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The General Sombor Index of Extremal Trees with a Given Maximum Degree

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Abstract

The general Sombor index of a graph G, denoted by $\mathcal{SO}_\alpha(G)$, is recently defined as:

$$\mathcal{SO}_\alpha(G) = \sum_{v_i v_j \in E(G)} \left(d_G(v_i)^2 + d_G(v_j)^2 \right)^\alpha ,$$

where $d_G(v_i)$ represents the degree of vertex v_i, and α is an arbitrary real number. This study focuses on identifying extremal trees for the general Sombor index within the class of n-vertex trees with maximum degree Δ. We analyze the general Sombor index across various intervals of α. Specifically, for $\alpha > 1$ and $\alpha \in [-1, 0)$, we determine the trees that maximize the general Sombor index. Moreover, for $\alpha < 0$ and $\alpha > 0$, we identify the trees that minimize the general Sombor index $\mathcal{SO}_\alpha$. Finally, the characterization of extremal trees for $\mathcal{SO}_\alpha$ in the remaining intervals of α remains an open problem and presents a promising direction for future research.

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1 Introduction

Let $G = (V, E)$ be a simple undirected graph, where $V(G)$ and $E(G)$ represent the vertex set and edge set of the graph G, respectively. The order and size of the graph, denoted by $n(G)$ (or simply n) and $m(G)$ (or simply m), correspond to the number of vertices and edges in G. For a vertex $v_i \in V(G)$, the degree of v_i is denoted by $d_G(v_i)$ (or simply d_i), and the set of vertices adjacent to v_i is denoted by $N_G(v_i)$ (or simply N_i). The maximum degree of a vertex in G is denoted by $\Delta(G)$ (or Δ). A tree is a connected acyclic graph of order n, commonly referred to as an n-vertex tree. Additionally, the path graph and star graph of order n are denoted by P_n and S_n, respectively. Denote by $\mathcal{T}(n, \Delta)$ the collection of all n-vertex trees with maximum degree Δ. The path P_n is the unique element of $\mathcal{T}(n, 2)$, and the star S_n is the unique element of $\mathcal{T}(n, n-1)$.

Molecular descriptors play a crucial role in mathematical chemistry, particularly in QSPR /QSAR studies. Among these, the degree-based topological indices hold a special place. Recently, Gutman [17] introduced a new degree-based topological index grounded in geometric principles, known as the Sombor index, defined as:

$$\mathcal{SO}(G) = \sum_{v_i v_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2},$$

where $d_G(v_i)$ is the degree of the vertex v_i in G. This index has gained significant attention, sparking extensive research into its mathematical properties [3–12, 18, 19, 22, 24, 26, 27, 29, 30, 36, 38–41] and its applications in chemistry [14, 23, 26, 35].

In the literature, the Randić index [2] and the sum-connectivity index [42] are widely popular in mathematical chemistry. Building on these indices, researchers have introduced the general Randić index and the general sum-connectivity index for graphs, offering a more versatile approach to studying graph structures and their chemical applications. Motivated by the above, Zhong and Hu [20] proposed the general Sombor index, defined as:

$$\mathcal{SO}_\alpha(G) = \sum_{v_i v_j \in E(G)} \Big(d_G(v_i)^2 + d_G(v_j)^2\Big)^\alpha,$$

where α is a real number. For $\alpha = 0$, $\mathcal{SO}_0(G)$ equals the number of edges m in graph G. For a tree T with n vertices, $\mathcal{SO}_0(T)$ is given by $n-1$. Consequently, it is customary to require that α be non-zero. When $\alpha = \frac{1}{2}$, $\mathcal{SO}_{\frac{1}{2}}$ represents the standard Sombor index, while for $\alpha = 1$, $\mathcal{SO}_1$ corresponds to the forgotten index, denoted as F [15].

Very recently, Dehgardi and Azari [13] studied on the lower bounds of geometric Sombor index for trees and unicyclic graphs, and also the extremal trees and unicyclic graphs that achieve the lower bound are characterized. Zhong and Hu [20] explored the maximum general Sombor index of unicyclic graphs with a specified diameter for the range $0 < \alpha < 1$. Maiteryi et al. [28] identified both the maximum and minimum general Sombor index among trees with a fixed number of pendant vertices when $0 < \alpha < 1$. This line of inquiry highlights a significant research focus: characterizing extremal graphs for degree-based topological indices under various parameters. A particular emphasis has been placed on trees within the class $\mathcal{T}(n, \Delta)$, where extensive studies have characterized these structures for various indices. Notably, the general sum-connectivity index and the general Randić index have been investigated across different intervals of α; see [1,21,32–34,37] and [25,37], respectively. Inspired by these works, this paper addresses the following extremal problem:

Problem 1. Characterize the extremal trees within $\mathcal{T}(n, \Delta)$ for the general Sombor index $\mathcal{SO}_\alpha$. Specifically:

- For $\alpha > 1$ and $\alpha \in [-1, 0)$, identify the trees that maximize the $\mathcal{SO}_\alpha$ index.
- For $\alpha < 0$ and $\alpha > 0$, determine the trees that minimize the $\mathcal{SO}_\alpha$ index.

Zhou et al. [41] solved Problem 1 for $\alpha = \frac{1}{2}$, focusing on minimizing the $\mathcal{SO}_\alpha$ index. We address Problem 1 by analyzing α across different intervals, each exhibiting distinct behavior.

The structure of the paper is as follows: Section 2 introduces key concepts and relevant lemmas, Section 3 presents the main results pertaining to Problem 1, and Section 4 concludes the paper.

2 Preliminaries and supporting lemmas

This section introduces the key terms, notation, and lemmas used throughout the paper. A **d-vertex** of a graph G is a vertex with degree d. Specifically, a **1-vertex** is called a **pendant vertex** (or a **leaf**) and the edge incident to a 1-vertex is referred to as a **pendant edge**. If $v_iv_j \in E(G)$, then $G - v_iv_j$ denotes the subgraph of G obtained by deleting the edge v_iv_j; similarly, $G + v_iv_j$ denotes the graph obtained from G by adding the edge v_iv_j if it is not already in $E(G)$. If $v_i \in V(G)$, then $G - v_i$ (or $G\backslash\{v_i\}$) denotes the subgraph of G obtained by deleting the vertex v_i and all edges incident to it. A **pendant path** in a graph G is a path where one end vertex has degree 1, the other end vertex has degree at least 3, and all internal vertices (if any) have degree 2. The length of a pendant path is the number of edges it contains. The distance between vertices v_i and v_j in G, denoted by $d_G(v_i, v_j)$, is the length of the shortest path connecting them. The **degree sequence** of a graph G, denoted by $D(G)$, is the sequence of vertex degrees in G listed in non-increasing order. Formally, $D(G) = (d_1, d_2, \ldots, d_n)$, where d_i represents the degree of the i-th vertex and $d_1 \geq d_2 \geq \cdots \geq d_n$.

Let $n_i(G)$ (or n_i) be the number of vertices of degree i and $e_{ij}(G)$ (or e_{ij}) the number of edges between vertices of degrees i and j. The following system of equations holds for any graph G:

$$i \cdot n_i(G) = 2 \cdot e_{ii}(G) + \sum_{\substack{j=1 \\ j \neq i}}^{\Delta} e_{ij}(G) \tag{1}$$

for each i, where $i \in \{1, 2, \ldots, \Delta\}$. For additional notations and terminologies, we refer to [16].

