

Some results in the multiplicative version of Sombor index

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Abstract

For a graph $\mathcal{A}$ including vertex set $V_{\mathcal{A}}$ and edge set $E_{\mathcal{A}}$, the Sombor index is defined as $SO(\mathcal{A}) = \sum_{wz \in E_{\mathcal{A}}} \sqrt{\eta_{\mathcal{A}}(w)^2 + \eta_{\mathcal{A}}(z)^2}$ where $\eta_{\mathcal{A}}(w)$ is the degree of w in $\mathcal{A}$.

This study focus on the multiplicative version of SO , namely the multiplicative Sombor index ($\mathfrak{M}_{SO}$) which defined as $\mathfrak{M}_{SO}(\mathcal{A}) = \prod_{wz \in E_{\mathcal{A}}} \sqrt{\eta_{\mathcal{A}}(w)^2 + \eta_{\mathcal{A}}(z)^2}$. In this work, sharp upper and lower bounds on $\mathfrak{M}_{SO}$ of trees in terms of order and given diameter are obtained. We identify the extremal trees for these bounds. Furthermore, the maximal trees are characterized with respect to order and given number of leaves. We determine sharp bounds of simple graphs for $\mathfrak{M}_{SO}$ in terms of graph parameters.

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1. Introduction

In this work, we deal only with graphs that are simple and finite. Consider $\mathcal{A} = (V_{\mathcal{A}}, E_{\mathcal{A}})$ as a graph in which $V_{\mathcal{A}}$ and $E_{\mathcal{A}}$ are the vertex and edge set, respectively. The cardinality of $V_{\mathcal{A}}$ and $E_{\mathcal{A}}$ are called the order and size of $\mathcal{A}$, respectively.

The set of the neighbors of the vertex $w \in V_{\mathcal{A}}$ is defined by $N_{\mathcal{A}}(w) = \{z \in V_{\mathcal{A}} : wz \in E_{\mathcal{A}}\}$ and $|N_{\mathcal{A}}(w)| = \eta_{\mathcal{A}}(w)$ is called the degree of w . Let $\Delta = \max_{w \in V_{\mathcal{A}}} \{\eta_{\mathcal{A}}(w)\}$ and $\delta = \min_{w \in V_{\mathcal{A}}} \{\eta_{\mathcal{A}}(w)\}$. If $\eta_{\mathcal{A}}(w) = 1$, then w is called a leaf in $\mathcal{A}$. The graph $\bar{\mathcal{A}}$ is called the complement graph of $\mathcal{A}$ with the exact same set of vertices as $\mathcal{A}$ and edges between vertices in $\mathcal{A}$ do not exist in $\bar{\mathcal{A}}$ and vice versa. A path $P = x_1x_2 \dots x_k$ in $\mathcal{A}$ is called a pendant path if $\eta_{\mathcal{A}}(x_1) \geq 3$, $\eta_{\mathcal{A}}(x_k) = 1$ and $\eta_{\mathcal{A}}(x_l) = 2$ for $2 \leq l \leq k - 1$. The diameter of $\mathcal{A}$ is defined as the maximum distance (shortest path length) between any two vertices in $\mathcal{A}$. For

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$w \in V_{\mathcal{A}}$, $\mathcal{A} - \{w\}$ is a subgraph of $\mathcal{A}$ derived by deleting vertex w and all edges that are incident to it. Given an edge $wz \in E_{\mathcal{A}}$, the graph $\mathcal{A} - \{wz\}$ is the graph derived by deleting the edge wz . For k edges $e_1, e_2, \dots, e_k$ in $E_{\mathcal{A}}$, $\mathcal{A} + \{e_1, \dots, e_k\}$ ($\mathcal{A} - \{e_1, \dots, e_k\}$) is the graph obtained from $\mathcal{A}$ by adding (deleting, resp.) the edges $e_1, \dots, e_k$ [1].

A topological index plays a significant role in theoretical chemistry and different sciences. Topological indices can predict physical and chemical properties of chemical compounds and are known as important tools in the development of QSPR and QSAR models [2].

