

Extremal trees for the general Sombor index

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Abstract: Recently, the Sombor index of a graph has been extended to general Sombor index. The general Sombor index of a simple graph G is defined as $SO_\alpha(G) =$

$\sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2]^{\alpha/2}$, where $d_G(u)$ denotes the degree of a vertex u in G and

α is a real number. In this paper, we obtain bounds for the general Sombor index of trees. We further determine the trees with the extremal general Sombor indices.

Keywords: Sombor index, general Sombor index, trees, degree

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1. Introduction

One generally associates various graph-theoretical invariants to molecular graphs in chemical graph theory. This way, one studies the correlation of the invariants with various properties of the corresponding molecules. In 1947, Wiener [20] introduced such index for the first time and used it to correlate boiling points of alkanes. Historically, the first vertex-degree-based indices are the Zagreb indices. In general,

the vertex-degree-based topological indices of a simple graph G are of the form

$\sum_{uv \in E(G)} f(d_G(u), d_G(v))$, where $d_G(u)$ denotes degree of the vertex u , $E(G)$ is the

edge set and f is an appropriately chosen function such that $f(x, y) = f(y, x)$. A

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number of invariants and their generalisations have been introduced in the literature with varying success in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies. In 1975, Randić introduced an index, now known as *Randić connectivity index*, which turned out to be the most widely used index in the QSPR and the QSAR studies [16]. Erdős and Bollobás extended the Randić connectivity index in 1998 [1], known as the *general Randić connectivity index*, and is defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} [d_G(u)d_G(v)]^\alpha$$

for any real number α . This extends the classical Randić index $R_{1/2}(G)$ and the second Zagreb index $R_1(G)$, another important index that is studied extensively [13]. Extremal results on trees for the general Randić connectivity index are studied extensively in the literature, namely in [3], [9], [8], [10], [12], [21] and [22]. Motivated by Randić connectivity and Zagreb indices, Zhou and Trinajstić defined *sum-connectivity index* $\chi(G)$ [24] and its generalisation known as *general sum-connectivity index* $\chi_\alpha(G)$ [25], which are defined as

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}}$$

and

$$\chi_\alpha(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^\alpha$$

for any real number α . Notice that $\chi_{-1/2}(G) = \chi(G)$ and $\chi_1(G) = M_1(G)$, the classical first Zagreb index. Thus the general sum-connectivity index extends the ordinary sum-connectivity index and the first Zagreb index. Extremal results on trees for the general sum-connectivity index are explored in [4], [6], [18] and [23].

In this paper, we explore extremal trees for the extension of the recently introduced index, the *Sombor index*, by Gutman [7]. The Sombor index is known to have a reasonable predictive potential in the QSPR and the QSAR studies [17] and its relation with the existing well known indices are studied in [2], [5], [14] and [19]. For extremal results and various bounds of the Sombor index, we refer the readers to a recent survey paper [11] and the references therein.

Recently in [15], the Sombor index is extended, known as the *general Sombor index*, and is defined as

$$SO_\alpha(G) = \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2]^{\alpha/2}$$

for any real number α . Notice that $SO_1(G) = SO(G)$, the usual Sombor index, and $SO_2(G) = F(G)$, the forgotten index. Thus the general Sombor index generalises both the ordinary Sombor index and the forgotten index. In [15], bounds in terms

of important graph parameters for general Sombor index have been reported and explored the Nordhaus-Gaddum-type results. It further explored its relations with general sum-connectivity and general Randić indices. In this paper, we derive bounds for the general Sombor index of trees. We further determine the trees with the extremal general Sombor indices.

2. Preliminaries

All graphs considered in this paper are finite and simple. For a graph G , we denote the vertex set of G by $V(G)$. A tree T is a graph which is connected and acyclic. We denote the n -vertex path and n -vertex star by P_n and S_n respectively. We now present the following lemmas that are crucial in proving our main results in the next section.

Lemma 1. *Let H be a connected graph of order at least 2. Let $a_1 \geq a_2 \geq 1$ and let $v \in V(H)$. Let H_1 be the graph obtained from H by attaching two paths P and P' of lengths a_1 and a_2 respectively to v ; and H_2 be the graph obtained from H by attaching a path P'' of length $a_1 + a_2$ to v . Then $SO_\alpha(H_1) > SO_\alpha(H_2)$ for $\alpha > 0$.*

Proof. Let $d_1 = d_{H_1}(v)$ and $d_u = d_{H_1}(u)$ for vertex of H_1 or H_2 that is also a vertex of H . Then $d_1 \geq 3$. Now, we consider the following three cases.