A tree is said to be **starlike** if exactly one of its vertices has degree greater than two. By $S(a_1, a_2, \ldots, a_\Delta)$ we denote the starlike tree which has a vertex v_1 of degree $\Delta \geq 3$ and which has the property

$$S(a_1, a_2, \ldots, a_\Delta) - v_1 = P_{a_1} \cup P_{a_2} \cup \ldots \cup P_{a_\Delta}.$$

This tree has $a_1 + a_2 + \cdots + a_\Delta + 1 = n$ vertices and assumed that $a_1 \geq a_2 \geq \cdots \geq a_\Delta \geq 1$. We say that the starlike tree $S(a_1, a_2, \ldots, a_\Delta)$ has Δ branches, the lengths of which are $a_1, a_2, \ldots, a_\Delta$ respectively. In particular, for $\Delta = n-1$, $S(a_1, a_2, \ldots, a_\Delta) \cong S_n$. To formulate our results, we define the following four trees:

- $S_{\Delta,n-\Delta}$: The double star graph formed by attaching $\Delta - 1$ pendant vertices to one vertex of the path P_2 and $n - \Delta - 1$ pendant vertices to the other vertex of P_2 (see, Fig. 1 (a)).
- $B_{n,\Delta}$: The broom graph constructed from $S(a_1, a_2, \ldots, a_\Delta)$ by attaching $\Delta - 1$ pendant vertices to one end of the path $P_{n-\Delta+1}$ (see, Fig. 1 (b)).
- $T_{n,\Delta}$ (for $n \leq 2\Delta$): A tree derived from $S(a_1, a_2, \ldots, a_\Delta)$ by attaching a pendant vertex to each of the $n - \Delta - 1$ pendant vertices of the star $S_{\Delta+1}$ (see, Fig. 1 (c)).
- T_Δ: A tree formed from $S(a_1, a_2, \ldots, a_\Delta)$ by attaching Δ pendant paths to a single vertex, with each pendant path having a length of at least 2 (see, Fig. 1 (d)).

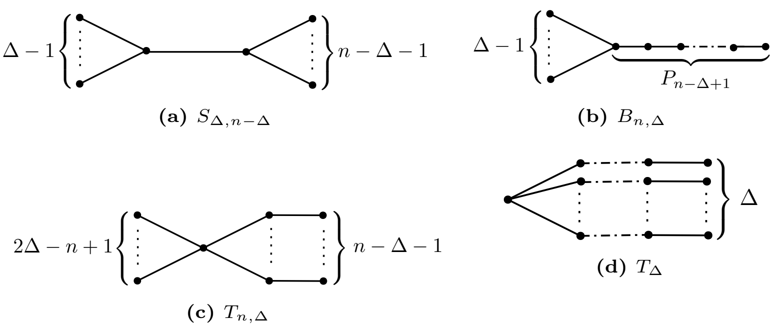

Figure 1. *The Trees* $S_{\Delta,n-\Delta}, B_{n,\Delta}, T_{n,\Delta}$ *and* T_Δ.

We now present several lemmas that will be frequently applied in the subsequent section. The following lemma is straightforward and can be easily derived.

Lemma 1. *For any $x > 0$, $c > d \geq 0$ and real number α, consider the function*

$$\Phi(x) = (x^2 + c^2)^\alpha - (x^2 + d^2)^\alpha.$$

(i) If $\alpha < 0$ or $\alpha > 1$, then $\Phi(x)$ strictly increases.

(ii) If $0 < \alpha < 1$, then $\Phi(x)$ strictly decreases.

Lemma 2. *If $x \geq 0$ and $\alpha \geq 1$, then the function*

$$f(x) = x\left[\Big((x+1)^2 + 1\Big)^\alpha - (x^2+1)^\alpha\right] + (x^2+1)^\alpha$$

strictly increases.

Proof. We obtain

$$f'(x) = \Big((x+1)^2 + 1\Big)^\alpha - (x^2+1)^\alpha + 2x\alpha\Big[\Big((x+1)^2+1\Big)^{\alpha-1}(x+1) - x(x^2+1)^{\alpha-1}\Big] + 2x\alpha(x^2+1)^{\alpha-1}.$$

Since $\alpha \geq 1$, it follows that $\Big((x+1)^2+1\Big)^\alpha > (x^2+1)^\alpha$, $(x+1)\Big((x+1)^2+1\Big)^{\alpha-1} > x(x^2+1)^{\alpha-1}$ and $2x\alpha(x^2+1)^{\alpha-1} \geq 0$. Thus $f'(x) > 0$ and hence $f(x)$ is strictly increasing on $x \geq 0$ and $\alpha \geq 1$. ■

Lemma 3. *If $p > 0$, $t \geq 2$ and $x > 1$, then*

(i) $\Big((t+1)^2 + p^2\Big)^x + \Big((t-1)^2 + p^2\Big)^x > 2\,(t^2+p^2)^x,$

(ii) $t\Big((t+1)^2+1\Big)^x + (t-2)\Big((t-1)^2+1\Big)^x > 2(t-1)\,(t^2+1)^x.$

Proof. *(i)* Let us consider a function

$$g(x) = \left(\frac{(t+1)^2+p^2}{t^2+p^2}\right)^x + \left(\frac{(t-1)^2+p^2}{t^2+p^2}\right)^x, \quad t \geq 2,\ p > 0 \text{ and } x > 1.$$

Then we have

$$g'(x) = \left(\frac{(t+1)^2+p^2}{t^2+p^2}\right)^x \ln\left(\frac{(t+1)^2+p^2}{t^2+p^2}\right) + \left(\frac{(t-1)^2+p^2}{t^2+p^2}\right)^x \times \ln\left(\frac{(t-1)^2+p^2}{t^2+p^2}\right).$$

and

$$g''(x) = \left(\frac{(t+1)^2+p^2}{t^2+p^2}\right)^x \left(\ln\left(\frac{(t+1)^2+p^2}{t^2+p^2}\right)\right)^2 + \left(\frac{(t-1)^2+p^2}{t^2+p^2}\right)^x \times \left(\ln\left(\frac{(t-1)^2+p^2}{t^2+p^2}\right)\right)^2 > 0.$$

Thus $g(x)$ is strictly convex for $t \geq 2$, $p > 0$ and $x > 1$. We have $g(0) = 2$ and $g(1) = 2\left(1 + \frac{1}{t^2+p^2}\right) > 2$. Hence $g(x) > 2$ for $t \geq 2$, $p > 0$ and $x > 1$, that is, $\left((t+1)^2+p^2\right)^x + \left((t-1)^2+p^2\right)^x > 2(t^2+p^2)^x$.

(ii) Similarly, we consider

$$h(x) = \frac{t}{t-1}\left(\frac{(t+1)^2+1}{t^2+1}\right)^x + \frac{t-2}{t-1}\left(\frac{(t-1)^2+1}{t^2+1}\right)^x, \quad t \geq 2 \text{ and } x > 1.$$

Then

$$h''(x) = \frac{t}{t-1}\left(\frac{(t+1)^2+1}{t^2+1}\right)^x \left(\ln\left(\frac{(t+1)^2+1}{t^2+1}\right)\right)^2 + \frac{t-2}{t-1} \times \left(\frac{(t-1)^2+1}{t^2+1}\right)^x \left(\ln\left(\frac{(t-1)^2+1}{t^2+1}\right)\right)^2 > 0.$$

Thus $h(x)$ is strictly convex for $t \geq 2$ and $x > 1$. We have $h(0) = 2$ and $h(1) = \frac{1}{(t-1)(t^2+1)}[2t^2(t-1) + 4(2t-1)]$. One can easily check that $h(1) > 2$, that is,

$$2t^2(t-1) + 4(2t-1) > 2(t-1)(t^2+1),$$

that is, $t \geq 2$, which is always true. Thus $h(x) > 2$ for $x > 1$. So

$$t\Big((t+1)^2+1\Big)^x+(t-2)\Big((t-1)^2+1\Big)^x>2(t-1)(t^2+1)^x.$$

This completes the proof. ■

Lemma 4. *If x is any real number, then*

(*i*) $3\cdot 8^x-2\cdot 13^x-5^x<0$ *for* $x>0$,

(*ii*) $2\cdot 8^x-5^x-20^x<0$ *for* $x>0$,

(*iii*) $3\cdot 8^x-2\cdot 13^x-5^x>0$ *for* $-1.5\le x<0$,

(*iv*) $2\cdot 8^x-5^x-20^x\ge 0$ *for* $-1\le x<0$.

Proof. Let us consider a function

$$f(x)=2\left(\frac{13}{8}\right)^x+\left(\frac{5}{8}\right)^x,\ x\ge -1.5.$$

Then we have

$$f'(x)=2\left(\frac{13}{8}\right)^x\ln\left(\frac{13}{8}\right)+\left(\frac{5}{8}\right)^x\ln\left(\frac{5}{8}\right)$$

and

$$f''(x)=2\left(\frac{13}{8}\right)^x\left(\ln\left(\frac{13}{8}\right)\right)^2+\left(\frac{5}{8}\right)^x\left(\ln\left(\frac{5}{8}\right)\right)^2>0.$$

Thus $f(x)$ is strictly convex for any real number x. We have $f(-1)<3$ and $f(0)=3$. Hence $f(x)>f(0)=3$ for any $x>0$, that is, $3\cdot 8^x-2\cdot 13^x-5^x<0$ for $x>0$, which gives (*i*). Moreover, we have $f(-1.5)<3$ and $f(0)=3$. Since $f(x)$ is strictly convex, we obtain $f(x)<3$ for $-1.5\le x<0$. This gives $3\cdot 8^x-2\cdot 13^x-5^x>0$ for $-1.5\le x<0$ and we obtain the result in (*iii*).