Recently, Gutman [3] in 2021 defined the Sombor index as

$$SO(\mathcal{A}) = \sum_{wz \in E_{\mathcal{A}}} \sqrt{\eta_{\mathcal{A}}(w)^2 + \eta_{\mathcal{A}}(z)^2}.$$

Chemical applications of the Sombor index are discussed in [4-10]. Several topological indices of a graph motivated by the definition of SO and some known topological indices were presented and studied. The extremal graphs in terms of SO on the set of chemical graphs are characterized in [11]. Rada et al. [12] determined some bounds of the Sombor indices. Also, they presented inequalities for these indices in terms of other topological indices. Liu in [13] explored the minimum Sombor indices of graphs with fixed order, given cut vertices, and at least one cycle. In [14], some bounds for SO in terms of matching number, graph energy and induced matching number are established. For more details and the mathematical properties of Sombor indices, we refer to [15-21].

In [22], the authors extended the topological invariants by defining the multiplicative version. Liu [32] introduced the multiplicative Sombor index as follows

$$\mathfrak{M}_{SO}(\mathcal{A}) = \prod_{wz \in E_{\mathcal{A}}} \sqrt{\eta_{\mathcal{A}}(w)^2 + \eta_{\mathcal{A}}(z)^2}.$$

He obtained extremal values of $\mathfrak{M}_{SO}$ of trees and unicyclic graphs. Sharma, Bhat, and Lal, [24] computed several multiplicative topological indices of the crystalline structure of cubic carbon. In [25], the multiplicative versions of some topological indices of Silicon-Carbon are investigated. Hassan in [26] calculated the multiplicative Zagreb connection indices of some nanostructures. More results of the applications on the multiplicative graph energy, Sombor indices are found in [24, 27, 28].

In this paper, our aim is to determine $\mathfrak{M}_{SO}$ of trees and simple graphs.

In the following, some modifications that will be utilized in the main results are defined.

Modification 1.1: [29] Let T_0 be a tree with a vertex $u \in V_{T_0}$ and S_{t+1} is a star graph where $t \geq 1$ with center vertex $v \in V_{S_{t+1}}$. Let T be the tree obtained from T_0 and S_{t+1} with the following vertex and edge sets (see Figure 1).

$$V_T = V_{T_0} \cup V_{S_{t+1}}, \quad E_T = E_{T_0} \cup E_{S_{t+1}} \cup \{uv\}.$$

Define $T^* = T - \{vu_1, vu_2, \dots, vu_{t+1}\} + \{uu_1, \dots, uu_t\}$ in which $u_1, \dots, u_t$ are pendant vertices of S_{t+1} (see Figure 1).

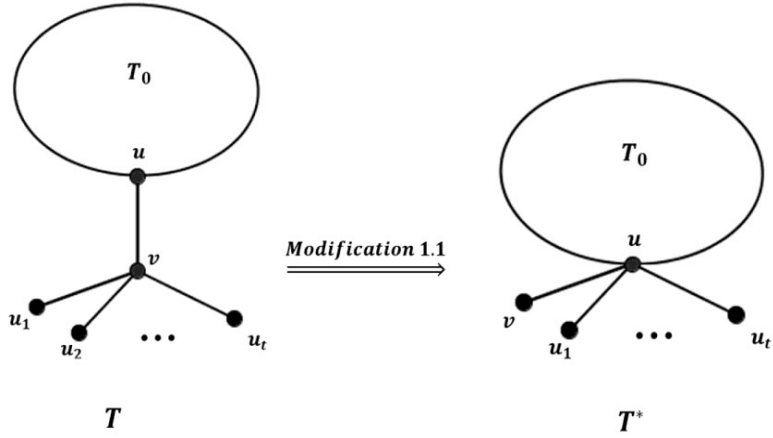


Figure 1
Trees T and T^* in Modification 1.1.

Modification 1.2: Assume that T_0 is a tree with a vertex $u \in V_{T_0}$ which $\eta_{T_0}(u) \geq 3$ and T is the tree obtained from T_0 and S_{t+s+1} by adding an edge between u and center vertex v of S_{t+s+1} , where $s, t \geq 1$.

Define $T^* = T - \{vu_2, \dots, vu_t, \dots, vu_{s+t}\} + \{u_1u_2, \dots, u_{t-1}u_t, u_tu_{t+1}, \dots, u_tu_{t+s}\}$ (see Figure 2).

