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On the Extremal General Sombor Index of Trees with Given Pendent Vertices

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Abstract

The General Sombor index of a graph G is given by,

$$SO_\alpha(G) = \sum_{xy\in E(G)} (d_G^2(x) + d_G^2(y))^\alpha,$$

where $d_G(x)$ represents the degree of vertex x in graph G. This paper focuses on determining the maximum and minimum General Sombor index among trees with given number of pendent vertices, where $\alpha \in (0,1)$. Additionally, the graphs that achieve the extremal index values are identified and described in this paper.

1 Introduction

Let G be a simple graph. This graph possesses a combination of vertices and edges, represented as $V(G)$ and $\mathcal{E}(G)$, respectively. We use the

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symbols m and n to represent the total number of edges and vertices, where $|\mathcal{E}(G)| = m$ and $|V(G)| = n$. We denote the degree of a specific vertex y within G, as $d_G(y)$ or simply $d(y)$, corresponds to the total count of the neighboring vertices attached to it. When vertices x and y are connected, the connecting edge is denoted as $e = xy$. In both mathematical and chemical literature, numerous graph invariants centered around vertex degrees (often termed "topological indices") has been introduced and thoroughly examined [10–12]. A numerical quantity, denoted as $TI(G)$, can be used to represent a topological index, which is computed or determined based on a (chemical) graph in a manner that preserves its value when considering graph isomorphism. These invariants can generally be expressed using the formula

$$TI(G) = \sum_{xy \in \mathcal{E}(G)} H(d_G(x), d_G(y)),$$

here $H(x, y)$ represents a function exhibiting the characteristic $H(x, y) = H(y, x)$. Numerous topological indices, explored within the realm of chemical graph theory, hold multiple significant applications in chemistry. This is evident from recent publications like [29, 33].

Another degree-based topological index, the Sombor index [11],

$$SO(G) = \sum_{xy \in \mathcal{E}(G)} \sqrt{(d_G^2(x) + d_G^2(y))}$$

was originally formulated based on geometric principles and rapidly captured substantial attention. While the Sombor index has been extensively explored for its mathematical attributes and chemical utility [1, 2, 6, 9, 13, 15, 19, 20, 26, 27], its geometric aspects have largely gone unnoticed. The maximal Sombor index has been investigated in relation to (chemical) trees [3, 4, 7, 8, 17, 18, 31, 32], chemical graphs [3, 9, 19, 22, 35], c-cyclic graphs [5, 14, 21, 22, 30], as well as its implications in chemical contexts [8, 19, 24, 28] and spectral characteristics [23, 24], among other areas.

In [16], X. Hu and L. Zhong defined the general Sombor index as,

$$SO_\alpha(G) = \sum_{xy \in \mathcal{E}(G)} (d_G^2(x) + d_G^2(y))^\alpha.$$

Inspired by the work in [36], we investigate the General Sombor index for the trees having a given number of pendent vertices. Let $N_G(x)$ (or $N(x)$), represent the collection of neighboring vertices for a given vertex $x \in V(G)$. Since the degree $d_G(x)$ (or $d(x)$) corresponds to the number of edges in G that are incident to x, it can also be denoted as $d_G(x) = |N_G(x)|$. Specifically, we define $\Delta(G)$ as the highest value among the degrees of vertices in G, i.e., the maximum degree in G. For any $y \in V(G)$, the $G - y$ graph is formed by eliminating vertex y and its connecting edges from G. The graph $G - xy$ is derived by removing the edge xy from G, where xy is an edge in the edge set $E(G)$.

A vertex with a degree of one is referred to as a pendent vertex. If the degree of a vertex x is r, it is termed as an r-vertex. The edges adjacent to the pendent vertices are called pendent edges. Consider an induced sub-path $P = y_0y_1...y_r$ within graph G, where P has a length of r. If $d(y_0)$ equals 1, $d(y_1)$ through $d(y_{r-1})$ are all equal to 2, and $d(y_r)$ is greater than or equal to 3, then we refer to the sub-path P as a pendent path within G. The collection containing all the pendent vertices in graph G is symbolized as $\mathcal{PV}(G)$ and we represent the collection of all pendent paths in graph G as $\mathcal{P}(G)$. In G, a vertex set $V(G) = \{d(y_1), d(y_2), \ldots, d(y_n)\}$, where $d(y_1) \geq d(y_2) \geq \ldots \geq d(y_n)$ holds, then the sequence $(d(y_1), d(y_2), ..., d(y_n))$ is termed the degree sequence of G.

When a connected graph $\mathcal{T}$ has $m = n - 1$, it is termed a tree. We can easily verify that every tree must have a minimum of two vertices having degree one, where star is the only tree having precisely $n - 1$ vertices that are pendent. For $2 \leq k \leq n - 1$, we define two collection : $\mathcal{T}_{n,k}$ for trees and $\mathcal{CT}_{n,k}$ for chemical trees, both of order n and k vertices that are pendent. If a tree $\mathcal{T}$ belongs to $\mathcal{T}_{n,k}$ and all its vertices which are not pendent vertices are 3-vertices, then we call $\mathcal{T}$ a $(k, 3)$-regular tree. It is observed directly that all the $(k, 3)$-regular tree consists of $2k - 2$ vertices, including exactly k pendent vertices.

In [36] Zhang et al. initially introduced three transformations for a tree $\mathcal{T}$ consisting of n vertices, which will hold significant significance throughout the main results.

Transformation I : The process of taking a fixed edge xy in $\mathcal{T}$ and constructing another tree $\mathcal{T}_{xy}$ having $n-1$ vertices, by merging the two vertices connected by the edge xy in $\mathcal{T}$ is referred as *Transformation I* (See figure 1).

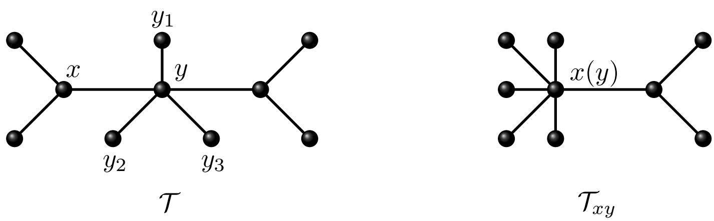

Figure 1. Illustration of Transformation I

Transformation II : Suppose $y \in V(\mathcal{T})$ with $N(y) = Y' \cup Y''$ satisfying $Y' \cap Y'' = \emptyset$, $|Y'| = b_1 \geq 1$, and $|Y''| = b_2 \geq 1$. We denote by $\mathcal{T}_{y\mapsto(b_1,b_2)}$, a new tree with $|V(\mathcal{T}_{y\mapsto(b_1,b_2)})| = |V(\mathcal{T})|+1$. The construction of $\mathcal{T}_{y\mapsto(b_1,b_2)}$ from $\mathcal{T}$ involves splitting the vertex y into two new vertices y' and y'' and adding an edge between y' and y'', joining y' and all vertices of Y', and then joining y'' and all vertices of Y''. In the subsequent discussions, we will refer to $\mathcal{T}_{y\mapsto(b_1,b_2)}$ as a result of *Transformation II* (See figure 2).