Similarly, we consider

$$g(x)=\left(\frac{5}{8}\right)^x+\left(\frac{5}{2}\right)^x,\quad x\ge -1.$$

Then

$$g''(x) = \left(\frac{5}{8}\right)^x \left(\ln\left(\frac{5}{8}\right)\right)^2 + \left(\frac{5}{2}\right)^x \left(\ln\left(\frac{5}{2}\right)\right)^2 > 0.$$

Thus $g(x)$ is strictly convex for any real number x. We have $g(-1) = 2 = g(0)$. Hence $g(x) > g(0) = 2$ for any $x > 0$, that is, $2 \cdot 8^x - 5^x - 20^x < 0$ for $x > 0$, which gives (ii). Moreover, we obtain $g(x) \leq 2$ for $-1 \leq x < 0$. Thus, it holds $2 \cdot 8^x - 5^x - 20^x \geq 0$ for $-1 \leq x < 0$. Hence we obtain the result in (iv). This completes the proof. ■

We now discuss certain graph transformations that can either increase or decrease the generalized Sombor index of a graph. When the graph under consideration is clear, we will use d_{v_i} and N_{v_i} in place of $d_G(v_i)$ and $N_G(v_i)$, respectively. In diagrams, a dotted circle around a vertex $v_i \in V(G)$ indicates that $d_{v_i} \geq 1$.

Lemma 5. *For a graph G, let $w, u \in V(G)$ with $d_G(w) > d_G(u) \geq 2$. Suppose $ww_0, uu_0 \in E(G)$, where w_0 is a 1-vertex, $N_G(u_0)\backslash\{u\} = \{u_1, \ldots, u_\ell\}$ ($\ell \geq 1$) and u_0 is not on the $w - u$ path (see, Fig. 2). Define G_1 as the graph obtained from G by removing the edges $\{u_0u_1, \ldots, u_0u_\ell\}$ and adding the edges $\{w_0u_1, \ldots, w_0u_\ell\}$.*

(i) If $\alpha < 0$ or $\alpha > 1$, then $\mathcal{SO}_\alpha(G_1) > \mathcal{SO}_\alpha(G)$,

(ii) If $0 < \alpha < 1$, then $\mathcal{SO}_\alpha(G_1) < \mathcal{SO}_\alpha(G)$.

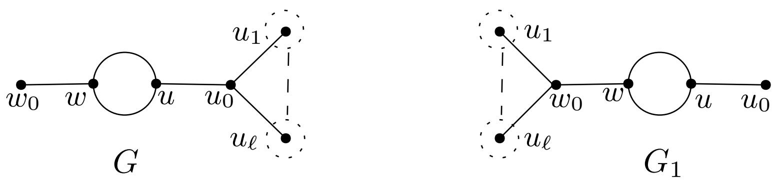

Figure 2. *Two graphs G and G_1.*

Proof. Note that w_0 and u_0 are the only vertices whose degrees are different in G and G_1. We have $d_{G_1}(u_0) = d_G(u_0) - \ell = 1$ and $d_{G_1}(w_0) = d_G(w_0) + \ell = \ell + 1$. Therefore

$$\mathcal{SO}_\alpha(G_1) - \mathcal{SO}_\alpha(G) = \Big((\ell+1)^2 + d_w^2\Big)^\alpha - (1+d_w^2)^\alpha + (1+d_u^2)^\alpha - \Big((\ell+1)^2 + d_u^2\Big)^\alpha. \tag{2}$$

(i) If $\alpha < 0$ or $\alpha > 1$, then using Lemma 1 (i) with $d_w > d_u$, (2) becomes

$$\mathcal{SO}_\alpha(G_1) - \mathcal{SO}_\alpha(G) > 0.$$

(ii) Similarly, for $0 < \alpha < 1$, using Lemma 1 (ii) with $d_w > d_u$, (2) becomes

$$\mathcal{SO}_\alpha(G_1) - \mathcal{SO}_\alpha(G) < 0.$$

This completes the proof of the lemma. ■

Lemma 6. *For a graph G, let $w, u \in V(G)$ with $d_G(w) > d_G(u) \geq 2$. Suppose $ww_0, uu_0 \in E(G)$, where u_0 is a 1-vertex, $N_G(w_0)\backslash\{w\} = \{w_1, \ldots, w_\ell\}$ $(\ell \geq 1)$ and w_0 is not on the $w-u$ path (see, Fig. 3). Define G_2 as the graph obtained from G by removing the edges $\{w_0w_1, \ldots, w_0w_\ell\}$ and adding the edges $\{u_0w_1, \ldots, u_0w_\ell\}$.*

(i) If $\alpha < 0$ or $\alpha > 1$, then $\mathcal{SO}_\alpha(G_2) < \mathcal{SO}_\alpha(G)$.

(ii) If $0 < \alpha < 1$, then $\mathcal{SO}_\alpha(G_2) > \mathcal{SO}_\alpha(G)$.

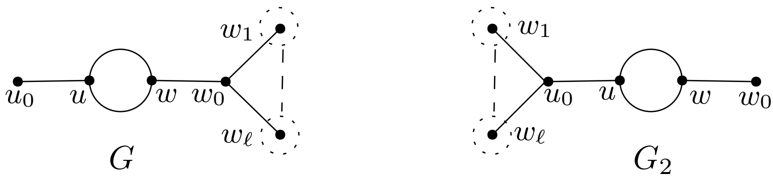

Figure 3. *Two graphs G and G_2.*

Proof. Note that $d_{G_2}(w_0) = 1$, $d_{G_2}(u_0) = \ell + 1$ and $d_{G_2}(v) = d_G(v)$ for all $v \in V(G)\backslash\{w_0, u_0\}$. Thus

$$\mathcal{SO}_\alpha(G_2) - \mathcal{SO}_\alpha(G) = \Big((\ell+1)^2 + d_u^2\Big)^\alpha - (1+d_u^2)^\alpha + (1+d_w^2)^\alpha - \Big((\ell+1)^2 + d_w^2\Big)^\alpha. \tag{3}$$

(i) If $\alpha < 0$ or $\alpha > 1$, then using Lemma 1 (i) (with $d_w > d_u$), we obtain

$$\mathcal{SO}_\alpha(G_2) - \mathcal{SO}_\alpha(G) < 0.$$

(ii) For $0 < \alpha < 1$, using Lemma 1 (ii) (with $d_w > d_u$), (3) becomes

$$\mathcal{SO}_\alpha(G_2) - \mathcal{SO}_\alpha(G) > 0.$$

This completes the proof of the result. ■

Lemma 7. *Consider the graph $Q_{s,t}$ with $s \geq t \geq 2$, as illustrated in Fig. 4. If $\alpha \geq 1$, then we have $\mathcal{SO}_\alpha(Q_{s,t}) < \mathcal{SO}_\alpha(Q_{s+1,t-1})$.*

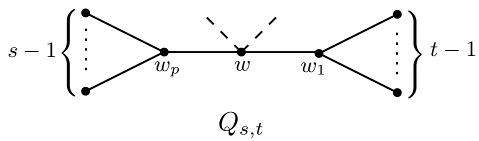

Figure 4. *The graph $Q_{s,t}$.*

Proof. Let w be a p-vertex in $Q_{s,t}$. Then we obtain:

$$\begin{aligned}
&\mathcal{SO}_\alpha(Q_{s+1,t-1}) - \mathcal{SO}_\alpha(Q_{s,t})\\
=&s\Big((s+1)^2+1\Big)^\alpha - (s-1)(s^2+1)^\alpha + \Big((s+1)^2+p^2\Big)^\alpha - (s^2+p^2)^\alpha\\
&+ (t-2)\Big((t-1)^2+1\Big)^\alpha - (t-1)(t^2+1)^\alpha + \Big((t-1)^2+p^2\Big)^\alpha\\
&- (t^2+p^2)^\alpha.
\end{aligned}$$