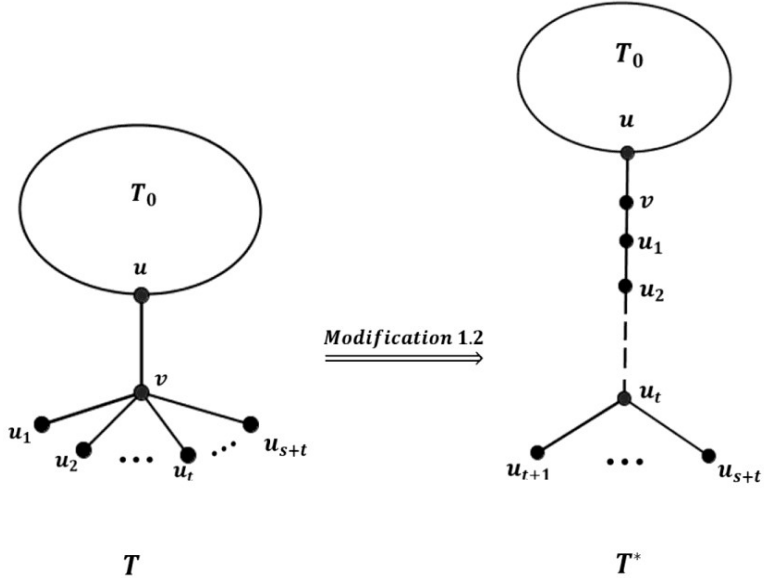


Figure 2
Trees T and T^* in Modification 1.2.

Modification 1.3: Assume that T is the tree shown in Figure 3 such that including subset T_0 with $u \in V_{T_0}$ where $\eta_{T_0}(u) \geq 3$. For $t, s \geq 1$ and $t_1 \leq t$, we define $T^* = T - \{u_{t_1+1}u_{t_1+2}, \dots, u_{t-1}u_t, u_t w_1, \dots, u_t w_s\} + \{u_{t_1}u_{t_1+1}, u_{t_1}u_{t_1+2}, \dots, u_{t_1}u_t, u_{t_1}w_1, \dots, u_{t_1}w_s\}$ (see Figure 3).

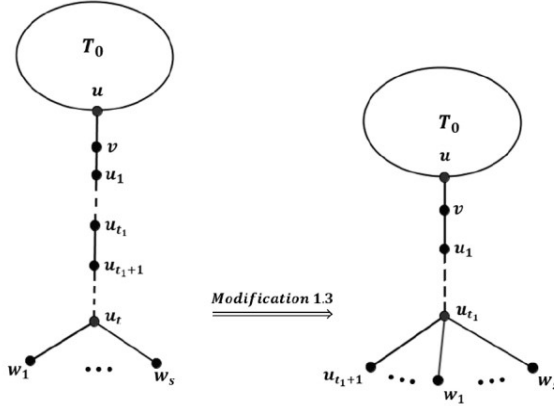


Figure 3
Trees T and T^* in Modification 1.3.

Modification 1.4: Let T be a tree and $x, y \in V_T$ belonging to the path $P = zy \dots xv$ of length at least one such that $\eta(z) \geq 3$, $\eta(y) \geq 3$, $\eta(v) = 1$, $\eta(x) = 2$ and other vertices on P equals two.

Define $T^* = T - \{yu: u \in V_{T_0}\} + \{xu: u \in V_{T_0}\}$ (see Figure 4).



Figure 4
Trees T and T^* in Modification 1.4.

2. Main Results

In this section, the sharp bounds on $\mathfrak{M}_{SO}$ in terms of order and given diameter are obtained. Also, a sharp upper bound on $\mathfrak{M}_{SO}$ of trees with given number of leaves is presented.