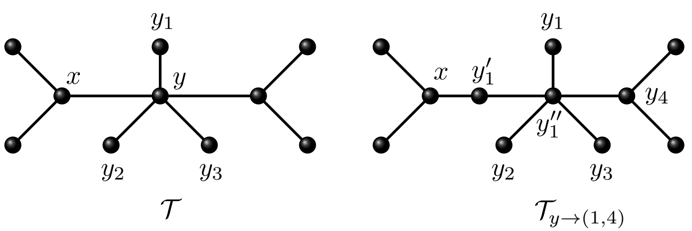

Figure 2. Illustration of Transformation II

Transformation III : Consider a tree $\mathcal{T}$ with a vertex y containing at least four vertices. We can construct a new tree $\mathcal{T}_{y\mapsto(3-reg)}$, by modifying $\mathcal{T}$. This transformation involves substituting the vertex $y \in \mathcal{T}$ with a $(b,3)$-tree H, such that we individually identify each vertex in the neighborhood of y and each pendent vertex in H. This process is referred to as *Transformation III* when applied to $\mathcal{T}$ (See figure 3).

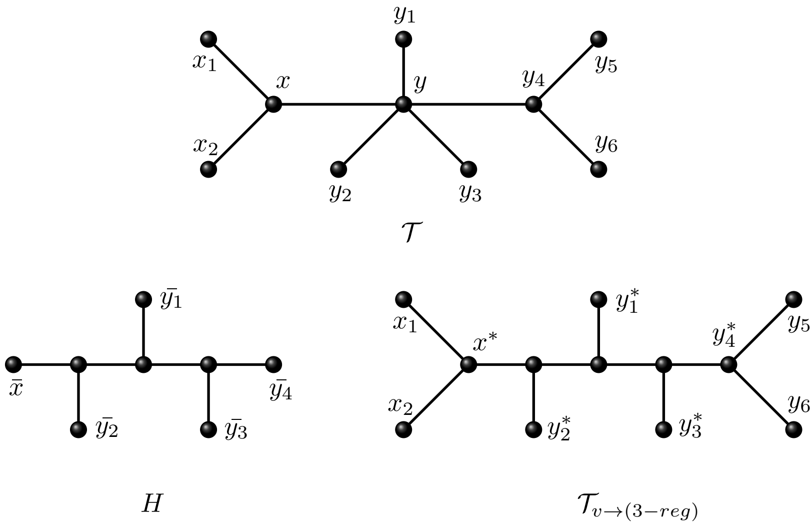

Figure 3. Illustration of Transformation III

We define $\eta_i(G)$ as the total count of vertices in graph G having i as it's degree, and the notation $e_{i,j}(G)$ signifies the count of edges in graph G linking a i-vertex with a j-vertex. When there is no risk of confusion, we will utilize the more concise notations η_i and $e_{i,j}$. Additionally, we denote the star with n vertices as S_n and the path with n vertices as P_n. The set $\mathcal{E}_2(G) = \{xy : xy \in \mathcal{E}(G) \text{ and } d(x) = d(y) = 2\}$. The expression $A := B$ signifies that B is identical to A.

2 Preliminaries

In this section, we present few lemmas that have a frequent application in the subsequent sections.

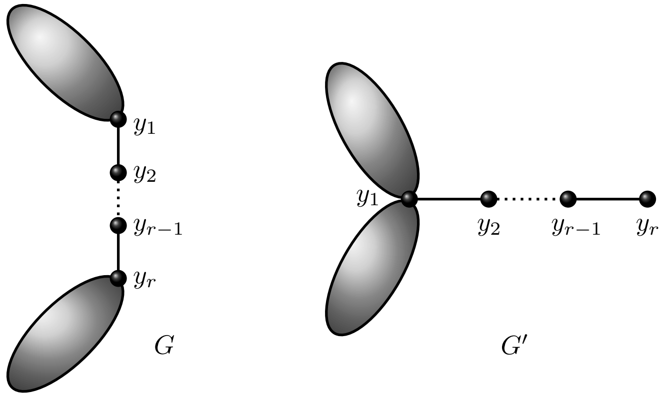

Figure 4. The graphs G and G' from Lemma 1

Lemma 1. *Consider a graph G and an induced sub-path $P = y_1y_2...y_r$ belonging to G, having the degrees of both y_1 and y_r are at least 2. A new graph G' is constructed as, $G' = G - \{y_rz : z \in N(y_r)\backslash y_{r-1}\} + \{y_1z : z \in N(y_r)\backslash y_{r-1}\}$ (refer to Figure 4 for a visual representation). Then we have $SO_\alpha(G) < SO_\alpha(G')$.*

Proof. Consider the function $\psi(p, q)$ defined as follows:

$$\psi(p, q) = (4 + p^2)^\alpha + (4 + q^2)^\alpha - (4 + (p + q - 1)^2)^\alpha - 5^\alpha,$$

where both p and q are greater than or equal to 2. It can be easily verified that:

$$\frac{\partial\psi(p, q)}{\partial p} = 2\alpha p(4 + p^2)^{\alpha-1} - 2\alpha(p + q - 1)(4 + (p + q - 1)^2)^{\alpha-1} < 0$$

implying that $\psi(p, q)$ strictly decreases as p increases while q is fixed and

$$\frac{\partial\psi(p, q)}{\partial q} = 2\alpha q(4 + q^2)^{\alpha-1} - 2\alpha(p + q - 1)(4 + (p + q - 1)^2)^{\alpha-1} < 0$$

This implies that $\psi(p, q)$ strictly decreases as q increases while p is fixed, implying $\psi(p, q)$ is strictly decreasing with fixed $q \geq 2$ and for $p \geq 2$, and strictly decreasing for fixed $p \geq 2$ and with $q \geq 2$. For convenience we assign the values $d_G(y_1) = p \geq 2$ and $d_G(y_r) = q \geq 2$ in the subsequent discussion.

Case 1 : $r > 2$

Consequently, we have

$$\begin{aligned}
&SO_\alpha(G) - SO_\alpha(G') \\
&= \sum_{z \in N_G(y_1) \setminus \{y_2\}} \left(p^2 + d_G^2(z)\right)^\alpha + \sum_{z \in N_G(y_r) \setminus \{y_{r-1}\}} \left(q^2 + d_G^2(z)\right)^\alpha \\
&\quad + (2^2 + p^2)^\alpha + (2^2 + q^2)^\alpha + -(1^2 + 2^2)^\alpha - (2^2 + (p+q-1)^2)^\alpha \\
&\quad - \sum_{z \in N_G(y_1) \cup N_G(y_r) \setminus \{y_2, y_{r-1}\}} \left((p+q-1)^2 + d_G^2(z)\right)^\alpha \\
&< (2^2 + p^2)^\alpha + (2^2 + q^2)^\alpha - (1^2 + 2^2)^\alpha - (2^2 + (p+q-1)^2)^\alpha = \psi(p,q) \\
&\leq \psi(2,2) = (2^2 + 2^2)^\alpha + (2^2 + 2^2)^\alpha - (1^2 + 2^2)^\alpha - (2^2 + (2+2-1)^2)^\alpha \\
&= 2 \cdot 8^\alpha - 5^\alpha - 13^\alpha < 0
\end{aligned}$$

implying $SO_\alpha(G) < SO_\alpha(G')$.