To begin with, note that for $\alpha = 1$, the expression $\mathcal{SO}_\alpha(Q_{s+1,t-1}) - \mathcal{SO}_\alpha(Q_{s,t})$ simplifies to $3(s^2-t^2) + 3(s+t)$ (with $s \geq t \geq 2$) and is positive. Moving on to $\alpha > 1$, while keeping in mind $s \geq t \geq 2$, we have:

$$\begin{aligned}
&\mathcal{SO}_\alpha(Q_{s+1,t-1}) - \mathcal{SO}_\alpha(Q_{s,t})\\
=&s\Big[\Big((s+1)^2+1\Big)^\alpha - (s^2+1)^\alpha\Big] + (s^2+1)^\alpha + \Big((s+1)^2+p^2\Big)^\alpha\\
&- (s^2+p^2)^\alpha - (t-1)(t^2+1)^\alpha + (t-2)\Big((t-1)^2+1\Big)^\alpha
\end{aligned}$$

$$+\Big((t-1)^2+p^2\Big)^\alpha-(t^2+p^2)^\alpha.$$

Utilizing Lemmas 1 (i), 2 and 3, it follows that

$$\begin{aligned}
&\mathcal{SO}_\alpha(Q_{s+1,t-1})-\mathcal{SO}_\alpha(Q_{s,t})\\
\geq& t\Big((t+1)^2+1\Big)^\alpha-(t-1)(t^2+1)^\alpha-(t^2+p^2)^\alpha+\Big((t+1)^2+p^2\Big)^\alpha\\
&+(t-2)\Big((t-1)^2+1\Big)^\alpha-(t-1)(t^2+1)^\alpha+\Big((t-1)^2+p^2\Big)^\alpha-(t^2+p^2)^\alpha\\
=&t\Big((t+1)^2+1\Big)^\alpha+(t-2)\Big((t-1)^2+1\Big)^\alpha-2(t-1)(t^2+1)^\alpha\\
&\quad+\Big((t+1)^2+p^2\Big)^\alpha+\Big((t-1)^2+p^2\Big)^\alpha-2(t^2+p^2)^\alpha>0.
\end{aligned}$$

Thus the proof is done. ■

3 Main results

In this section we focus on the extremal graphs of $\mathcal{SO}_\alpha(T)$ in the class of $\mathcal{T}(n,\Delta)$ for $\Delta\geq 3$.

Theorem 1. *Let $T\in\mathcal{T}(n,\Delta)$ be a tree of order n and $\Delta\geq 3$. Then*
(i) for $\alpha>0$,

$$\mathcal{SO}_\alpha(T)\geq\mathcal{SO}_\alpha\Big(S(a_1,a_2,\ldots,a_\Delta)\Big) \tag{4}$$

with equality if and only if $T\cong S(a_1,a_2,\ldots,a_\Delta)$,
(ii) for $-1\leq\alpha<0$,

$$\mathcal{SO}_\alpha(T)\leq\mathcal{SO}_\alpha\Big(S(a_1,a_2,\ldots,a_\Delta)\Big) \tag{5}$$

with equality if and only if $T\cong S(a_1,a_2,\ldots,a_\Delta)$.

Proof. If $T\cong S(a_1,a_2,\ldots,a_\Delta)$, then the equalities in (4) and (5) hold. Otherwise, $T\ncong S(a_1,a_2,\ldots,a_\Delta)$. Then T contains at least two vertices of degree greater than 2. Without loss of generality, we can assume that w is a Δ-vertex, and u is the farthest vertex from w with degree $p\geq 3$. Let $N_T(u)=\{u_1,u_2,\ldots,u_p\}$, where u_p is a vertex adjacent to u lies on the $u-w$ path (the vertices u_p and w may coincide). Since u is the furthest vertex from w with degree $p\,(\geq 3)$, the vertex u has $p-1$ pendant paths with $d_T(u_j)\in\{1,2\}$ for $j=1,2,\ldots,p-1$. Without loss of generality, we can assume that $d_T(u_1)\leq d_T(u_2)\leq\cdots\leq d_T(u_{p-1})\leq d_T(u_p)$. We now distinguish three cases in (i) and (ii):

(i) **Case 1:** $d_T(u_1)=d_T(u_2)=\cdots=d_T(u_{p-1})=1$.

Then we can obtain a tree $T_1\in\mathcal{T}(n,\Delta)$ from T by deleting the edges $uu_2,\ldots,uu_{p-1}$ and adding the new edges $u_1u_2,u_2u_3,\ldots,u_{p-2}u_{p-1}$, that is,

$$T_1=T-\{uu_2,uu_3,\ldots,uu_{p-1}\}+\{u_1u_2,u_2u_3,\ldots,u_{p-2}u_{p-1}\}.$$

Now we have $d_T(u)=p$, $d_T(u_j)=1$ for $j\in\{1,\ldots,p-2\}$, $d_{T_1}(u)=2$, $d_{T_1}(u_j)=2$ for $j\in\{1,\ldots,p-2\}$, $d_T(u_p)=d_{T_1}(u_p)=d_{u_p}$ and the degrees of other vertices remain the same in T and T_1. One can easily see that $E(T_1-\{uu_1,u_1u_2,u_2u_3,\ldots,u_{p-2}u_{p-1},uu_p\})=E(T\backslash\{u\})$. Thus we obtain

$$\begin{aligned}\mathcal{SO}_\alpha(T_1)=&\sum_{xy\in E(T\backslash\{u\})}\Big(d_{T_1}(x)^2+d_{T_1}(y)^2\Big)^\alpha+(d_{T_1}(u_p)^2+4)^\alpha\\&+\sum_{j=1}^{p-2}\Big(d_{T_1}(u_j)^2+d_{T_1}(u_{j+1})^2\Big)^\alpha+\Big(d_{T_1}(u)^2+d_{T_1}(u_1)^2\Big)^\alpha\\=&\sum_{xy\in E(T\backslash\{u\})}\Big(d_T(x)^2+d_T(y)^2\Big)^\alpha+(p-2)\,8^\alpha+5^\alpha\\&+(d_{T_1}(u_p)^2+4)^\alpha\end{aligned}$$

and

$$\begin{aligned}&\mathcal{SO}_\alpha(T)\\&=\sum_{xy\in E(T\backslash\{u\})}\Big(d_T(x)^2+d_T(y)^2\Big)^\alpha+\sum_{u_j\in N_T(u)}\Big(d_T(u)^2+d_T(u_j)^2\Big)^\alpha\\&=\sum_{xy\in E(T\backslash\{u\})}\Big(d_T(x)^2+d_T(y)^2\Big)^\alpha+(p-1)(p^2+1)^\alpha+\Big(p^2+d_{u_p}^2\Big)^\alpha.\end{aligned}$$

From the above two results, we obtain

$$\mathcal{SO}_\alpha(T_1) - \mathcal{SO}_\alpha(T) = (4 + d_{u_p}^2)^\alpha - (p^2 + d_{u_p}^2)^\alpha + (p-2)[8^\alpha - (p^2+1)^\alpha] + 5^\alpha - (p^2+1)^\alpha.$$

Since $p \geq 3$ and $\alpha > 0$, it follows that

$$\mathcal{SO}_\alpha(T_1) - \mathcal{SO}_\alpha(T) < 0, \quad \text{that is, } \mathcal{SO}_\alpha(T) > \mathcal{SO}_\alpha(T_1).$$

Case 2: When u is adjacent to at least one pendant vertex but not more than $p-2$ pendant vertices.

Without loss of generality, we can assume that u_1 is a pendant vertex and u_2 is a vertex of degree 2, both of which are adjacent to u in T. Let $v_1\,(\neq u_1)$ be a pendant vertex connected to u on a pendant path that includes u_2, and let v_2 be adjacent to v_1 (where v_2 may coincide with u_2). Define $T_2 \in \mathcal{T}(n,\Delta)$ as the graph obtained from T by deleting the edge uu_1 and adding the new edge v_1u_1. Thus we have $d_{T_2}(v_1) = 2$, $d_{T_2}(u) = p-1$, and the degrees of other vertices remain the same in T and T_2. Then

$$\mathcal{SO}_\alpha(T_2) - \mathcal{SO}_\alpha(T) = 5^\alpha - (1+p^2)^\alpha + 8^\alpha - 5^\alpha + \sum_{j=2}^{p}\left[\left((p-1)^2 + d_{u_j}^2\right)^\alpha - (p^2 + d_{u_j}^2)^\alpha\right].$$

Since $p \geq 3$ and $\alpha > 0$, it follows that

$$\mathcal{SO}_\alpha(T_2) - \mathcal{SO}_\alpha(T) < 0, \quad \text{that is, } \mathcal{SO}_\alpha(T) > \mathcal{SO}_\alpha(T_2).$$

Case 3: $d_T(u_1) = d_T(u_2) = \cdots = d_T(u_{p-1}) = 2$.