Lemma 2.1: For trees T and T^* described in Modification 1.1,

$$\mathfrak{M}_{SO}(T) < \mathfrak{M}_{SO}(T^*).$$

Proof: Suppose that $N_{T_0}(u) = \{v_1, \dots, v_s\}$ where $s \geq 1$. Since for each $w \in V_{T_0} \setminus \{u\}$, $\eta_T(w) = \eta_{T^*}(w)$ and for $t \geq 3$, $s \geq 1$ we have $\sqrt{\eta_T(v_h)^2 + (s+1)^2} < \sqrt{\eta_T(v_h)^2 + (s+1+t)^2}$, then

$$\begin{aligned} \frac{\mathfrak{M}_{SO}(T)}{\mathfrak{M}_{SO}(T^*)} &= \frac{\prod_{h=1}^s \sqrt{\eta_T(v_h)^2 + (s+1)^2} \times \sqrt{(t+1)^2 + (s+1)^2} \times \prod_{h=1}^t \sqrt{(t+1)^2 + 1}}{\prod_{h=1}^s \sqrt{\eta_T(v_h)^2 + (s+1+t)^2} \times \prod_{h=1}^{t+1} \sqrt{(s+t+1)^2 + 1}} \\ &< \frac{\sqrt{(t+1)^2 + (s+1)^2}}{\sqrt{(s+t+1)^2 + 1}} \times \left(\frac{\sqrt{(t+1)^2 + 1}}{\sqrt{(s+t+1)^2 + 1}} \right)^t \\ &< 1. \end{aligned}$$

Thus, $\mathfrak{M}_{SO}(T) < \mathfrak{M}_{SO}(T^*)$.

Lemma 2.2: For trees T and T^* described in Modification 1.2,

$$\mathfrak{M}_{SO}(T) > \mathfrak{M}_{SO}(T^*).$$

Proof: According to the structure of trees T and T^* depicted in Figure 2, we have $\eta_T(u) \geq 3$, $\eta_T(v) = s+t+1$, $\eta_{T^*}(v) = 2$, $\eta_T(u_t) = 1$, $\eta_{T^*}(u_t) = s+1$ and for any vertex $x \in V(T_0)$, $\eta_T(x) = \eta_{T^*}(x)$.

Therefore, we get

$$\begin{aligned} \frac{\mathfrak{M}_{SO}(T)}{\mathfrak{M}_{SO}(T^*)} &= \frac{\sqrt{\eta_T(u)^2 + \eta_T(v)^2} \times (\sqrt{\eta_T(v)^2 + 1})^{s+t}}{\sqrt{\eta_{T^*}(u)^2 + 4} \times (\sqrt{\eta_{T^*}(u_t)^2 + 1})^s \times (\sqrt{\eta_{T^*}(u_t)^2 + 4}) \times (\sqrt{8})^{t-1}} \\ &= \frac{\sqrt{\eta_T(u)^2 + (s+t+1)^2}}{\sqrt{\eta_T(u)^2 + 4}} \times \left(\frac{\sqrt{(s+t+1)^2 + 1}}{\sqrt{(s+1)^2 + 1}} \right)^s \\ &\quad \times \left(\frac{\sqrt{(s+t+1)^2 + 1}}{\sqrt{8}} \right)^{t-1} \times \left(\frac{\sqrt{(s+t+1)^2 + 1}}{\sqrt{(s+1)^2 + 4}} \right) \\ &> 1. \end{aligned}$$

Therefore, $\mathfrak{M}_{SO}(T) > \mathfrak{M}_{SO}(T^*)$.

Lemma 2.3: For trees T and T^* described in Modification 1.3,

$$\mathfrak{M}_{SO}(T^*) > \mathfrak{M}_{SO}(T).$$

Proof: According to the trees depicted in Figure 3, for $t, s \geq 1$, $\eta_T(u_{t_1}) = 2$, $\eta_{T^*}(u_{t_1}) = s+t-t_1+1$, $\eta_T(u_t) = s+1$, $\eta_{T^*}(u_t) = 1$, $\eta_T(u_{t_1+1}) = \eta_T(u_{t_1+2}) = \dots = \eta_T(u_{t-1}) = 2$ and $\eta_{T^*}(u_{t_1+1}) = \eta_{T^*}(u_{t_1+2}) = \dots = \eta_{T^*}(u_{t-1}) = 1$. Therefore, we have

$$\begin{aligned} \frac{\mathfrak{M}_{SO}(T^*)}{\mathfrak{M}_{SO}(T)} &= \frac{(\sqrt{(s+t-t_1+1)^2 + 1})^{s+t-t_1} \times (\sqrt{(s+t-t_1+1)^2 + 4}) \times (\sqrt{8})^{t_1-1}}{(\sqrt{(s+1)^2 + 1})^s \times (\sqrt{(s+1)^2 + 4}) \times (\sqrt{8})^{t-1}} \\ &= \left(\frac{\sqrt{(s+t-t_1+1)^2 + 1}}{\sqrt{(s+1)^2 + 1}} \right)^s \times \left(\frac{\sqrt{(s+t-t_1+1)^2 + 4}}{\sqrt{(s+1)^2 + 4}} \right) \\ &\quad \times \left(\frac{\sqrt{(s+t-t_1+1)^2 + 1}}{\sqrt{8}} \right)^{t-t_1} \\ &> 1. \end{aligned}$$

