# Extremal trees for Maximum Sombor index with given degree sequence

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**Abstract**

Let $G = (V, E)$ be a simple graph with vertex set $V$ and edge set $E$. The Sombor index of the graph $G$ is a degree-based topological index, defined as

$$SO(G) = \sum_{uv \in E} \sqrt{d(u)^2 + d(v)^2},$$

in which $d(x)$ is the degree of the vertex $x \in V$ for $x = u, v$.
In this paper, we characterize the extremal trees with a given degree sequence that maximizes the Sombor index.

**Keywords:** Sombor index, tree, degree sequence.
**AMS Subj. Class.:** 05C35, 05C90.

## 1 Introduction

In [1], Gutman defined a new vertex degree-based topological index, named the Sombor index, and defined for a graph $G$ as follows

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2},$$

where $d(u)$ and $d(v)$ denote the degree of vertices $u$ and $v$ in $G$, respectively.

Other versions of the Sombor index are induced and studied in [1–5]. Guman [1] showed that the Sombor index is minimized by the path and maximized by the star among general trees of the same size. In [6] the extremal values of the Sombor index of trees and unicyclic graphs with a given maximum degree are obtained. Deng et al. [7] obtained a sharp upper bound for the Sombor index and the reduced Sombor

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index among all molecular trees with fixed numbers of vertices, and characterized those molecular trees achieving the extremal value. In [8] characterized the extremal graphs with respect to the Sombor index among all the trees of the same order with a given diameter. Réti et al. [9] characterized graphs with the maximum Sombor index in the classes of all connected unicyclic, bicyclic, tricyclic, tetracyclic, and pentacyclic graphs of a given order. In this paper, we focus on the following natural extremal problem of Sombor index.

**Problem 1.** Find extremal trees of Sombor indices with a given degree sequence and characterize all extremal trees which attain the extremal values.

Let $T = (V, E)$ be a simple and undirected tree with vertex set $V(G) = \{v_1, \dots, v_n\}$ and the edge set $E(G) = \{e_1, \dots, e_m\}$. The set $N_T(u) = \{v \in V | uv \in E\}$ is called the neighborhood of vertex $u \in V$ in tree $T$. The number of edges incident to vertex $u$ in $G$ is denoted $d(u) = d_u$. A leaf is a vertex with degree 1 in tree $T$. The minimum degree and the maximum degree of $T$ are denoted by $\delta$ and $\Delta$, respectively. The distance between vertices $u$ and $v$ is the minimum number of edges between $u$ and $v$ and is denoted by $d(u, v)$. The degree sequence of the tree is the sequence of the degrees of non-leaf vertices arranged in non-increasing order. Therefore, we consider $(d_1, d_2, \dots, d_k)$ as a degree sequence of the tree $T$ where $d_1 \geq d_2 \geq \cdots \geq d_k \geq 2$. A tree is called a maximum optimal tree if it maximizes the Sombor index among all trees with a given degree sequence.

In this paper, we investigate the extremal trees which attain the maximum Sombor index among all trees with given degree sequences.

## 2 Preliminaries

In this section, We prove Some lemmas that are used in the next main results.

**Lemma 2.1** *For function $g(x, y) = \sqrt{x^2 + y^2}$, if $x \leq y$ then $g(x, 1) \leq g(y, 1)$.*

**Proof.** If $x \leq y$, then $x^2 + 1 \leq y^2 + 1$ and consequently, $\sqrt{x^2 + 1} \leq \sqrt{y^2 + 1}$. Therefore, $g(x, 1) \leq g(y, 1)$. □

**Lemma 2.2** *Let $f(x) = \sqrt{x^2 + a^2} - \sqrt{y^2 + b^2}$ with $a, b, x \geq 1$. Then $f(x)$ is an increasing function for every $a \leq b$ and a decreasing function for every $a > b$.*

**Proof.** We have that

$$f'(x) = \frac{x}{\sqrt{x^2 + a^2}} - \frac{x}{\sqrt{x^2 + b^2}}.$$

We consider function $\hat{f}(y) = \frac{x}{\sqrt{x^2+y^2}}$ where $y \geq 1$. The derivative of function $\hat{f}(y)$ is $\hat{f}'(y) = \frac{-xy}{(x^2+y^2)\sqrt{x^2+y^2}} < 0$. Therefore, $\hat{f}(y)$ is a decreasing function for every $y \geq 1$. Hence, if $a \leq b$, $\frac{x}{\sqrt{x^2+a^2}} = \hat{f}(a) \geq \hat{f}(b) = \frac{x}{\sqrt{x^2+b^2}}$. Consequently, $f'(x) > 0$ and the function $f(x)$ is an increasing function for $a \leq b$. similarity, if $a > b$, then $f(x)$ is a decreasing function for every $x \geq 1$. $\square$