In this case we transform the tree T into $T_3 \in \mathcal{T}(n,\Delta)$ by replacing the $p-1$ pendant paths of length at least 2 from u with a single pendant path of length at least $2(p-1)$. Thus we have $d_T(u) = p$, $d_{T_3}(u) = 2$, the degrees of $p-2$ pendant vertices that are connected to u on pendant paths in T becomes 2 in T_3, and the degrees of other vertices remain the same in T and T_3. Thus we obtain

$$\begin{aligned}\mathcal{SO}_\alpha(T_3) - \mathcal{SO}_\alpha(T) &= (4 + d_{u_p}^2)^\alpha - (p^2 + d_{u_p}^2)^\alpha + (2p-3)8^\alpha \\ &\qquad - (p-1)(p^2+4)^\alpha - (p-2)5^\alpha \\ &< (2p-3)8^\alpha - (p-1)(p^2+4)^\alpha - (p-2)5^\alpha \qquad (6)\end{aligned}$$

as $p \geq 3$. For $p = 3$ and $\alpha > 0$, by Lemma 4 (i), from the above, we obtain

$$\mathcal{SO}_\alpha(T_3) - \mathcal{SO}_\alpha(T) < 3 \cdot 8^\alpha - 2 \cdot 13^\alpha - 5^\alpha < 0.$$

Otherwise, $p \geq 4$ and $\alpha > 0$, from (6), we obtain

$$\begin{aligned}\mathcal{SO}_\alpha(T_3) - \mathcal{SO}_\alpha(T) &< (p-1)[2 \cdot 8^\alpha - 5^\alpha - (p^2+4)^\alpha] \\ &< (p-1)[2 \cdot 8^\alpha - 5^\alpha - 20^\alpha] < 0\end{aligned}$$

as $8^\alpha > 5^\alpha$, and by Lemma 4 (ii). Thus $\mathcal{SO}_\alpha(T) > \mathcal{SO}_\alpha(T_3)$.

After applying the **Cases** $1-3$, we obtain a tree $T' \in \mathcal{T}(n, \Delta)$. If $T' \cong S(a_1, a_2, \ldots, a_\Delta)$, then we are done. Otherwise, $T' \ncong S(a_1, a_2, \ldots, a_\Delta)$. Then T' contains two vertices of degree greater than 2. Using the above three cases we obtain $T'' \in \mathcal{T}(n, \Delta)$ from T'. If $T'' \cong S(a_1, a_2, \ldots, a_\Delta)$, then we are done. Otherwise, continuing the same procedure, finally, we obtain

$$\mathcal{SO}_\alpha(T) > \mathcal{SO}_\alpha(T') > \mathcal{SO}_\alpha(T'') > \cdots > \mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big).$$

(ii) **Cases** 1 and 2 follow similarly from the proof of (i) (and are therefore omitted). We now proceed to discuss **Case** 3. In this case we have $d_T(u_1) = d_T(u_2) = \cdots = d_T(u_{p-1}) = 2$. Using the same transformation mentioned in **Case** 3 of (i), we obtain

$$\begin{aligned}\mathcal{SO}_\alpha(T_3) - \mathcal{SO}_\alpha(T) &= (4 + d_{u_p}^2)^\alpha - (p^2 + d_{u_p}^2)^\alpha + (2p-3)8^\alpha \\ &\qquad - (p-1)(p^2+4)^\alpha - (p-2)5^\alpha \\ &> (2p-3)8^\alpha - (p-1)(p^2+4)^\alpha - (p-2)5^\alpha \qquad (7)\end{aligned}$$

as $p \geq 3$. For $p = 3$ and $-1 \leq \alpha < 0$, by Lemma 4 (iii), (7) becomes

$$\mathcal{SO}_\alpha(T_3) - \mathcal{SO}_\alpha(T) > 3 \cdot 8^\alpha - 2 \cdot 13^\alpha - 5^\alpha > 0.$$

Otherwise, $p \geq 4$ and $-1 \leq \alpha < 0$, from (7), we obtain

$$\begin{aligned}\mathcal{SO}_\alpha(T_3) - \mathcal{SO}_\alpha(T) &> (p-1)[2 \cdot 8^\alpha - 5^\alpha - (p^2+4)^\alpha] \\ &> (p-1)[2 \cdot 8^\alpha - 5^\alpha - 20^\alpha] \geq 0\end{aligned}$$

as $5^\alpha > 8^\alpha$, and by Lemma 4 (iv). Thus $\mathcal{SO}_\alpha(T) < \mathcal{SO}_\alpha(T_3)$.

By using the same arguments as given in (i), we obtain

$$\mathcal{SO}_\alpha(T) < \mathcal{SO}_\alpha(T') < \mathcal{SO}_\alpha(T'') < \cdots < \mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big).$$

This completes the proof of the theorem. ■

Proposition 2. *Let $S(a_1, a_2, \ldots, a_\Delta) \in \mathcal{T}(n, \Delta)$ be a star-like tree of order n and $\Delta \geq 3$.*
(i) *If $0 < \alpha < 1$, then*

$$\mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big) \geq \begin{cases} (n-\Delta-1)\Big[5^\alpha + (\Delta^2+4)^\alpha\Big] + (2\Delta - n + 1)(\Delta^2+1)^\alpha & \text{if } \Delta \geq \lfloor \frac{n+1}{2} \rfloor, \\ \Delta\Big[(\Delta^2+4)^\alpha + 5^\alpha\Big] + (n - 2\Delta - 1)8^\alpha & \text{if } 3 \leq \Delta \leq \lfloor \frac{n-1}{2} \rfloor \end{cases}$$

with equality if and only if $S(a_1, a_2, \ldots, a_\Delta) \cong T_{n,\Delta}$ for $\Delta \geq \lfloor \frac{n+1}{2} \rfloor$, and $S(a_1, a_2, \ldots, a_\Delta) \cong T_\Delta$ for $3 \leq \Delta \leq \lfloor \frac{n-1}{2} \rfloor$.

(ii) If $-1 \le \alpha < 0$*, then*

$$\mathcal{SO}_\alpha\Big(S(a_1, a_2, \dots, a_\Delta)\Big)$$
$$\le \begin{cases} (n-\Delta-1)\Big[5^\alpha + (\Delta^2+4)^\alpha\Big] + (2\Delta-n+1)(\Delta^2+1)^\alpha \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{if } \Delta \ge \lfloor\frac{n+1}{2}\rfloor, \\ \Delta\Big[(\Delta^2+4)^\alpha + 5^\alpha\Big] + (n-2\Delta-1)8^\alpha \quad \text{if } 3 \le \Delta \le \lfloor\frac{n-1}{2}\rfloor \end{cases}$$

with equality if and only if $S(a_1, a_2, \dots, a_\Delta) \cong T_{n,\Delta}$ *for* $\Delta \ge \lfloor\frac{n+1}{2}\rfloor$*, and* $S(a_1, a_2, \dots, a_\Delta) \cong T_\Delta$ *for* $3 \le \Delta \le \lfloor\frac{n-1}{2}\rfloor$*.*

Proof. If $S(a_1, a_2, \dots, a_\Delta) \cong T_{n,\Delta}$ or $S(a_1, a_2, \dots, a_\Delta) \cong T_\Delta$, then the equality holds in (i) and (ii). Otherwise, $T_{n,\Delta} \ncong S(a_1, a_2, \dots, a_\Delta) \ncong T_\Delta$. Then $S(a_1, a_2, \dots, a_\Delta)$ has a pendant path of length at least 3 and a pendant vertex adjacent to the maximum degree vertex.

$$\textbf{Transformation I:}\quad S(a_1, a_2, \dots, a_\Delta) \to T_1,$$

where T_1 is a star-like tree obtained from $S(a_1, a_2, \dots, a_\Delta)$ by replacing the pendant path of length 1 with a pendant path of length 2, and a pendant path of length $\ell\,(\ge 3)$ with a pendant path of length $\ell-1$. Then we obtain

$$\mathcal{SO}_\alpha(T_1) - \mathcal{SO}_\alpha\Big(S(a_1, a_2, \dots, a_\Delta)\Big) = (\Delta^2+4)^\alpha - (\Delta^2+1)^\alpha + 5^\alpha - 8^\alpha. \tag{8}$$

(i) Setting $c = 2$, $d = 1$ in Lemma 1 (ii), it follows that $\Phi(\Delta) = (\Delta^2 + 4)^\alpha - (\Delta^2+1)^\alpha < 8^\alpha - 5^\alpha = \Phi(2)$ as $0 < \alpha < 1$. Using this result in (8), we obtain $\mathcal{SO}_\alpha\Big(S(a_1, a_2, \dots, a_\Delta)\Big) > \mathcal{SO}_\alpha(T_1)$.