(i) Let $a_1 = a_2 = 1$. Then

$$\begin{aligned} SO_\alpha(H_1) - SO_\alpha(H_2) &= 2(d_1^2 + 1)^{\alpha/2} + \sum_{uv \in E(H)} (d_1^2 + d_u^2)^{\alpha/2} - 5^{\alpha/2} \\ &\quad - [(d_1 - 1)^2 + 2^2]^{\alpha/2} - \sum_{uv \in E(H)} [(d_1 - 1)^2 + d_u^2]^{\alpha/2} \\ &= \left[(d_1^2 + 1)^{\alpha/2} - [d_1^2 + 5 - 2d_1]^{\alpha/2} \right] + \left[(d_1^2 + 1)^{\alpha/2} - 5^{\alpha/2} \right] \\ &\quad + \sum_{uv \in E(H)} \left[(d_1^2 + d_u^2)^{\alpha/2} - [(d_1 - 1)^2 + d_u^2]^{\alpha/2} \right] \\ &> 0 \end{aligned}$$

(ii) Let $a_1 \geq 2$ and $a_2 = 1$. Then

$$\begin{aligned} SO_\alpha(H_1) - SO_\alpha(H_2) &= (d_1^2 + 1)^{\alpha/2} - 8^{\alpha/2} + (d_1^2 + 4)^{\alpha/2} - [(d_1 - 1)^2 + 4]^{\alpha/2} \\ &\quad + \sum_{uv \in E(H)} \left[(d_1^2 + d_u^2)^{\alpha/2} - [(d_1 - 1)^2 + d_u^2]^{\alpha/2} \right] > 0 \end{aligned}$$

(iii) Let $a_1 \geq 2$ and $a_2 \geq 2$. Then

$$SO_\alpha(H_1) - SO_\alpha(H_2) = 2(d_1^2 + 1)^{\alpha/2} + 5^{\alpha/2} - [(d_1 - 1)^2 + 4]^{\alpha/2} - 2 \times 8^{\alpha/2} \\ + \sum_{uv \in E(H)} \left[(d_1^2 + d_u^2)^{\alpha/2} - [(d_1 - 1)^2 + d_u^2]^{\alpha/2} \right] > 0$$

Hence $SO_\alpha(H_1) > SO_\alpha(H_2)$ for $\alpha > 0$. □

We recall few basic definitions that are needed for the next section. A graph G is said to be r -regular if $d_G(u) = r$ for all vertices $u \in V(G)$ and it is said to be *bi-degreed* if it has two distinct vertex degrees. A connected graph G is said to be *bi-regular* or *semi-regular bipartite* if G is a bipartite graph with two partite sets A and B assuming minimal degree for each vertex in A and maximal degree for each vertex in B . Now, we state necessary and sufficient conditions for non-regular graphs to be bi-regular which is proven in [15].

Lemma 2. [15] *Let G be a connected non-regular graph. Then the following statements are equivalent.*

(i) G is bi-regular.

(ii) G is bi-degreed and the absolute values of $d_G(u) - d_G(v)$ is a non-zero constant for all edges uv of G .

(iii) $d_G(u)^2 + d_G(v)^2 > 0$ is constant for all edges uv of G .

We present the following inequality which we require in the next section.

Lemma 3. $10^a + 8^a - 13^a - 5^a \geq 0$ for $0 < a \leq 1$.

Proof. Notice that $10^a + 8^a - 13^a - 5^a = 0$ if $a = 1$. Let $0 < a < 1$. Consider the function

$$f(x, y) = 2^a x^a + (x + y)^a - (x + y + 5)^a - x^a, \quad \forall x \geq 1, y \geq 0.$$

Then

$$\frac{\partial f}{\partial x} = a[x^{a-1}(2^a - 1) + (x + y)^{a-1} - (x + y + 5)^{a-1}] > 0$$

and

$$\frac{\partial f}{\partial y} = a[(x + y)^{a-1} - (x + y + 5)^{a-1}] > 0.$$

Thus

$$10^a + 8^a - 13^a - 5^a = f(5, 3) > f(5, 0) = 0.$$

□

3. Main Results

In this section, we determine the extremal trees for the general Sombor index SO_α when $\alpha > 0$. We further present the trees with the second minimum general Sombor index SO_α when $\alpha > 0$. First, we prove that the maximum and minimum general Sombor index SO_α when $\alpha > 0$ is attained by the star and path respectively.