**Lemma 2.3** *Let $g(x,y) = \sqrt{x^2+y^2}$ with $y \geq 2$. Then $f(x,y)$ is an increasing function for every $x \geq 1$.*

**Proof.** We have $f'(x,y) = \frac{x}{\sqrt{x^2+y^2}}$. Since $x \geq 1$, $f'(x,y) > 0$ and function $f(x,y)$ is an increasing function for every $x \geq 1$. $\square$

# 3 Extremal trees with the maximum Sombor index

In this section, we characterize the extremal trees with maximum Sombor index among the trees with given degree sequence. We propose a technique to construct these trees. to do this, we first state some properties of a maximum optimal tree.

**Theorem 3.1** *Let $T$ be a maximum optimal tree with a path $v_0v_1v_2\cdots v_kv_{k+1}$ in $T$, where $v_0$ and $v_{k+1}$ are leaves. For $i \leq \frac{t+1}{2}$ and $i+1 \leq j \leq k-i+1$*

*(i) if $i$ is odd, then $d(v_i) \geq d(v_{k-i+1}) \geq d(v_j)$,*

*(ii) if $i$ is even, then $d(v_i) \leq d(v_{k-i+1}) \leq d(v_j)$.*

**Proof.** Let $T$ be a maximum optimal tree with the degree sequence $D$. We prove the result by induction on $i$. For $i = 1$, we show that $d(v_1) \geq d(v_k) \geq d(v_j)$ where $2 \leq j \leq k$. We suppose for contradiction that $d(v_1) < d(v_j)$ for some $2 \leq j \leq k$. We consider a new tree $T'$ obtained from $T$ by changing edges $v_0v_1$ and $v_jv_{j+1}$ to edges $v_0v_j$ and $v_1v_{j+1}$ such that no other edges are changed. Note that $T$ and $T'$ have the same degree sequence. Therefore, using Lemmas 2.1-2.3, and since $d(v_{j+1}) > 1$, we have

$$\begin{aligned}
SO(T') - SO(T) &= \sqrt{d(v_0)^2 + d(v_j)^2} + \sqrt{d(v_1)^2 + d(v_{j+1})^2} \\
&- \left(\sqrt{d(v_0)^2 + d(v_1)^2} - \sqrt{d(v_j)^2 + d(v_{j+1})^2}\right) \\
&= \left(\sqrt{d(v_j)^2 + 1} - \sqrt{d(v_1)^2 + 1}\right) \\
&+ \left(\sqrt{d(v_1)^2 + d(v_{j+1})^2} - \sqrt{d(v_j)^2 + d(v_{j+1})^2}\right) \\
&= f(1) - f(d(v_{j+1})) > 0,
\end{aligned}$$

which is a contradiction with the maximum optimality $T$. Thus, $d(v_1) \geq d(v_j)$ for every $2 \leq j \leq k$. similarity, we can get $d(v_1) \geq d(v_k)$ and $d(v_k) \geq d(v_j)$. Therefore, we have $d(v_1) \geq d(v_k) \geq d(v_j)$ where $2 \leq j \leq k$. So, we suppose that the result holds for smaller values of $i$.
If $i \geq 2$ is even, then $i-1$ is odd and by the induction hypothesis, $d(v_{i-1}) \geq d(v_{k-i+1}) \geq d(v_j)$ for $i+1 \leq j \leq k-i+1$. We suppose for contradiction that $d(v_i) > d(v_j)$ for some $i+1 \leq j \leq k-i+1$. We consider a new tree $T''$ obtained from $T$ by changing edges $v_{i-1}v_i$ and $v_jv_{j+1}$ to edges $v_{i-1}v_j$ and $v_iv_{j+1}$ with the degree sequence $D$. Also, in tree $T''$, other edges are the same edges in tree $T$.
By the induction hypothesis, $d(v_{i-1}) \geq d(v_{j+1})$. Therefore, by applying Lemma 2.2, we have