Case 2 : $r = 2$

To begin, it's important to observe that for values of $p \geq 2$ and $q \geq 2$, the expression $1 + (p+q-1)^2 - (p^2 + q^2) = 2(pq - p - q) + 1$ is greater than zero. By this fact, we can now state that:

$$\begin{aligned}
&SO_\alpha(G) - SO_\alpha(G') \\
&\quad = \sum_{z \in N_G(y_1) \setminus \{y_2\}} \left(p^2 + d_G^2(z)\right)^\alpha + \sum_{z \in N_G(y_2) \setminus \{y_1\}} \left(q^2 + d_G^2(z)\right)^\alpha \\
&\qquad - \sum_{z \in N_G(y_1) \cup N_G(y_2) \setminus \{y_1, y_2\}} \left((p+q-1)^2 + d_G^2(z)\right)^\alpha \\
&\qquad + (p^2 + q^2)^\alpha - (1^2 + (p+q-1)^2)^\alpha \\
&\quad < (p^2 + q^2)^\alpha - (1^2 + (p+q-1)^2)^\alpha < 0
\end{aligned}$$

Thus the proof is completed. ■

Corollary 1. *Consider a tree $\mathcal{T}$ with a total of n vertices, where n is greater than or equal to 3. We have,*

$$8^{\alpha}(n-3)+2\cdot 5^{\alpha} \leq SO_{\alpha}(\mathcal{T}) \leq (n-1)(n^2-2n+2)^{\alpha}$$

The left inequality is achieved iff $\mathcal{T}$ is identical to P_n, and the right side inequality is achieved iff $\mathcal{T}$ is identical to S_n.

Proof. If we have a tree $\mathcal{T}$ that is distinct from the star graph S_n, then it is possible to transform $\mathcal{T}$ into the star graph S_n through a series of finite steps using the transformation from Lemma 1. Consequently, according to Lemma 1, we can establish that $SO_{\alpha}(\mathcal{T})$ is bounded by $SO_{\alpha}(S_n)$, which equals $(n-1)(n^2-2n+2)^{\alpha}$.

Conversely, if $\mathcal{T}$ is not isomorphic to the path graph P_n, then by applying the transformation from Lemma 1 to P_n a suitable number of times, we can eventually obtain the desired tree $\mathcal{T}$. Again, by Lemma 1, we can deduce that $SO_{\alpha}(\mathcal{T})$ is greater than or equal to $SO_{\alpha}(P_n)$, which equals $8^{\alpha}(n-3)+2\cdot 5^{\alpha}$. ■

Lemma 2. *If r is greater than or equal to 1, and $\alpha \in (0,1)$, then the function $f(u)=(u^2+r^2)^{\alpha}-u^{\alpha}$ strictly decreases for $u \geq 1$.*

Proof. One can readily observe that, for values of r greater than or equal to 1 and $\alpha \in (0,1)$, the derivative $f'(u)$, is expressed as follows: $f'(u) = 2\alpha u\Big[(u+r)^{\alpha-1}-u^{\alpha-1}\Big]$, and it consistently remains negative. As a result, the lemma remains valid. ■

Lemma 3. *Consider a tree $\mathcal{T}$ from the collection $\mathcal{T}_{n,k}$ and y be a vertex with degree 2 in $\mathcal{T}$. If the two neighbor vertices of z are not pendent and $\alpha \in (0,1)$, then there exists a tree $\mathcal{T}^*$ of $\mathcal{T}_{n,k}$ so that $SO_{\alpha}(\mathcal{T}) \geq SO_{\alpha}(\mathcal{T}^*)$ with equality if and only if y is adjacent to at least one vertex with degree 2.*

Proof. Let $N(y)=\{x,z\}$ where $d(x)=s\geq 2$ and $d(z)=t\geq 2$. Assume that p is a pendent vertex and q is the only neighbor of p in the tree $\mathcal{T}$ with $d(q)=r\geq 2$. Define $\mathcal{T}_{xy}$ as a result of applying Transformation I to $\mathcal{T}$ and let $\mathcal{T}^*$ be the graph constructed from $\mathcal{T}_{xy}$ by introducing a new edge to the pendent vertex p. It follows that $\mathcal{T}^* \in \mathcal{T}_{n,k}$. Since $s, t, r \geq 2$, and $\alpha \in (0,1)$ we have,

$$\begin{aligned}
&SO_\alpha(\mathcal{T}) - SO_\alpha(\mathcal{T}^*) \\
&= (s^2+2^2)^\alpha + (t^2+2^2)^\alpha + (u^2+1)^\alpha - (s^2+t^2)^\alpha - (u^2+2^2)^\alpha - 10^\alpha \\
&= \Big[(s^2+2^2)^\alpha + (t^2+2^2)^\alpha - (s^2+t^2)^\alpha\Big] - \Big[(u^2+2^2)^\alpha - (u^2+1)^\alpha\Big] - 10^\alpha
\end{aligned}$$

Let $\phi(s,t) = (s^2+2^2)^\alpha + (t^2+2^2)^\alpha - (s^2+t^2)^\alpha$ having $s, t \geq 2$, and $\alpha \in (0,1)$ then

$$\frac{\partial f(s,t)}{\partial s} = 2\alpha s\Big[(s^2+2^2)^{\alpha-1} - (s^2+t^2)^{\alpha-1}\Big] \geq 0$$

and

$$\frac{\partial f(s,t)}{\partial t} = 2\alpha t\Big[(t^2+2^2)^{\alpha-1} - (s^2+t^2)^{\alpha-1}\Big] \geq 0$$

implying $f(s,t)$ increases for both s and t with $s, t \geq 2$. From Lemma 2, it follows that

$$SO_\alpha(\mathcal{T}) - SO_\alpha(\mathcal{T}^*) = \phi(s,t) - f(u^2+1) - 10^\alpha \geq \phi(2,2) - f(3) - 10^\alpha = 0$$

■

Lemma 4. *Consider a tree $\mathcal{T}$ from the collection $\mathcal{T}_{n,k}$, and let pq represent an edge within $\mathcal{T}$ such that the $d(p) = b \geq 3$, and $d(q) = 1$. For $\alpha \in (0,1)$ and the collection $\mathcal{E}_2(\mathcal{T})$ is non-empty, there exists another $\mathcal{T}^*$ in $\mathcal{T}_{n,k}$ so that $SO_\alpha(\mathcal{T}) > SO_\alpha(\mathcal{T}^*)$ holds.*