3.1. Extremal trees for SO_α when $\alpha > 0$.

Theorem 1. *Let T be a tree of order $n \geq 4$. If $\alpha > 0$, then*

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

where the left equality holds if and only if $T = P_n$; and the right equality holds if and only if $T = S_n$.

Proof. Notice that $SO_\alpha(P_n) = 2 \times 5^{\alpha/2} + (n-3)8^{\alpha/2}$. Now if $T \neq P_n$, then by Lemma 1 we can conclude that $SO_\alpha(T) > SO_\alpha(P_n)$ for $\alpha > 0$.

To prove the upper bound, we note that $d_T(u) + d_T(v) \leq n$ for all edges uv of T . Moreover, $d_T(u)^2 + d_T(v)^2 \leq 1 + (n-1)^2$ for all edges uv of T . Thus

$$SO_\alpha(T) \leq \sum_{uv \in E(T)} [1 + (n-1)^2]^{\alpha/2} = (n-1)(n^2 - 2n + 2)^{\alpha/2}$$

where the equality holds if and only if $d_T(u)^2 + d_T(v)^2 = 1 + (n-1)^2$ i.e., by Lemma 2, T is bi-regular. Notice that a tree that is also bi-regular is a star. Hence, the maximal general Sombor index $SO_\alpha(T)$ is attained by the star S_n when $\alpha > 0$. This completes the proof. \square

3.2. Trees with second minimal SO_α when $0 < \alpha \leq 2$.

Finally, we determine the trees with the second minimum general Sombor index SO_α when $0 < \alpha \leq 2$.

Remark 1. For $n = 5$, there are only three nonisomorphic trees: P_5 , S_5 and the tree T as shown in Fig. 1 (and thus T has the second minimum general Sombor index).

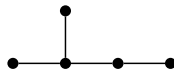


Figure 1. 5-vertex tree T with the second minimum general Sombor index.

Remark 2. For $n = 6$, apart from P_6 and S_6 , we have four nonisomorphic trees as shown in Fig. 2.

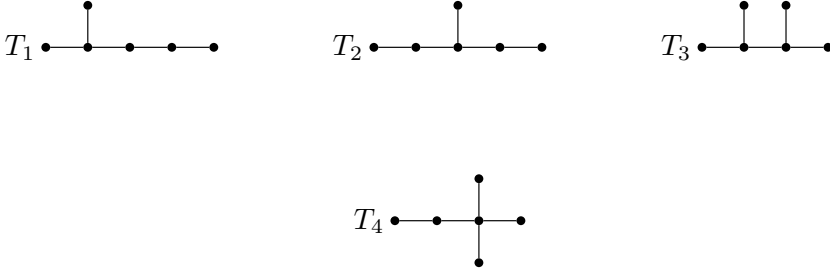


Figure 2. 6-vertex tree with the second minimum general Sombor index.

It can be easily seen with direct computation that the second minimum general Sombor index is attained by the tree T_2 shown in Fig. 2.

Let $n \geq 7$ and $s \geq 2$. Let T_{rs} denotes the n -vertex tree with a maximal degree vertex 3 such that $r + s = n$ and if $P_r = v_1 v_2 \dots v_{r-1} v_r$ is a longest path in T_{rs} with $d_{T_{rs}}(v_j) = 3$ for $3 \leq j \leq r - 2$, then deleting v_j we get three paths $v_1 v_2 \dots v_{j-1}$, $v_{j+1} \dots v_{r-1} v_r$ and $P_s = u_1 \dots u_{s-1} u_s$. The tree T_{rs} is shown in Fig. 3 below.