$$\begin{aligned}
SO(T'') - SO(T) &= \sqrt{d(v_{i-1})^2 + d(v_j)^2} + \sqrt{d(v_i)^2 + d(v_{j+1})^2} \\
&- \left( \sqrt{d(v_{i-1})^2 + d(v_i)^2} - \sqrt{d(v_j)^2 + d(v_{j+1})^2} \right) \\
&= \left( \sqrt{d(v_j)^2 + d(v_j)^2} - \sqrt{d(v_{i-1})^2 + d(v_i)^2} \right) \\
&+ \left( \sqrt{d(v_{j+1})^2 + d(v_i)^2} - \sqrt{d(v_{j+1})^2 + d(v_j)^2} \right) \\
&= f(d(v_{i-1}) - f(d(v_{j+1})) > 0.
\end{aligned}$$

This contradiction with the maximum optimality of $T$. Therefore, $d(v_i) \leq d(v_j)$ for $i+1 \leq j \leq k-i+1$. Similarity, we have $d(v_i) \leq d(v_{k-i+1})$ and $d(v_{k-i+1}) \leq d(v_j)$. Consequently, for $i$ even, $d(v_i) \leq d(v_{k-i+1}) \leq d(v_j)$ where $i+1 \leq j \leq k-i+1$. For odd $i > 2$, with similarity technique, we can get $d(v_i) \geq d(v_{k-i+1}) \geq d(v_j)$ for $i+1 \leq j \leq k-i+1$. □

Suppose that $L_i$ denotes the set of vertices adjacent to the closet leaf at a distance $i$. Thus, $L_0$ and $L_1$ denote the set of leaves and the set of vertices that are adjacent to the leaves. Let $d^m = min\{d(u) \ : \ u \in L_1\}$ and $L_1^m$ be the set of leaves whose adjacent vertices have degree $d^m$ in $T$. We suppose that $\overline{L_1^m}$ denote the set of leaves $v$ such that $v \notin L_1^m$.
We construct a new tree $T_i'$ from tree $T$ and tree $T_i$ rooted at $v_i$ by identifying the root $v_i$ with a vertex $v \in L_1^m$.

**Theorem 3.2** *Let $T_1'$ and $T_2'$ are obtained from $T$ by identifying the root $v_i$ of $T_i$ with $u' \in L_1^m$ and $v' \in \overline{L_1^m}$, respectively. Then, $SO(T_1') \geq SO(T_2')$.*

**Proof.** We suppose that $u$ and $v$ are adjacent to $u'$ and $v'$, respectively. Using Theorem 3.1, $d(u) \leq d(v)$. Therefore, we have

$$
\begin{aligned}
SO(T_1') - SO(T_2') &= \sqrt{(d(v_i)+1)^2 + d(u)^2} + \sqrt{d(u)^2+1} \\
&- \left(\sqrt{(d(v_i)+1)^2 + d(v)^2} - \sqrt{d(v)^2+1}\right) \\
&= \left(\sqrt{(d(v_i)+1)^2 + d(u)^2} - \sqrt{(d(v_i)+1)^2 + d(v)^2}\right) \\
&+ \left(\sqrt{d(v)^2+1} - \sqrt{d(u)^2+1}\right) \\
&= f(1) - f(d(v_i)+1) > 0.
\end{aligned}
$$

Therefore, $SO(T_1') \geq SO(T_2')$. □

We use a similar technique in [10], for constructing tree $T$ with a fixed degree sequence $D$ such that $T$ is the maximum optimal tree among the trees with degree sequence $D$. We propose the following algorithms to construct such trees.

**Algorithm 1.** (Construction of subtrees)

1. Given the degree sequence of the non-leaf vertices as $D = \big(d_1, d_2, \ldots, d_m\big)$ in descending order.

2. If $d_m \geq m-1$, then using Theorem 3.1, the vertices with degrees $d_1, d_2, \ldots, d_{m-1}$ are in $L_1$. Tree $T$ produces by rotted at $u$ with $d_m$ children whose their degrees are $d_1, d_2, \ldots, d_{m-1}$ and $d_m - m + 1$ leaves adjacent to $u$.

3. If $d_m \leq m-2$, then we produce subtree $T_1$ by rotted at $u_1$ with $d_m - 1$ children with degrees $d_1, d_2, \ldots, d_{d_{m-1}}$ such that $u_1 \in L_2$ and the children of $u_1$ are in $L_1$. Subtree $T_2$ is constructed by rooted at $u_2$ with $d_{m-1} - 1$ children whose degrees are $d_{d_m}, d_{d_m+1}, \ldots, d_{(d_m-1)+(d_{m-1}-1)}$. Then do the same to get subtrees $T_3, T_4, \ldots$ until $T_k$ satisfies the condition of step (2). In this case, we have $d(v_k) = d_{m-k+1}$.