Since $s, t \geq 1$ and $t_1 \leq t$, thus $\mathfrak{M}_{SO}(T^*) > \mathfrak{M}_{SO}(T)$.

Denote $T_{n,d}$ to be a family of trees with diameter d and n vertices. We consider $\mathcal{T}_{n,d}$ for the family of trees $T \in T_{n,d}$ obtained from the union of path $P_{d-1} = x_1 x_2 \dots x_{d-1}$ and star graph S_{n-d+1} with center vertex u and pendant vertices $u_1 u_2 \dots u_{n-d}$ by adding the edge $x_{d-1} u_1$. Therefore for $T \in \mathcal{T}_{n,d}$,

$$\begin{aligned} V_T &= V_{P_{d-1}} \cup V_{S_{n-d+1}}, \\ E_T &= E_{P_{d-1}} \cup E_{S_{n-d+1}} \cup \{x_{d-1} u_1\}. \end{aligned}$$

Theorem 2.4: For a tree $T \in T_{n,d}$ where $3 \leq d \leq n-2$,

$$\mathfrak{M}_{SO}(T) \leq \sqrt{5}(\sqrt{8})^{d-3} \times \sqrt{(n-d+1)^2 + 4} \times (\sqrt{(n-d+1)^2 + 1})^{n-d}.$$

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

Proof: To simplify the computations, we consider

$$f(n, d) = \sqrt{5}(\sqrt{8})^{d-3} \times \sqrt{(n-d+1)^2 + 4} \times (\sqrt{(n-d+1)^2 + 1})^{n-d}.$$

Assume that $T \in T_{n,d}$ where $d \geq 3$ such that has the maximum multiplicative Sombor index among all trees in $T_{n,d}$. Consider the path $P_{d+1} = v_0 v_1 \dots v_{d-1} v_d$ in T .

Using Lemma 2.1, for any $w \in V_T \setminus V_{P_{d+1}}$, $\eta(w) = 1$ and w is adjacent to exactly one of vertices P_{d+1} .

Suppose there is a vertex $v_k \in V_T$ such that $k \neq 1, d-1$ where $\eta(v_k) \geq 3$. Without loss of generality, let $\eta(v_h) = 2$ for any vertex v_h ($h \neq 0, d, k$). Denote $N(v_k) = \{u_1, \dots, u_t\}$ where $\eta(u_h) = 1$ for $1 \leq h \leq t$. We take $T' = T - \{v_k u_1, \dots, v_k u_t\} + \{v_1 u_1, \dots, v_1 u_t\}$. Clearly, $T' \in T_{n,d}$. According to the structure of trees T and T' , one can easily see that $\eta_{T'}(v_1) = t+1$, $\eta_T(v_1) = 2$, $\eta_{T'}(v_k) = 2$, $\eta_T(v_k) = t+2$ and for any vertex $u \in V_T \setminus \{v_1, v_k\}$, $\eta_T(u) = \eta_{T'}(u)$.

With putting $E' = \{v_0 v_1, v_1 v_2, v_{k-1} v_k, v_k v_{k+1}\} \subseteq E$, we have

$$\begin{aligned} \frac{\mathfrak{M}_{SO}(T')}{\mathfrak{M}_{SO}(T)} &= \frac{\prod_{wz \in E_{T'} \setminus E'} \sqrt{\eta_{T'}(w)^2 + \eta_{T'}(z)^2} \times \sqrt{5} \times (\sqrt{(t+2)^2 + 1})^{t+1} \times (\sqrt{(t+2)^2 + 4}) \times (\sqrt{8})^2}{\prod_{wz \in E_T \setminus E'} \sqrt{\eta_T(w)^2 + \eta_T(z)^2} \times (\sqrt{5})^2 \times (\sqrt{(t+2)^2 + 1})^t \times (\sqrt{(t+2)^2 + 4})^2 \times (\sqrt{8})} \\ &= \frac{\sqrt{(t+2)^2 + 1} \times \sqrt{8}}{\sqrt{(t+2)^2 + 4} \times \sqrt{5}} > 1. \end{aligned}$$