Proof. Consider that $\mathcal{E}_2(\mathcal{T})$ is not an empty set. Consequently, it is possible to create $\mathcal{T}^*$ containing $n-1$ vertices derived from $\mathcal{T}$ by merging any edge from $\mathcal{E}_2(\mathcal{T})$ and subsequently introducing a new vertex to the edge pq. Thus, $\mathcal{T}^*$ belongs to the set $\mathcal{T}_{n,k}$. According to Lemma 2, this leads to

$$\begin{aligned}
SO_\alpha(\mathcal{T}) - SO_\alpha(\mathcal{T}^*) &= 8^\alpha + (b^2+1)^\alpha - (b^2+2^2)^\alpha - 5^\alpha \\
&= \Big[8^\alpha - 5^\alpha\Big] - \Big[(b^2+2^2)^\alpha - (b^2+1)^\alpha\Big] > 0
\end{aligned}$$

Hence the lemma holds. ■

Lemma 5. *Consider a tree $\mathcal{T}$ belonging to the collection $\mathcal{T}_{n,k}$ and a vertex x within $\mathcal{T}$ that has a degree of 4. Furthermore, let y_1, y_2, y_3, and y_4 denote four vertices that are neighbors of x, so that $d(y_4) \leq 5$ and $d(y_1) \leq d(y_2) \leq d(y_3) \leq 3$. If $\alpha \in (0,1)$ and the collection $\mathcal{E}_2(\mathcal{T})$ is not empty, then there exists another $\mathcal{T}^*$ in the set $\mathcal{T}_{n,k}$ so that $SO_\alpha(\mathcal{T}) > SO_\alpha(\mathcal{T}^*)$.*

Proof. Note that $\mathcal{E}_2(\mathcal{T})$ is not an empty set. As a result, we have the ability to create $\mathcal{T}'$ with a total of $n-1$ vertices by merging any edge from the set $\mathcal{E}_2(\mathcal{T})$. Subsequently, we can generate an additional tree labeled as $\mathcal{T}^* := \mathcal{T}^*_{y \mapsto (3-reg)}$ from $\mathcal{T}'$ through Transformation III, while ensuring $\mathcal{T}^*$ remains within the set $\mathcal{T}_{n,k}$. Given that $d(y_1) \leq d(y_2) \leq d(y_3) \leq 3$ and $d(y_4) \leq 5$, and in accordance with Lemma 2, we have

$$\begin{aligned} SO_\alpha(\mathcal{T}) - SO_\alpha(\mathcal{T}^*) &= 8^\alpha + \sum_{i=1}^{4} \Big[(4^2 + d^2(y_i))^\alpha - (3^2 + d^2(y_i))^\alpha\Big] - 18^\alpha \\ &\geq 8^\alpha + 3\Big[25^\alpha - 18^\alpha\Big] + 41^\alpha - 34^\alpha - 18^\alpha \\ &= 8^\alpha - 4 \cdot 18^\alpha + 3 \cdot 25^\alpha + 41^\alpha - 34^\alpha \end{aligned}$$

Let $\phi(\alpha) = 8^\alpha - 4 \cdot 18^\alpha + 3 \cdot 25^\alpha + 41^\alpha - 34^\alpha$ with $\alpha \in (0,1)$. It is easy to check that $\phi(\alpha) > 0$ for $\alpha \in (0,1)$. (see Figure 5)

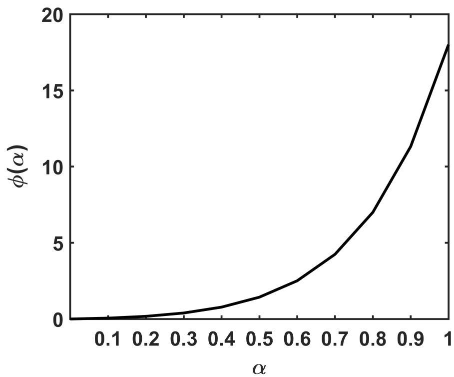

Figure 5. $\phi(\alpha)$ from Lemma 5

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Lemma 6. *If $\mathcal{T}$ represents a tree from the collection $\mathcal{T}_{n,k}$, and let x be one of the vertices in $\mathcal{T}$, with a degree of at least 4. If $|\mathcal{E}_2(\mathcal{T})| \geq b-3$ and the neighbors of x are denoted as $N(x) = \{y_1, y_2, ..., y_b\}$ such that $d(y_1) \leq d(y_2) \leq ... \leq d(y_b)$. For $\alpha \in (0,1)$ if we consider $\mathcal{T}$, satisfying either of the following two conditions:*
(i) When $d(y_{b-1}) \leq 3$ and $b \geq 5$.
(ii) When $3 \leq d(y_{b-1}) \leq 4$ and $b \geq 8$.
then we can find another $\mathcal{T}^*$ of $\mathcal{T}_{n,k}$ so that $SO_\alpha(\mathcal{T}) > SO_\alpha(\mathcal{T}^*)$.

Proof. Let $d(y_{b-1}) = a$. It's important to note that $|\mathcal{E}_2(\mathcal{T})| \geq b-3$. Consequently, new $\mathcal{T}'$ can be constructed by taking $\mathcal{T}$ and contracting $b-3$ arbitrary edges from $\mathcal{E}_2(\mathcal{T})$. When we consider Transformation III, another tree denoted as $\mathcal{T}^* := \mathcal{T}^*_{y\mapsto(3-reg)}$,can be constructed from $\mathcal{T}'$. Also note that, the tree $\mathcal{T}^*$ belongs to the collection $\mathcal{T}_{n,k}$. Since $b \geq 4$, $\alpha \in (0,1)$,and by Lemma 2, we have

$$
\begin{aligned}
& SO_\alpha(\mathcal{T}) - SO_\alpha(\mathcal{T}^*) \\
&= (b-3)8^\alpha + \sum_{i=1}^{b}\Big[(d^2(y_i)+b^2)^\alpha - (d^2(y_i)+3^2)^\alpha\Big] - (b-3)\cdot 18^\alpha \\
&\geq (b-3)\Big[8^\alpha - 18^\alpha\Big] + (b-1)\Big[(a^2+b^2)^\alpha - (a^2+3^2)^\alpha\Big] \\
&+ \Big[(d^2(y_b)+b^2)^\alpha - (d^2(y_b)+3^2)^\alpha\Big] \\
&> (b-3)\Big[8^\alpha - 18^\alpha\Big] + (b-1)\Big[(a^2+b^2)^\alpha - (a^2+3^2)^\alpha\Big] \qquad (1)
\end{aligned}
$$

Let $\phi(a,b) = (b-3)\Big[8^\alpha - 18^\alpha\Big] + (b-1)\Big[(a^2+bq^2)^\alpha - (a^2+3^2)^\alpha\Big]$ where $\alpha \in (0,1)$, $a \geq 1$ and $b \geq 4$.

By Lemma 2, $\phi(a,b)$ strictly decreases on a.