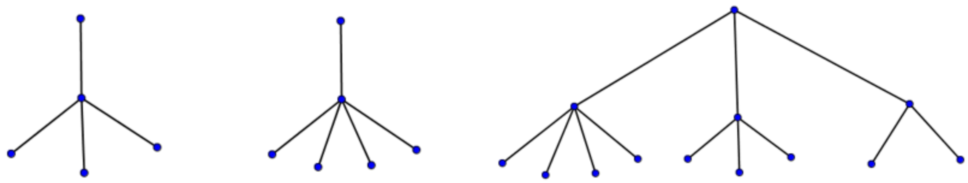
**Algorithm 2.** (Merge of subtrees)

1. Set $T = T_i$ and $i = k$. We produce a new tree $T'_{i-1}$ from $T$ and $T_{i-1}$ rooted at $v_{i-1}$ by identifying the root $v_{i-1}$ with a vertex $v \in L_1^m$. Using Theorem 3.2, tree $T'_{i-1}$ is a maximum optimal tree among trees with the same degree sequence.

2. Consider $i = k-1, k-2, \ldots, 1$ and $T = T_i$. Tree $T'_{i-1}$ from $T$ and $T_{i-1}$ by the same method of step (1). We construct trees $T'_{k-2}, T'_{k-3}, \ldots, T'_1$.

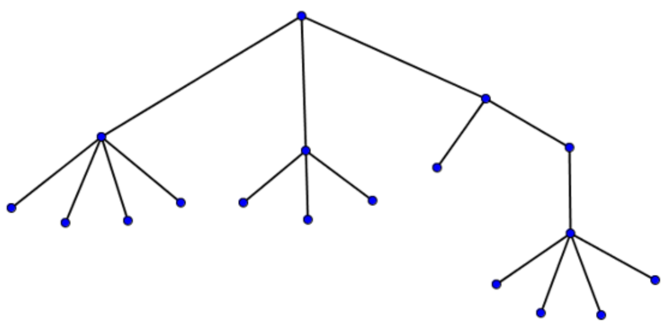
3. $T = T'_1$ is the maximum optimal tree with given degree sequence $D = \big(d_1, d_2, \ldots, d_m\big)$.

**Example 3.3** In this example, we propose a maximum optimal tree with given degree sequence $D = \big(5, 5, 5, 4, 3, 3, 2, 2\big)$. Using step (3) of Algorithm 1, we have subset $T_1$



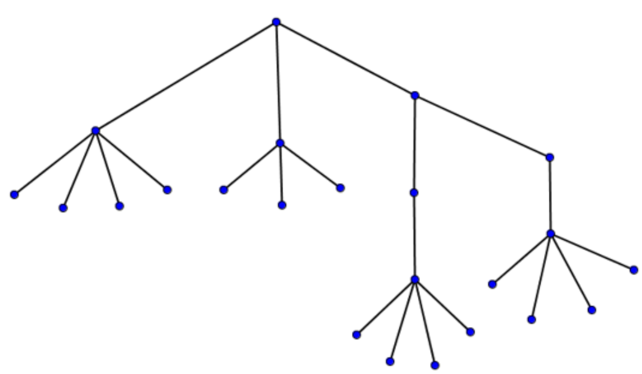
$T_1$ $T_2$ $T_3$

Figure 1: Construction of subtrees using Algorithm 1



$T'_2$

Figure 2: Merge of subtrees using Algorithm 2



$T'_1 = T$

Figure 3: A maximum optimal tree $T$ with degree sequence $\big(5, 5, 5, 4, 3, 3, 2, 2\big)$.

with 1 child whose has degree 5. For new degree sequence $D_1 = \big(5,5,4,3,3,2\big)$, we construct tree $T_2$ and have new degree sequence $D = \big(5,4,3,3\big)$ (Figure 1). It is easily seen that $D_2$ satisfies the condition of step (2).
Using Algorithm 2, we attach subtrees $T_2$ to $T_3$ for constructing $T_2'$ (Figure 2) and $T_2$ to $T_2'$ for constructing the maximum optimal tree $T_1' = T$ (Figure 3).

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