First we assume that $\Delta \ge \lfloor\frac{n+1}{2}\rfloor$. Thus we have $n \le 2\Delta$, that is, $n_1 + n_2 + 1 \le 2\Delta = 2n_1$ as T_1 is a star-like tree of order n. Thus we have $n_2 < n_1$. From this, we conclude that star-like tree T_1 contains a pendant vertex adjacent to the maximum degree vertex. If $T_1 \cong T_{n,\Delta}$, then we are done. Otherwise, $T_1 \ncong T_{n,\Delta}$. Then T_1 contains a pendant path of length $\ell \ge 3$. Using the same **Transformation I**, we obtain star-like tree T_2 from star-like tree T_1. Similarly, we get $\mathcal{SO}_\alpha(T_1) > \mathcal{SO}_\alpha(T_2)$. Continuing the same procedure, finally, we obtain

$$\mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big) > \mathcal{SO}_\alpha(T_1) > \mathcal{SO}_\alpha(T_2) > \cdots > \mathcal{SO}_\alpha(T_{n,\Delta}),$$

where

$$\mathcal{SO}_\alpha(T_{n,\Delta}) = (n - \Delta - 1)\left[5^\alpha + (\Delta^2 + 4)^\alpha\right] + (2\Delta - n + 1)(\Delta^2 + 1)^\alpha.$$

Next we assume that $3 \le \Delta \le \lfloor \frac{n-1}{2} \rfloor$. Thus we have $n_1 + n_2 + 1 = n \ge 2\Delta + 1 = 2n_1 + 1$, that is, $n_2 \ge n_1$. If $n_2 = n_1$, then $T_1 \cong T_\Delta$. Otherwise, $n_2 \ge n_1 + 1$. Then star-like tree T_1 has a path of length at least 3. For $T_1 \cong T_\Delta$, we are done. Now we suppose that $T_1 \ncong T_\Delta$. Then T_1 has a pendant vertex adjacent to the maximum degree vertex. Using the same **Transformation I**, we obtain star-like tree T_2' from star-like tree T_1. Similarly, we get $\mathcal{SO}_\alpha(T_1) > \mathcal{SO}_\alpha(T'_2)$. Continuing the same procedure, finally, we obtain

$$\mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big) > \mathcal{SO}_\alpha(T_1) > \mathcal{SO}_\alpha(T'_2) > \cdots > \mathcal{SO}_\alpha(T_\Delta),$$

where

$$\mathcal{SO}_\alpha(T_\Delta) = \Delta\left[(\Delta^2 + 4)^\alpha + 5^\alpha\right] + (n - 2\Delta - 1)8^\alpha.$$

(ii) Setting $c = 2$, $d = 1$ in Lemma 1 (i), it follows that $\Phi(\Delta) = (\Delta^2 + 4)^\alpha - (\Delta^2 + 1)^\alpha > 8^\alpha - 5^\alpha = \Phi(2)$ as $-1 \le \alpha < 0$. Using this result in (8), we obtain $\mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big) < \mathcal{SO}_\alpha(T_1)$.

For $\Delta \ge \lfloor \frac{n+1}{2} \rfloor$, by using the same arguments as given in the proof of (i), we obtain

$$\mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big) < \mathcal{SO}_\alpha(T_1) < \mathcal{SO}_\alpha(T_2) < \cdots < \mathcal{SO}_\alpha(T_{n,\Delta}).$$

For $3 \le \Delta \le \lfloor \frac{n-1}{2} \rfloor$, by using the same arguments as given in the proof of (i), we obtain

$$\mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big) < \mathcal{SO}_\alpha(T_1) < \mathcal{SO}_\alpha(T_2) < \cdots < \mathcal{SO}_\alpha(T_\Delta).$$

Thus the proof is complete. ■

Corollary 1. *Let $S(a_1, a_2, \ldots, a_\Delta) \in \mathcal{T}(n, \Delta)$ be a star-like tree of order n and $\Delta \geq 3$.*
(i) If $S(a_1, a_2, \ldots, a_\Delta)$ with minimum $\mathcal{SO}_\alpha$ for $0 < \alpha < 1$ contains a pendant path of length 1, then it does not contain a pendant path longer than 2.
(ii) If $S(a_1, a_2, \ldots, a_\Delta)$ with maximum $\mathcal{SO}_\alpha$ for $-1 \leq \alpha < 0$ contains a pendant path of length 1, then it does not contain a pendant path longer than 2.

The next theorem directly follows from Theorem 1 and Proposition 2.

Theorem 3. *Let $T \in \mathcal{T}(n, \Delta)$ be a tree of order n and $\Delta \geq 3$.*
(i) If $0 < \alpha < 1$, then

$$\mathcal{SO}_\alpha(T) \geq \begin{cases} (n-\Delta-1)\left[5^\alpha + (\Delta^2+4)^\alpha\right] + (2\Delta - n + 1)(\Delta^2+1)^\alpha & \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{if } \Delta \geq \lfloor \frac{n+1}{2} \rfloor, \\ \Delta\left[(\Delta^2+4)^\alpha + 5^\alpha\right] + (n-2\Delta-1)8^\alpha \quad \text{if } 3 \leq \Delta \leq \lfloor \frac{n-1}{2} \rfloor \end{cases}$$

with equality if and only if $T \cong T_{n,\Delta}$ for $\Delta \geq \lfloor \frac{n+1}{2} \rfloor$, and $T \cong T_\Delta$ for $3 \leq \Delta \leq \lfloor \frac{n-1}{2} \rfloor$.
(ii) If $-1 \leq \alpha < 0$, then

$$\mathcal{SO}_\alpha(T) \leq \begin{cases} (n-\Delta-1)\left[5^\alpha + (\Delta^2+4)^\alpha\right] + (2\Delta - n + 1)(\Delta^2+1)^\alpha & \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{if } \Delta \geq \lfloor \frac{n+1}{2} \rfloor, \\ \Delta\left[(\Delta^2+4)^\alpha + 5^\alpha\right] + (n-2\Delta-1)8^\alpha \quad \text{if } 3 \leq \Delta \leq \lfloor \frac{n-1}{2} \rfloor \end{cases}$$

with equality if and only if $T \cong T_{n,\Delta}$ for $\Delta \geq \lfloor \frac{n+1}{2} \rfloor$, and $T \cong T_\Delta$ for $3 \leq \Delta \leq \lfloor \frac{n-1}{2} \rfloor$.

Theorem 4. *Let $T \in \mathcal{T}(n, \Delta)$ be a tree of order n and $3 \leq \Delta \leq n-2$. If $\alpha > 1$, then*

$$\mathcal{SO}_\alpha(T) \geq (\Delta-1)(\Delta^2+1)^\alpha + (\Delta^2+4)^\alpha + (n-\Delta-2)8^\alpha + 5^\alpha$$

with equality if and only if $T \cong B_{n,\Delta}$.

Proof. First we prove the following result:

Claim 1.

$$\begin{aligned} \mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big) \geq (\Delta-1)(\Delta^2+1)^\alpha + (\Delta^2+4)^\alpha \\ + (n-\Delta-2)8^\alpha + 5^\alpha \end{aligned} \tag{9}$$

with equality if and only if $S(a_1, a_2, \ldots, a_\Delta) \cong B_{n,\Delta}$.