Since $\alpha \in (0,1)$, then $\dfrac{\partial^2\phi(a,b)}{\partial b^2} \geq \alpha(a^2+b^2)^{\alpha-2}(2a^2+2b^2-b+1) > 0$

Hence $\dfrac{\partial\phi(a,b)}{\partial b}$ strictly increases on b. Now, the subsequent cases are examined.

Case (i) : $\mathcal{T}$ satisfies (i). i.e., $b \geq 5$ and $a \leq 3$ and so $\phi(a,b) \geq \phi(3,b)$.

$$
\frac{\partial\phi(3,b)}{\partial b} \geq \frac{\partial\phi(3,b)}{\partial b}\bigg|_{b=5} = 34^{\alpha-1}\Big[4\alpha+34\Big] + 34^\alpha - 2\cdot 18^\alpha > 0
$$

where in Figure 6 (a), the last strict inequality is indicated. Thus, $\phi(3, b)$ strictly increases on $b \geq 5$. Combining this with (1), we have

$$SO_\alpha(\mathcal{T}) - SO_\alpha(\mathcal{T}^*) > \phi(a, b) \geq \phi(3, b) \geq \phi(3, 5) = 2 \cdot 8^\alpha - 6 \cdot 18^\alpha + 4 \cdot 34^\alpha > 0$$

where in Figure 6 (b), the last strict inequality is indicated.

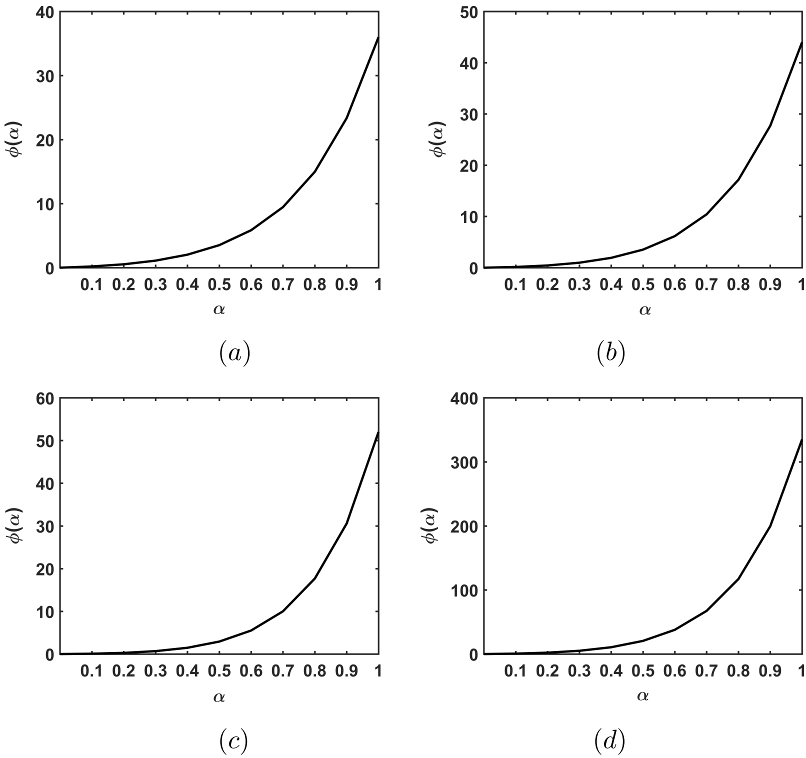


Figure 6. The four functions $\phi(\alpha)$ from Lemma 6

Case (ii) : $\mathcal{T}$ satisfies (ii). i.e., $a \leq 4$ and $b \geq 8$ and so $\phi(a, b) \geq \phi(4, b)$

$$\frac{\partial \phi(4, b)}{\partial b} \geq \left. \frac{\partial \phi(4, b)}{\partial b} \right|_{b=8} = 8^\alpha - 18^\alpha - 25^\alpha + 80^{\alpha-1}\Big[80 + 7\alpha\Big] > 0$$

where in Figure 6 (c), the last strict inequality is indicated. Thus, $\phi(4, b)$

strictly increases $b \geq 8$. We have,

$$SO_\alpha(\mathcal{T}) - SO_\alpha(\mathcal{T}') > \phi(a,b) \geq \phi(4,b) \geq \phi(4,8)$$
$$= 5(8^\alpha - 18^\alpha) + 7(80^\alpha - 25^\alpha) > 0$$

where in Figure 6 (d), the last strict inequality is indicated. ■

Lemma 7. *[34] Let $\mathcal{T}$ be a tree of $\mathcal{T}_{n,k}$. If $3 \leq k \leq \left\lfloor \frac{n+2}{3} \right\rfloor$ and $\mathcal{E}_2(\mathcal{T}) \subseteq E(\mathcal{P}(\mathcal{T}))$, then*

$$|\mathcal{E}_2(\mathcal{T})| \geq \eta_4 + 2\eta_5 + \cdots + (\Delta(\mathcal{T}) - 3)\eta_{\Delta(\mathcal{T})}.$$

3 Main results

Within this section, our focus is on identifying the maximum and minimum General Sombor indices for trees that have a specified number of vertices that are pendent.

3.1 The maximum general Sombor index of trees with given number of pendent vertices

Within this context, we denote a tree known as the broom graph as $\mathbb{Y}_{n,k}$. This broom graph is essentially created by taking the star graph S_k and substituting one of the edge that is pendent with a path P_{n-k}. We establish the broom graph $\mathbb{Y}_{n,k}$ as the unique tree within the collection $\mathcal{T}_{n,k}$ that achieves the maximum general Sombor index.

Theorem 1. *Suppose we have a tree denoted as $\mathcal{T}$ in the collection $\mathcal{T}_{n,k}$. For any value of $\alpha \in (0,1)$, then*

$$SO_\alpha(\mathcal{T}) \leq (k-1)(1+k^2)^\alpha + (4+k^2)^\alpha + (n-k-2) \cdot 8^\alpha + 5^\alpha$$

and the inequality holds if and only if $\mathcal{T}$ is isomorphic to the tree $\mathbb{Y}_{n,k}$.

Proof. When k equals either 2 or $n-1$, it means that $\mathcal{T}$ takes the form of either $P_n = \mathbb{Y}_{n,2}$ or $S_n = \mathbb{Y}_{n,n-1}$. Therefore, theorem is true for

these specific cases when k is 2 or $n-1$. Now, let's proceed with the assumption $3 \leq k \leq n-2$, and that the result has already been established for trees within $\mathcal{T}_{n',k'}$, where $n' \leq n-1$ and $k' \leq p-1$. Suppose we have a tree $\mathcal{T}$ belonging to $\mathcal{T}_{n,k}$ and a vertex y within $\mathcal{PV}(\mathcal{T})$. If x serves as the neighbor of y, and the set $N_{\mathcal{T}}(x) = \{y, x_1, x_2, ..., x_{t-1}\}$, then we know that $d_{\mathcal{T}}(x) = t$, which is less than or equal to k. Moreover, within the neighborhood set $N_{\mathcal{T}}(x)$, there is at least a vertex having a degree exceeding two. For the sake of simplicity, we can make the assumption, without compromising generality, that $d_{\mathcal{T}}(x_1)$ is greater than or equal to two, and for $i = 1, 2, ..., t-1$, $d_{\mathcal{T}}(x_i) \geq 1$.
Now, we obtain $\mathcal{T}'$, by eliminating y from $\mathcal{T}$, i.e., $\mathcal{T}' = \mathcal{T} - y$.