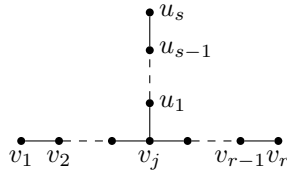


Figure 3. T_{rs}

Notice that

$$SO_\alpha(T_{rs}) = 3 \times 5^{\alpha/2} + (n - 7)8^{\alpha/2} + 3 \times 13^{\alpha/2}.$$

We now prove that the second minimum general Sombor index SO_α is attained by the tree T_{rs} when $0 < \alpha \leq 2$. We first give an outline of the proof.

Outline of the proof: We noticed above that the path P_n has the least general Sombor index. So, we consider any n -vertex tree T , which is not P_n and T_{rs} , and we proof the theorem by way of contradiction. Such consideration of trees are done based on the degree of the vertex along the longest path in the tree. More precisely, if $P_r = v_1 v_2 \dots v_{r-1} v_r$ is a longest path in T , then we proceed our argument on the basis of the degree of v_2 or v_{r-1} .

We assume that the tree T has the second minimum general Sombor index. Considering (upto isomorphism) different possibilities of T , we could produce another tree (which could also be T_{rs}) with lesser general Sombor index contradicting our assumption that T has second minimum general Sombor index. Such trees are constructed by attaching only the pendant vertices at some vertices. These are sufficient to conclude our argument as one can notice that the trees with a combination of pendant and non-pendant vertices could also be similarly argued. We make this point clear at one place in *Case 1* of the proof below.

Theorem 2. *Let T be a tree of order $n \geq 7$ and $0 < \alpha \leq 2$. If $T \neq P_n$, then*

$$SO_\alpha(T) \geq 3 \times 5^{\alpha/2} + (n - 7)8^{\alpha/2} + 3 \times 13^{\alpha/2}$$

where equality holds if and only if $T = T_{rs}$.

Proof. Let $T \neq P_n$ and $T \neq T_{rs}$ be an n -vertex tree with the second minimum SO_α when $0 < \alpha \leq 2$. Let $P_r = v_1v_2 \dots v_{r-1}v_r$ be a path in T of largest length and let $d(v) = d_T(v)$ for $v \in V(T)$. We consider the following three cases depending on the degree of v_2 or v_{r-1} .

Case 1. Let $d(v_2) = 2 = d(v_{r-1})$.

Since $T \neq P_n$ and $T \neq T_{rs}$ there exists a vertex v_j for some $3 \leq j \leq r - 2$ such that $d(v_j) \geq 4$ as shown in the left of Fig. 4. Notice that u_1, \dots, u_s are all pendant vertices. We delete edges $u_2v_j, \dots, u_s v_j$ ($s \geq 2$) from T and add them as shown on the right of Fig. 4 to get a new tree T' . Notice that even if some of the u_i 's are non-pendant, the construction of T' is similar (i.e., attaching the path $u_1u_2 \dots u_s$ to v_j) and thus the effect on $SO_\alpha(T) - SO_\alpha(T')$ remains unchanged.

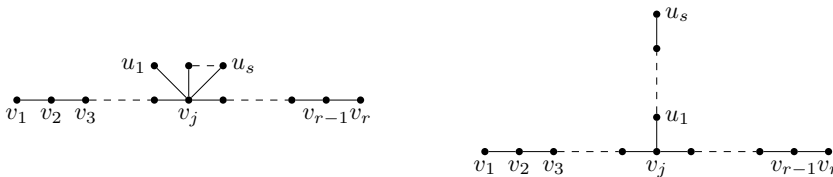


Figure 4. The trees T (left) and T' (right), respectively.

Then

$$\begin{aligned} SO_\alpha(T) - SO_\alpha(T') &= [d(v_{j-1})^2 + (s + 2)^2]^{\alpha/2} + [d(v_{j+1})^2 + (s + 2)^2]^{\alpha/2} \\ &\quad + s[1 + (s + 2)^2]^{\alpha/2} - [d(v_{j-1})^2 + 9]^{\alpha/2} - [d(v_{j+1})^2 + 9]^{\alpha/2} \\ &\quad - 13^{\alpha/2} - (s - 2)8^{\alpha/2} - 5^{\alpha/2} \\ &= [d(v_{j-1})^2 + (s + 2)^2]^{\alpha/2} - [d(v_{j-1})^2 + 9]^{\alpha/2} \\ &\quad + [d(v_{j+1})^2 + (s + 2)^2]^{\alpha/2} - [d(v_{j+1})^2 + 9]^{\alpha/2} \end{aligned}$$

$$\begin{aligned}
& + (s-2) \left[[1 + (s+2)^2]^{\alpha/2} - 8^{\alpha/2} \right] \\
& + 2[1 + (s+2)^2]^{\alpha/2} - 13^{\alpha/2} - 5^{\alpha/2}
\end{aligned}$$

Since $s \geq 2$ notice that $SO_\alpha(T) - SO_\alpha(T') > 0$, which is a contradiction to our assumption that T has the second minimum SO_α .