Proof of Claim 1. If $S(a_1, a_2, \ldots, a_\Delta) \cong B_{n,\Delta}$, then we obtain

$$\mathcal{SO}_\alpha(S(a_1, a_2, \ldots, a_\Delta)) = (\Delta-1)(\Delta^2+1)^\alpha + (\Delta^2+4)^\alpha + (n-\Delta-2)8^\alpha + 5^\alpha$$

and hence the equality holds in (9). Otherwise, $S(a_1, a_2, \ldots, a_\Delta) \ncong B_{n,\Delta}$. Then $S(a_1, a_2, \ldots, a_\Delta)$ contains at least two pendant paths of length $\ell_1 \geq 2$ and $\ell_2 \geq 2$, respectively. Let T_1 be a star-like tree derived from $S(a_1, a_2, \ldots, a_\Delta)$ by replacing the pendant path of length $\ell_1 \geq 2$ with a pendant path of length 1, and the pendant path of length $\ell_2 \geq 2$ with a pendant path of length $\ell_1 + \ell_2 - 1$. Then we obtain

$$\begin{aligned} \mathcal{SO}_\alpha(T_1) - \mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big) = (\Delta^2+1)^\alpha - (\Delta^2+4)^\alpha \\ + 8^\alpha - 5^\alpha. \end{aligned} \tag{10}$$

Setting $c = 2$, $d = 1$ in Lemma 1 (i), it follows that $\Phi(\Delta) = (\Delta^2+4)^\alpha - (\Delta^2+1)^\alpha > 8^\alpha - 5^\alpha = \Phi(2)$ as $\alpha > 1$. Using this result in (10), we obtain $\mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big) > \mathcal{SO}_\alpha(T_1)$. If $T_1 \cong B_{n,\Delta}$, then the inequality in (9) holds strictly. Otherwise, $T_1 \ncong B_{n,\Delta}$. Then T_1 contains at least two pendant paths of length greater than 1. Using the above transformation we obtain star-like tree T_2 from star-like tree T_1. Similarly, we obtain $\mathcal{SO}_\alpha(T_1) > \mathcal{SO}_\alpha(T_2)$. By continuing the same procedure for a sufficient number of times, finally, we obtain

$$\mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big) > \mathcal{SO}_\alpha(T_1) > \mathcal{SO}_\alpha(T_2) > \cdots > \mathcal{SO}_\alpha(B_{n,\Delta}),$$

where

$$\mathcal{SO}_\alpha(B_{n,\Delta}) = (\Delta-1)(\Delta^2+1)^\alpha + (\Delta^2+4)^\alpha + (n-\Delta-2)8^\alpha + 5^\alpha,$$

which gives the **Claim 1**.

By Theorem 1(i), we obtain $\mathcal{SO}_\alpha(T) \geq \mathcal{SO}_\alpha\Big(S(a_1, a_2, \ldots, a_\Delta)\Big)$ with equality if and only if $T \cong S(a_1, a_2, \ldots, a_\Delta)$. This result with **Claim 1**, we get the lower bound on $\mathcal{SO}_\alpha(T)$. Moreover, the equality holds if and only if $T \cong B_{n,\Delta}$. ■

We now focus on establishing the lower and upper bounds for trees in $\mathcal{T}(n, \Delta)$ with respect to the $\mathcal{SO}_\alpha$ index for $\alpha < 0$ and $\alpha > 1$, respectively. Note that the following result, which is useful for determining the bounds we are focusing on:

Proposition 5. *Let $T \in \mathcal{T}(n, \Delta)$ be a tree. If $\Delta \geq \lceil \frac{n}{2} \rceil$, then the maximum degree vertex w is adjacent to at least one pendant vertex.*

Proof. Assume to the contrary that there is no pendant vertex adjacent to the maximum degree vertex w. This implies that every neighbor of w is adjacent to at least one vertex other than w. Consequently, w, its Δ neighbors, and the vertices adjacent to these Δ neighbors (excluding w) account for at least $2\Delta + 1$ vertices. However, this contradicts the condition that $\Delta \geq \lceil \frac{n}{2} \rceil$. Therefore, we conclude that w must have at least one pendant neighbor. ■

Theorem 6. *Let $T \in \mathcal{T}(n, \Delta)$ be a tree of order n and $3 \leq \lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$. If $\alpha > 1$, then*

$$\mathcal{SO}_\alpha(T) \leq (\Delta-1)(\Delta^2+1)^\alpha + (n-\Delta-1)\Big((n-\Delta)^2+1\Big)^\alpha + \Big((n-\Delta)^2+\Delta^2\Big)^\alpha.$$

Equality occurs if and only if $T \cong S_{\Delta,n-\Delta}$.

Proof. Let $T' \in \mathcal{T}(n, \Delta)$ be a tree with $3 \leq \lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$ such that $\mathcal{SO}_\alpha(T')$ is maximum for $\alpha > 1$. Let $w \in V(T')$ be a Δ-vertex, where

$\Delta \geq \lceil \frac{n}{2} \rceil \geq 3$. According to Proposition 5, let w_0 be a pendant vertex adjacent to w. We now proceed with the following claims:

Claim 2. Each non-pendant neighbor of w has w as its only non-pendant neighbor.

Proof of Claim 2. Suppose, for the sake of contradiction, that there exists a non-pendant neighbor u of w which has another non-pendant neighbor u_0 distinct from w in T'. Let $N_{T'}(u_0)\backslash\{u\} = \{u_1, \ldots, u_\ell\}$, where $\ell \geq 1$. Since T' contains at least Δ pendant vertices and $\Delta \geq \lceil \frac{n}{2} \rceil$, it follows that $d_{T'}(u) \leq n - \Delta - 1 \leq \lfloor \frac{n}{2} \rfloor - 1 < \Delta = d_{T'}(w)$. We can construct a tree $T_1 \in \mathcal{T}(n, \Delta)$ by deleting the edges $u_0u_1, \ldots, u_0u_\ell$ and adding the new edges $w_0u_1, \ldots, w_0w_\ell$ in T'. By Lemma 5, it follows that $\mathcal{SO}_\alpha(T_1) > \mathcal{SO}_\alpha(T')$, which contradicts as $\mathcal{SO}_\alpha(T')$ is maximum. This proves the **Claim 2**.

Claim 3. The vertex w has a unique non-pendant neighbor.

Proof of Claim 3. Assume to the contrary that w_1 with degree $s \geq 2$ and w_p with degree $t \geq 2$ are the neighboring vertices of w in T'. Without loss of generality, assume that $s \geq t$. According to **Claim 2**, both $N_{T'}(w_1)$ and $N_{T'}(w_p)$ include only one non-pendant neighbor, which is w. This implies that $T' \cong Q_{s,t}$ (see, Fig. 4). By Lemma 7, it follows that

$$\mathcal{SO}_\alpha(T') = \mathcal{SO}_\alpha(Q_{s,t}) < \mathcal{SO}_\alpha(Q_{s+1,t-1}) < \cdots < \mathcal{SO}_\alpha(Q_{s+t-1,1}).$$

Furthermore, taking into account the inequality $(s-1)+(t-1)+(\Delta+1) \leq n$ and the assumption $\Delta \geq \lceil \frac{n}{2} \rceil$, it follows that $s+t-1 \leq n-\Delta \leq \lfloor \frac{n}{2} \rfloor \leq \Delta$. Thus $Q_{s+t-1,1} \in \mathcal{T}(n, \Delta)$ with $\mathcal{SO}_\alpha(Q_{s+t-1,1}) > \mathcal{SO}_\alpha(T')$, contradicting the maximality of $\mathcal{SO}_\alpha(T')$. Therefore, w must have a unique non-pendant neighbor. This proves the **Claim 3**.

Hence the **Claims 2 and 3** together imply that T' is isomorphic to $S_{\Delta,n-\Delta}$. By direct calculations, we get

$$\begin{aligned}\mathcal{SO}_\alpha(S_{\Delta,n-\Delta}) = (\Delta-1)(\Delta^2+1)^\alpha + (n-\Delta-1)\Big((n-\Delta)^2+1\Big)^\alpha \\ + \Big((n-\Delta)^2+\Delta^2\Big)^\alpha.\end{aligned}$$

Thus the result is established. ■

Theorem 7. *Let $T \in \mathcal{T}(n, \Delta)$ be a tree with order n and $3 \leq \lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$. If $\alpha < 0$, then*

$$\mathcal{SO}_\alpha(T) \geq (\Delta - 1)(\Delta^2 + 1)^\alpha + (n - \Delta - 1)\Big((n-\Delta)^2 + 1\Big)^\alpha + \Big((n-\Delta)^2 + \Delta^2\Big)^\alpha$$

with equality if and only if $T \cong S_{\Delta, n-\Delta}$.