If $d_{\mathcal{T}}(x) = 2$, it implies that $d_{\mathcal{T}'}(x) = 1$, and as a result, $\mathcal{T}'$ belongs to the set $\mathcal{T}_{n-1,k}$. Using the induction hypothesis, we can now derive the following:
$SO_\alpha(\mathcal{T}') \leq SO_\alpha(\mathbb{Y}_{n-1,k}) = (k-1)(1+k^2)^\alpha + (4+k^2)^\alpha + (n-k-2)8^\alpha + 5^\alpha$.
Hence,

$$\begin{aligned} SO_\alpha(\mathcal{T}) &= SO_\alpha(\mathcal{T}') + 5^\alpha + (d^2_{\mathcal{T}}(x_1) + 2^2)^\alpha - (d^2_{\mathcal{T}}(x_1) + 1^2)^\alpha \\ &\leq (k-1)(1+k^2)^\alpha + (4+k^2)^\alpha + (n-k-2)8^\alpha + 5^\alpha + 8^\alpha - 5^\alpha \\ &= (k-1)(1+k^2)^\alpha + (4+k^2)^\alpha + (n-k-2)8^\alpha + 5^\alpha \end{aligned}$$

The equality is valid if and only if $\mathcal{T}' = \mathbb{Y}_{n,k-1}$, and $d_{\mathcal{T}}(x_1) = 2$ implying $\mathcal{T}$ is isomorphic to $\mathbb{Y}_{n,k}$. Now, when $d_{\mathcal{T}}(x) \geq 3$, it implies that $d_{\mathcal{T}'}(x) \geq 2$, consequently we have, $\mathcal{T}' \in \mathcal{T}_{n-1,k-1}$. Applying the induction hypothesis, we obtain:

$$\begin{aligned} &SO_\alpha(\mathcal{T}) \\ &= SO_\alpha(\mathcal{T}') + (t^2 + 1^2)^\alpha + \sum_{i=1}^{t-1}(t^2 + d^2_{\mathcal{T}}(x_i))^\alpha - \sum_{i=1}^{t-1}((t-1)^2 + d^2_{\mathcal{T}}(x_i))^\alpha \\ &\leq SO_\alpha(\mathbb{Y}_{n-1,k-1}) + (t^2 + 1^2)^\alpha \\ &\quad + \sum_{i=1}^{t-1}\Big[(t^2 + d^2_{\mathcal{T}}(x_i))^\alpha - ((t-1)^2 + d^2_{\mathcal{T}}(x_i))^\alpha\Big] \end{aligned}$$

$$\leq SO_\alpha(\mathbb{Y}_{n-1,k-1}) + (t^2+1^2)^\alpha + (t-2)\Big[(t^2+1)^\alpha - ((t-1)^2+1)^\alpha\Big]$$
$$- ((t-1)^2+4)^\alpha + (t^2+4)^\alpha$$
$$= SO_\alpha(\mathbb{Y}_{n-1,k-1}) + (t^2+1^2)^\alpha + (t-2)\phi(t,1) + \phi(t,2)$$
$$\leq SO_\alpha(\mathbb{Y}_{n-1,k-1}) + (k^2+1^2)^\alpha + (k-2)\phi(k,1) + \phi(k,2) \quad \text{(Since } t \leq k\text{)}$$
$$= (k-1)(1+k^2)^\alpha + (4+k^2)^\alpha + (n-k-2)\cdot 8^\alpha + 5^\alpha$$

The equalities mentioned above are valid if and only if certain conditions holds: firstly, $\mathcal{T}' \cong \mathbb{Y}_{n-1,k-1}$, secondly, the degrees of all the vertices in the collection $x_1, x_2, ..., x_{t-1}$ within $\mathcal{T}$ must be equal to 1, and finally, the value of $\mathcal{T}$ must equal k. Consequently, we can conclude that $\mathcal{T} \cong \mathbb{Y}_{n,k}$, thereby completing the proof. ■

Observe that Theorem 1, generalize the findings of Chen et al. [2] (see Theorem 3.5 in [2]), where the maximum Sombor index of trees in $\mathcal{T}_{n,k}$ (for $3 \leq k \leq \lfloor \frac{n+2}{3} \rfloor$) are determined.

3.2 The minimum general Sombor index of trees with given number of pendent vertices

We now represent the collection of trees on n vertices as $\mathcal{T}^*_{n,k}$ constructed from a $(k,3)$-regular tree by replacing each pendent edge with a path of length at least 2. It can be easily verified that $\mathcal{T}^*_{n,k}$ has exactly k pendent vertices, $n-2k+2$ vertices of degree 2 and $k-2$ vertices of degree 3.

For any tree, $\mathcal{T}$, belonging to the set $\mathcal{T}^*_{n,k}$, as per the definition of $\mathcal{T}^*_{n,k}$, it can be deduced that the following conditions hold :

- The cardinality of vertices in $\mathcal{T}$, denoted as $|V(\mathcal{T})|$, equals n.
- The maximum degree of any vertex in $\mathcal{T}$, represented as $\Delta(\mathcal{T})$, is 3.
- Each neighboring vertex of a vertex with a degree of 3 is either another vertex with a degree of 3 or a vertex with a degree of 2.

Consequently, leading to $\eta_1(\mathcal{T}) = k$, $\eta_2(\mathcal{T}) = n + 2 - 2k$, and $\eta_3(\mathcal{T}) = k - 2$. For instance, consider the class $\mathcal{T}^*_{13,4}$, which contains exactly four distinct trees, as illustrated in Figure 7. To simplify further, when combined with the sets $\mathcal{T}_{n,2} = \mathcal{CT}_{n,2} = P_n$, $\mathcal{T}_{n,n-1} = S_n$, and $\mathcal{CT}_{n,n-1} = \{S_n | 3 \leq n \leq 5\}$, we limit our focus to cases where $3 \leq k \leq n - 2$.