Case 2. Let $d(v_2) = 3$ or $d(v_{r-1}) = 3$.

Without loss of generality, let $d(v_2) = 3$. Following the argument as in *Case 1*, it is enough to consider the following two subcases (involving pendant vertices).

Subcase 2.1. Since $T \neq P_n$ and $T \neq T_{rs}$ we consider the subcase when $d(v_j) = 2$ for all $3 \leq j \leq r-2$. Let T be the tree as shown on the left of Fig. 5. We delete the edge v_2u from T and add it to the vertex v_3 to get a new tree T' as shown on the right of Fig. 5.



Figure 5. The trees T (left) and T' (right), respectively.

Then

$$SO_\alpha(T) - SO_\alpha(T') = 10^{\alpha/2} + 8^{\alpha/2} - 5^{\alpha/2} - 13^{\alpha/2}.$$

Thus by Lemma 3 we have $SO_\alpha(T) \geq SO_\alpha(T')$ for $0 < \alpha \leq 2$, which is a contradiction to our assumption that T has the second minimum SO_α .

Subcase 2.2. Since $T \neq P_n$ and $T \neq T_{rs}$ there exists a vertex v_j for some $3 \leq j \leq r-2$ such that $d(v_j) \geq 3$. The tree T is shown on the left of Fig. 6. We delete the edges $uv_2, u_2v_j, \dots, u_s v_j$ and add them as shown on the right of Fig. 6 to get a new tree T' .

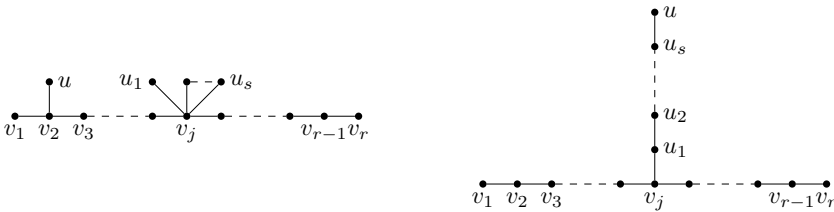


Figure 6. The trees T (left) and T' (right), respectively.

Then

$$\begin{aligned}
SO_\alpha(T) - SO_\alpha(T') & = 2 \times 10^{\alpha/2} + [9 + d(v_3)^2]^{\alpha/2} + [d(v_{j-1})^2 + (s+2)^2]^{\alpha/2} \\
& + [d(v_{j+1})^2 + (s+2)^2]^{\alpha/2} + s[1 + (s+2)^2]^{\alpha/2} - 2 \times 5^{\alpha/2}
\end{aligned}$$

$$\begin{aligned}
& - [4 + d(v_3)^2]^{\alpha/2} - [d(v_{j-1})^2 + 9]^{\alpha/2} - [d(v_{j+1})^2 + 9]^{\alpha/2} \\
& - 13^{\alpha/2} - (s-1)8^{\alpha/2} \\
& = [d(v_{j-1})^2 + (s+2)^2]^{\alpha/2} - [d(v_{j-1})^2 + 9]^{\alpha/2} \\
& + [d(v_{j+1})^2 + (s+2)^2]^{\alpha/2} - [d(v_{j+1})^2 + 9]^{\alpha/2} \\
& + [9 + d(v_3)^2]^{\alpha/2} - [4 + d(v_3)^2]^{\alpha/2} + 2(10^{\alpha/2} - 5^{\alpha/2}) \\
& + (s-1) \left[[1 + (s+2)^2]^{\alpha/2} - 8^{\alpha/2} \right] + [1 + (s+2)^2]^{\alpha/2} - 13^{\alpha/2} \\
& > 0,
\end{aligned}$$

which is a contradiction to our assumption that T has the second minimum SO_α .