Proof. Let $T' \in \mathcal{T}(n, \Delta)$ be a tree with $3 \leq \lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$ such that $\mathcal{SO}_\alpha(T')$ is minimum for $\alpha < 0$. Let $w \in V(T')$ be a Δ-vertex, where $\Delta \geq 3$. According to Proposition 5, let w' be a pendant vertex adjacent to w. We now proceed with the following claims:

Claim 4. The vertex w has a unique non-pendant neighbor.

Proof of Claim 4. Let u be a non-pendant vertex adjacent to a pendant vertex u_0 in T'. Suppose, contrary to the claim, that w has at least two non-pendant neighbors. This implies the existence of at least one non-pendant vertex $w_0 \in N_{T'}(w)$ such that w_0 does not lie on the $w - u$ path (the vertices u and w may adjacent). Let $N_{T'}(w_0) \backslash \{w\} = \{w_1, \ldots, w_\ell\}$, where $\ell \geq 1$. Since T' contains at least Δ pendant vertices and $\Delta \geq \lceil \frac{n}{2} \rceil$, it follows that $d_{T'}(u) \leq n - \Delta - 1 \leq \lfloor \frac{n}{2} \rfloor - 1 < \Delta = d_{T'}(w)$. We can construct a tree $T_1 \in \mathcal{T}_{n,\Delta}$ by deleting the edges $w_0w_1, \ldots, w_0w_\ell$ and adding the new edge $u_0w_1, \ldots, u_0w_\ell$ in T'. By applying Lemma 6, we obtain that $\mathcal{SO}_\alpha(T_1) < \mathcal{SO}_\alpha(T')$. This contradicts the assumption that $\mathcal{SO}_\alpha(T')$ is minimum. This proves the **Claim 4**.

From **Claim 4**, $T' - w$ contains only one non-trivial component. We denote this unique non-trivial component of $T' - w$ as X.

Claim 5. The component X of $T' - w$ is a star.

Proof of Claim 5. Suppose, for the sake of contradiction, that there exist at least one non-pendant edge $uu' \in E(T')$ (where u and u' are distinct from w) such that $d_{T'}(w, u)$ is as large as possible, and u has only one non-pendant neighbor u'. Let $d_{T'}(u) = t \geq 2$ and $d_{T'}(u') = s \geq 2$. Let $u_1, u_2, \ldots, u_{t-1}$ be the all pendant neighbors of u. We now define a tree

$T_2 \in \mathcal{T}(n,\Delta)$ by removing the edges $uu_1,\ldots,uu_{t-1}$ and adding the new edges $u'u_1,\ldots,u'u_{t-1}$ in T'. Note that $d_{T_2}(u)=1$, $d_{T_2}(u')=s+t-1$ and $d_{T_2}(v_i)=d_{T'}(v_i)=d_{v_i}$ for all $v_i \in V(T')\backslash\{u,u'\}$. Then

$$\begin{aligned}&\mathcal{SO}_\alpha(T')-\mathcal{SO}_\alpha(T_2)\\=&(t-1)\Big[(1+t^2)^\alpha-\Big(1+(s+t-1)^2\Big)^\alpha\Big]-\Big((s+t-1)^2+1\Big)^\alpha+(s^2+t^2)^\alpha\\&\qquad+\sum_{v_i\in N_{T'}(u')\backslash\{u\}}\Big[(d_{v_i}^2+s^2)^\alpha-\Big(d_{v_i}^2+(s+t-1)^2\Big)^\alpha\Big].\end{aligned}$$

Since $\alpha<0$ and $1+t^2<1+(s+t-1)^2$, it follows that $(1+t^2)^\alpha>\Big(1+(s+t-1)^2\Big)^\alpha$. Similarly, $(d_v^2+s^2)^\alpha>(d_v^2+(s+t-1)^2)^\alpha$, and $(s^2+t^2)^\alpha>\Big((s+t-1)^2+1\Big)^\alpha$ $\Big((s+t-1)^2+1>s^2+t^2$, that is, $st+1>s+t$, which is true as $s\geq 2$, $t\geq 2\Big)$. Therefore $\mathcal{SO}_\alpha(T')>\mathcal{SO}_\alpha(T_2)$, which contradicts the assumption that $\mathcal{SO}_\alpha(T')$ is minimum. This proves the **Claim 5**.

Thus from **Claims 4** and **5**, it follows that T' is isomorphic to $S_{\Delta,n-\Delta}$. Direct calculations yield

$$\begin{aligned}\mathcal{SO}_\alpha(S_{\Delta,n-\Delta})=(\Delta-1)(\Delta^2+1)^\alpha+(n-\Delta-1)\Big((n-\Delta)^2+1\Big)^\alpha\\+\Big((n-\Delta)^2+\Delta^2\Big)^\alpha.\end{aligned}$$

This completes the proof of the theorem. ∎

4 Concluding remarks

Within this work, we identified the trees that maximize the $\mathcal{SO}_\alpha$ index for $-1\leq\alpha<0$ and $\alpha>1$, as well as those that minimize the $\mathcal{SO}_\alpha$ index for $\alpha<0$ and $\alpha>0$. We also characterized the pertinent extremal trees.

By Theorem 1, the tree $S(a_1,a_2,\ldots,a_\Delta)\in\mathcal{T}(n,\Delta)$ minimizes the $\mathcal{SO}_\alpha$ index for $\alpha>0$ with degree sequence $(\Delta,\underbrace{2,\ldots,2}_{n-\Delta-1},\underbrace{1,\ldots,1}_{\Delta})$. Specifically, for $\alpha = 1$ we have $\mathcal{SO}_1 = F$. So

$$F\Big(S(a_1, a_2, \ldots, a_\Delta)\Big) = \sum_{v_i v_j \in E(S(a_1,a_2,\ldots,a_\Delta))} (d_{v_i}^2 + d_{v_j}^2) = \sum_{v_i \in V(S(a_1,a_2,\ldots,a_\Delta))} d_{v_i}^3 = \Delta^3 + 8n - 7\Delta - 8.$$

To maximize $\mathcal{SO}_1 = F = \sum_{v_i \in V(T)} d_{v_i}^3(T)$, a tree with degrees x and y (where $x \leq y$) yields a smaller $\mathcal{SO}_1$ than one with degrees $x-1$ and $y+1$. Among trees with given n and $\lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$, a tree with the degree sequence $(\Delta, n-\Delta, \underbrace{1, \ldots, 1}_{n-2})$ maximizes $\mathcal{SO}_1 = F$, represented uniquely by $S_{\Delta,n-\Delta}$. The following table summarizes our main results. and highlights key findings for future study.

α	Maximizes $\mathcal{SO}_\alpha$	Minimizes $\mathcal{SO}_\alpha$
$(-\infty, 0)$	$T_{n,\Delta}$ if $-1 \leq \alpha < 0$ and $\lfloor \frac{n+1}{2} \rfloor < \Delta \leq n-1$ T_Δ if $3 \leq \Delta \leq \lfloor \frac{n-1}{2} \rfloor$	$S_{\Delta,n-\Delta}$ if $3 \leq \lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$
$(0, 1)$	?	$T_{n,\Delta}$ if $\lfloor \frac{n+1}{2} \rfloor < \Delta \leq n-1$ T_Δ if $3 \leq \Delta \leq \lfloor \frac{n-1}{2} \rfloor$
$\{1\}$	$S_{\Delta,n-\Delta}$ if $3 \leq \lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$	$S(a_1, a_2, \ldots, a_\Delta)$ if $3 \leq \Delta \leq n-1$
$(1, \infty)$	$S_{\Delta,n-\Delta}$ if $3 \leq \lceil \frac{n}{2} \rceil \leq \Delta \leq n-2$	$B_{n,\Delta}$ if $3 \leq \Delta \leq n-2$

Table 1. *Trees maximize and minimize the $\mathcal{SO}_\alpha$ index in $\mathcal{T}(n, \Delta)$ for different intervals of α.*

The characterization of extremal trees for $\mathcal{SO}_\alpha$ index in the remaining intervals of α remains an open problem and presents a promising direction for future research.

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