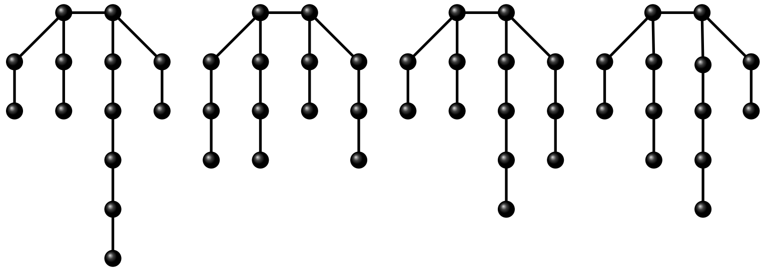


Figure 7. The elements of the collection $\mathcal{T}^*_{13,4}$

Theorem 2. *Consider a tree $\mathcal{T}$ belonging to the collection $\mathcal{T}_{n,k}$, where $3 \leq k \leq \left\lfloor \frac{n+2}{3} \right\rfloor$. When $\alpha \in (0,1)$, then,*

$$SO_\alpha(\mathcal{T}) \geq (5^\alpha + 13^\alpha)\ k + 8^\alpha\ (n + 2 - 3k) + 18^\alpha\ (k - 3).$$

and the equality holds if and only if $\mathcal{T}$ belongs to the collection $\mathcal{T}^*_{n,k}$.

Proof. We assume throughout the proof that there exists a tree denoted as $T^* \in \mathcal{T}_{n,k}$ which possesses the minimum general Sombor index within this collection . Given that k is greater than or equal to 3, it follows that $\Delta(T^*) \geq 3$. We will now proceed to establish certain assertions.

Assertion 1: Along a pendent path, each vertex in T^* with degree two is situated.

Proof for Assertion 1: To illustrate this assertion through a proof by contradiction, let's assume that there exists a vertex, denoted as x_0, in $\mathcal{T}^*$ with a degree of 2 but is not part of any pendent path. In such a case, all neighboring vertices of x_0 are non-pendent vertices. In accordance with Lemma 3, it follows that within the collection $\mathcal{T}_{n,k}$, there exists a tree $\mathcal{T}_1$ for which $SO_\alpha(\mathcal{T}^*) \geq SO_\alpha(\mathcal{T}_1)$, with equality only if x_0 is connected to at least one vertex of degree 2.

Through successive application of the transformations from Lemma 3, we can obtain a collection of trees denoted as $\{\mathcal{T}_i | i \geq 0\}$ within the collection $\mathcal{T}_{n,k}$, with $\mathcal{T}_0$ defined as $\mathcal{T}^*$. Simultaneously, we can form a sequence of vertices $\{x_i | i \geq 0\}$, so that every vertex x_i having a degree two is not situated on any pendent path of $\mathcal{T}_i$, and furthermore, the general Sombor index $SO_\alpha(\mathcal{T}_i)$ is greater than or equal to $SO_\alpha(\mathcal{T}_{i+1})$ for all $i \geq 0$.

As the count of 2-vertices not located on pendent paths in $\mathcal{T}_{i+1}$ consistently remains one less than that in $\mathcal{T}_i$, this series of transformations will ultimately conclude after a finite number of iterations. In simpler terms, there exists a non-negative integer b such that every 2-vertex within $\mathcal{T}_{b+1}$ is located on a pendent path. Consequently, we can identify x_b as the only 2-vertex in $\mathcal{T}_b$ that doesn't belong to any pendent path. As a result, x_b is connected to two vertices in $\mathcal{T}_b$, both of which have degrees of at least 3. This establishes a descending sequence of inequalities: $SO_\alpha(\mathcal{T}_0) \geq SO_\alpha(\mathcal{T}_1) \geq ... \geq SO_\alpha(\mathcal{T}_b) > SO_\alpha(\mathcal{T}_{b+1})$, which contradicts the initial choice of $\mathcal{T}^*$.

According to Assertion 1, it can be deduced that $\mathcal{E}_2(T^*)$ is a subset of $E(\mathcal{P}(\mathcal{T}^*))$. Now, we will proceed to illustrate that

$$\Delta(\mathcal{T}^*) = 3 \tag{2}$$

To the contrary, we suppose (2) is not true, i.e., $\Delta(T^*) \geq 4$. By Lemma 7, it follows that

$$|\mathcal{E}_2(T^*)| \geq \eta_4 + 2\eta_5 + ... + (\Delta(T^*) - 3)\eta_{\Delta(T^*)} \geq \Delta(T^*) - 3 \geq 1.$$

Assume that there exists $y_0 \in V(\mathcal{T}^*)$, where $d(y_0) = \Delta(\mathcal{T}^*)$ is at least 4. Let $P := y_0, y_1, \ldots, y_t$ be a path within $\mathcal{T}^*$,where $d(y_t)$ is greater than or equal to 4. We can make the assumption that the length of this path P is maximized. In the case where $t = 0$, we can deduce from Lemmas 5 and 6(i) that there is a tree within $\mathcal{T}_{n,k}$ with a smaller Sombor index compared to $\mathcal{T}^*$. However, this contradicts the $\mathcal{T}^*$, defined above. Hence, it must concluded that $t \geq 1$. According to assertion 1, it follows that when $t \geq 2$, the minimum value among the collection of $d(y_i)$ for $1 \leq i \leq t-1$ is at least 3.

When $t = 1$, define $N^*(y_{t-1}) = N(y_{t-1})$. For $t \geq 2$, define $N^*(y_{t-1})$ as the result of removing y_{t-2} from the collection $N(y_{t-1})$ ie., $N^*(y_{t-1}) := N(y_{t-1}) \backslash \{y_{t-2}\}$. It's evident that y_t belongs to the collection $N^*(y_{t-1})$.

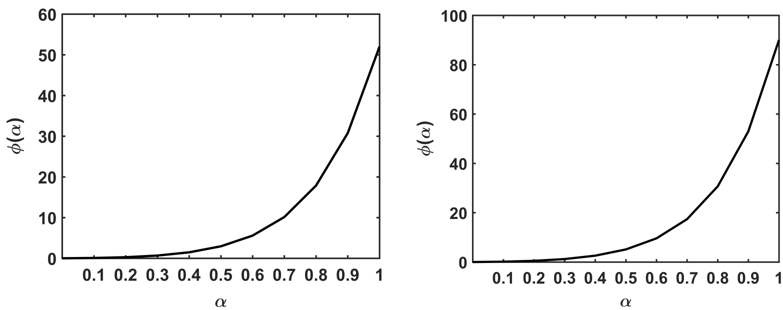
Assertion 2 : The maximum number of edges connected to any vertex in $\mathcal{T}^*$, which belongs to the set $N^*(y_{t-1})$, is 4, and the degree of the vertex y_t is equal to 4.

Proof for Assertion 2: Suppose there exists a vertex denoted as w in the neighborhood of y_{t-1}, and let the set $N(w)$ be defined as $\{w_1, w_2, ..., w_b\}$, where the degrees of these vertices are arranged as $d(w_1) \leq d(w_2) \leq ... \leq d(w_b)$. Thus we have, $|\mathcal{E}_2(\mathcal{T}^*)| \geq \Delta(\mathcal{T}^*) - 3 \geq b - 3$. Remember that we have already maximized the length of path P. Consequently, we have $d(w_{b-1}) \leq 3$. When $t = 1$ (in this case, $y_{t-1} = y_0$), we observe that $d(y_{t-1}) = \Delta(\mathcal{T}^*) \geq 4$, which is greater than $d(w_{b-1})$. Additionally, when $t \geq 2$, we have $d(y_{t-1}) \geq 3$, which is also greater than or equal to $d(w_{b-1})$. Hence, we can assume that $w_b = y_{t-1}$. Considering the selection of $\mathcal{T}^*$ and referring to Lemma 6(i), we can conclude that the degree of vertex w is at most 4. Notably, as y_t belongs to the neighborhood of y_{t-1} and has a degree of at least 4, it follows that $d(y_t) = 4$. This concludes the proof of assertion 2.