Case 3. Let $d(v_2) \geq 4$ or $d(v_{r-1}) \geq 4$.

If $d(v_3) = 1$, then T is a star graph in which case it has the maximum general Sombor index. Thus $SO_\alpha(T) \geq SO_\alpha(T_{rs})$, which is a contradiction to the choice of T . Let $d(v_3) \geq 2$. Then there exists a vertex v_j for some $4 \leq j \leq r-2$ such that $d(v_j) \geq 2$. In this case, it is enough to consider the following two subcases.

Subcase 3.1. Let $d(v_j) = 2$ for all $3 \leq j \leq r-2$. The tree T is shown on the left of Fig. 7 and we delete the edges v_2u_1, \dots, v_2u_s and add them at v_j as shown on the right of Fig. 7 to get a new tree T' .

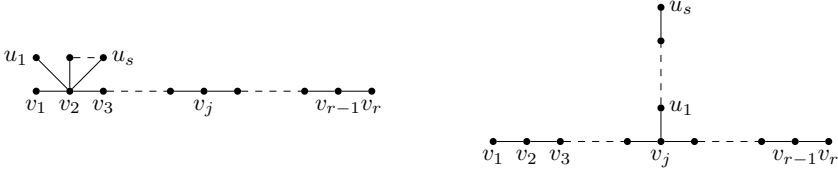


Figure 7. The trees T (left) and T' (right), respectively.

Then

$$\begin{aligned}
SO_\alpha(T) - SO_\alpha(T') &= (s+1)[1 + (s+2)^2]^{\alpha/2} + [4 + (s+2)^2]^{\alpha/2} + 2 \times 8^{\alpha/2} \\
& - 2 \times 5^{\alpha/2} - 3 \times 13^{\alpha/2} - (s-1)8^{\alpha/2} \\
& > (s-3)[(1 + (s+2)^2)^{\alpha/2} - 8^{\alpha/2}] + 2 \times [(1 + (s+2)^2)^{\alpha/2} - 5^{\alpha/2}] \\
& + 3 \times [(1 + (s+2)^2)^{\alpha/2} - 13^{\alpha/2}] \\
& > 0,
\end{aligned}$$

which is a contradiction to our assumption that T has the second minimum SO_α .

Subcase 3.2. Let $d(v_j) \geq 3$. Then the tree T is as shown on the left of Fig. 8 and we delete the edges v_2u_1, \dots, v_2u_s and add them at v_j as shown on the right of Fig. 8 to get a new tree T' . A simple computation get us that $SO_\alpha(T) \geq SO_\alpha(T')$, which is a contradiction to the choice of T .

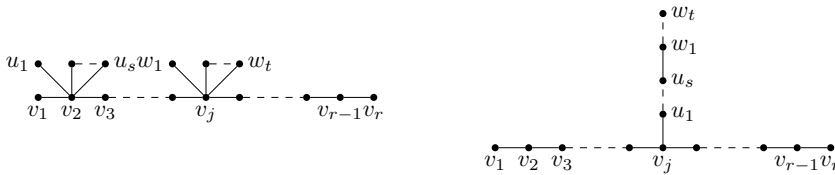


Figure 8. The trees T (left) and T' (right), respectively.

Thus, considering all the cases above, we can conclude that the second minimum general Sombor index tree is attained by the tree T_{r_s} and this completes the proof. \square

4. Conclusion

In this paper, we obtain bounds for the general Sombor index of trees. We further determine the trees with the extremal general Sombor index SO_α when $\alpha > 0$. More precisely, for $\alpha > 0$ we prove that the path and the star graph have the minimum and the maximum general Sombor index respectively. Further, we determine the tree with the second minimum general Sombor index SO_α when $0 < \alpha \leq 2$.

Following the same argument as in Theorem 1, we note that the lower bound for the general Sombor index is attained by the star when $\alpha < 0$. Notice that

$$(n-1)(n^2-2n+2)^{\alpha/2} \leq SO_\alpha(T)$$

for a tree T of order $n \geq 4$ and $\alpha < 0$, where the left equality holds if and only if $T = S_n$. Determining the extremal trees for the general Sombor index for $\alpha < 0$ is an attractive future work.

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Data Availability: Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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