sequence of scores. Recalling that $\operatorname{scr}(1) > \cdots > \operatorname{scr}(n)$ by Lemma 2.1, we see that such tree is actually the greedy tree GT_D , and this is the only tree that attains the minimum pseudo-Sombor index in \mathcal{T}_D . We can now complete the proof of Theorem 1.1.

PROOF OF THEOREM 1.1. If n = 1, then D = (0) is the only non-increasing sequence of non-negative integers in \mathbb{N}_0^1 for which $\mathfrak{T}_D \neq \emptyset$. In such a case we actually have $\mathfrak{T}_D = \{K_1\}$. Since K_1 is also a greedy tree, the minimum Sombor index is clearly attained by the greedy tree in this case.

For $n \geq 2$, suppose that $D \in \mathbb{N}_0^n$ is an arbitrarily chosen non-increasing sequence of non-negative integers such that $\mathcal{T}_D \neq \emptyset$. Now, Lemmas 3.2 and 3.3 guarantee that the greedy tree GT_D attains the minimum pseudo-Sombor index in \mathcal{T}_D . Lemma 2.3 then dictates that GT_D must also attain the minimum Sombor index in \mathcal{T}_D , which completes the proof.

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