Now, let's focus on the vertex y_{t-1}. However, from assertion 2, every vertex in $N(y_{t-1})$ excluding y_{t-2} (for $t \geq 2$) having degrees of maximum 4 within $\mathcal{T}^*$. Considering Lemma 6(ii) by taking into account our choice of $\mathcal{T}^*$, it shall be concluded that $d(y_{t-1})$ is at most 7. Moreover, based on assertion 2, it can be inferred that every vertex in $N(y_t)$ excluding y_{t-1} within $\mathcal{T}^*$ has a degree not exceeding 3. Now, considering $d(y_t) = 4$ and our choice of $\mathcal{T}^*$, Lemma 5 indicates that $d(y_{t-1})$ must be at least six. As a result, we can determine that $6 \leq d(y_{t-1}) \leq 7$.

Suppose we have $d(y_{t-1}) = a$, and the neighborhood of y_{t-1} is denoted as $N(y_{t-1}) = \{z_1, z_2, ..., z_a\}$. Based on assertion 2, it can be inferred that $d(z_i) \leq 4$ for $1 \leq i \leq a - 1$. Given that $|\mathcal{E}_2(\mathcal{T}^*)| \geq 1$, we have the opportunity to create a new tree $\bar{\mathcal{T}}$ by contracting an edge from $\mathcal{E}_2(\mathcal{T}^*)$ within $\mathcal{T}^*$. Applying Transformation II, we can subsequently form another tree denoted as $\mathcal{T}' := \bar{\mathcal{T}}_{y_{t-1}\mapsto(3,a-3)}$ belonging to $\mathcal{T}_{n,k}$, originating from $\bar{\mathcal{T}}$. By Combining $6 \le a \le 7$ and Lemma 2, we have

$$\begin{aligned}
&SO_\alpha(\mathcal{T}^*) - SO_\alpha(\mathcal{T}') \\
&\quad = 8^\alpha + \sum_{i=1}^{3}\Big[(d^2(z_i)+a^2)^\alpha - (d^2(z_i)+4^2)^\alpha\Big] \\
&\qquad + \sum_{i=4}^{a}\Big[(d^2(z_i)+a^2)^\alpha - (d^2(z_i)+(a-2)^2)^\alpha\Big] - (a^2+2^2)^\alpha \\
&\quad \ge 8^\alpha + 3\Big[(a^2+4^2)^\alpha - 32^\alpha\Big] + (a-4)\Big[(a^2+4^2)^\alpha - (a^2+2^2)^\alpha\Big] \\
&\qquad + (d^2(z_a)+a^2)^\alpha - (d^2(z_a)+(a-2)^2)^\alpha - (a^2+2^2)^\alpha \\
&\quad > 8^\alpha + 3\Big[(a^2+4^2)^\alpha - 32^\alpha\Big] + (a-4)\Big[(a^2+4^2)^\alpha - (a^2+2^2)^\alpha\Big] \\
&\qquad - (a^2+2^2)^\alpha \\
&\quad = (a-1)(a^2+4^2)^\alpha + 8^\alpha - 3\cdot 32^\alpha - (a-3)(a^2+2^2)^\alpha
\end{aligned}$$



(a) $a = 6$ $\qquad$ (b) $a = 7$

Figure 8. $\phi(a)$ from Theorem 2

Let $\phi(a) = (a-1)(a^2+4^2)^\alpha + 8^\alpha - 3\cdot 32^\alpha - (a-3)(a^2+2^2)^\alpha$. When $a = 6$, we find that $\phi(6) > 0$. Similarly, when $a = 7$, we also have $\phi(7) > 0$, in Figure 8, the last strict inequality is indicated. Consequently, we can deduce that for any value of $6 \le a \le 7$, the expression $SO_\alpha(\mathcal{T}^*) - SO_\alpha(\mathcal{T}')$ is greater than 0. This contradicts the initial assumption. Therefore, we can affirm that (2) is valid.

By referring to (2), we can establish the equations $\eta_1 + \eta_2 + \eta_3 = n$ and $\eta_1 + 2\eta_2 + 3\eta_3 = 2(n-1)$. It's worth noting that η_1 is equivalent to k, where $3 \le k \le \lfloor \frac{n+2}{3} \rfloor$. Consequently, η_2 can be expressed as $n - 2k + 2$, which is also greater than or equal to k. Considering both assertion (1) and assertion (2), to conclude the proof, it is necessary to demonstrate that every vertex with degree one is connected to 2-vertex. To the contrary, suppose a vertex with degree one denoted as x in $\mathcal{T}^*$ that is adjacent to a vertex with degree 3 exists. As $\eta_2 \ge k$ and in accordance with the assertion (1), we can conclude that $\mathcal{E}_2(\mathcal{T}^*) \neq \phi$. However, based on our selection of $\mathcal{T}^*$ and in consideration of Lemma 4, this assumption leads to a contradiction. Hence, it follows that every vertex with degree one in $\mathcal{T}^*$ should be connected to a 2-vertex. Through straightforward calculations, it is evident that :

$$SO_\alpha(\mathcal{T}^*) = (5^\alpha + 13^\alpha)\ k + 8^\alpha\ (n + 2 - 3k) + 18^\alpha\ (k - 3)$$

Hence the theorem. ■

Given that all trees in $\mathcal{T}^*_{n,k}$ exhibit a maximum degree of 3, it follows that $\mathcal{T}^*_{n,k} \subseteq \mathcal{CT}_{n,k} \subseteq \mathcal{T}_{n,k}$. Consequently, the subsequent result can be established (the detailed proof is omitted due to the similarity of ideas):

Theorem 3. *For any tree $\mathcal{T} \in \mathcal{CT}_{n,k}$ where $3 \le k \le \lfloor \frac{n+2}{3} \rfloor$ and $0 < \alpha < 1$, then*

$$SO_\alpha(\mathcal{T}) \ge (5^\alpha + 13^\alpha)\ k + 8^\alpha\ (n + 2 - 3k) + 18^\alpha\ (k - 3)$$

Equality holds if and only if $\mathcal{T} \in \mathcal{T}^*_{n,k}$.

Observe that Theorem 2 and Theorem 3 generalize the findings of Maitreyi et al. [25] (see Theorem 3.1 in [25]) and Liu et al. [19] (see Theorem 3.5 in [19]), where the minimum Sombor indices of trees in $\mathcal{T}_{n,k}$ and chemical trees in $\mathcal{CT}_{n,k}$ (for $3 \le k \le \lfloor \frac{n+2}{3} \rfloor$) are determined, respectively.

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