This implies that $\mathfrak{M}_S(T') > \mathfrak{M}_{SO}(T)$, which is a contradiction. Hence, $\eta(v_h) = 2$ for any $1 \leq h < d-1$ or $1 < h \leq d-1$. Therefore, $T \in \mathcal{T}_{n,d}$.

If $T \in \mathcal{T}_{n,d}$, then $\mathfrak{M}_{SO}(T) = f(n, d)$.

Lemma 2.5: For trees T and T^* described in Modification 1.4,

$$\mathfrak{M}_{SO}(T^*) > \mathfrak{M}_{SO}(T).$$

Proof: For any vertex $w \in V_{T_0}$, $\eta_T(u) = \eta_{T^*}(u)$, and any $w \in V_{T_1}$, we have $\eta_T(w) = \eta_{T^*}(w)$. Suppose that $\eta_{T_0}(y) = t$. Then $\eta_T(y) = t+2 = \eta_{T^*}(x)$ and $\eta_{T^*}(y) = 2 = \eta_T(x)$. Consequently, we get

$$\begin{aligned}\frac{\mathfrak{M}_{SO}(T^*)}{\mathfrak{M}_{SO}(T)} &= \frac{\sqrt{\eta_{T^*}(z)^2 + 4 \times \sqrt{8} \times \sqrt{(t+2)^2 + 4} \times \sqrt{(t+1)^2 + 1}}}{\sqrt{\eta_T(z)^2 + (t+2)^2} \times \sqrt{(t+2)^2 + 4} \times \sqrt{8} \times \sqrt{5}} \\ &= \frac{\sqrt{\eta_{T^*}(z)^2 + 4}}{\sqrt{5}} \times \frac{\sqrt{(t+2)^2 + 1}}{\sqrt{\eta_T(z)^2 + (t+2)^2}}.\end{aligned}$$

Let $f(x) = \frac{\sqrt{x^2+1}}{\sqrt{x^2+c^2}}$ where $c \geq 2$ is fixed. Since $f'(x) = \frac{x(c^2-1)}{\sqrt{x^2+1}(x^2+c^2)^{\frac{3}{2}}} > 0$, $f(x)$ is an increasing function. Therefore,

$$\begin{aligned}\frac{\mathfrak{M}_{SO}(T^*)}{\mathfrak{M}_{SO}(T)} &= \frac{\sqrt{\eta_{T^*}(z)^2 + 4}}{\sqrt{5}} \times \frac{\sqrt{(t+2)^2 + 1}}{\sqrt{\eta_T(z)^2 + (t+2)^2}} \\ &\geq \frac{\sqrt{\eta_{T^*}(z)^2 + 4}}{\sqrt{5}} \times \frac{\sqrt{10}}{\sqrt{\eta_T(z)^2 + 9}} \\ &= \frac{2\left(\sqrt{\eta_{T^*}(z)^2 + 4}\right)}{\sqrt{\eta_T(z)^2 + 9}} > 1.\end{aligned}$$

Hence, $\mathfrak{M}_{SO}(T^*) > \mathfrak{M}_{SO}(T)$.

Theorem 2.6: For a tree $T \in T_{n,d}$ where $n \geq 5$ and $d \geq 4$ is even,

- (i) if $d = 2$, then $\mathfrak{M}_{SO}(T) = \left(\sqrt{(n-1)^2 + 1}\right)^{n-2}$,
- (ii) if $d = 4$, then $\mathfrak{M}_{SO}(T) = 65\left(\sqrt{(n-5)^2 + 1}\right)^{n-6} \times \left(\sqrt{(n-5)^2 + 9}\right)$,
- (iii) if $d \geq 6$, then $\mathfrak{M}_{SO}(T) \geq 65\sqrt{13}\left(\sqrt{8}\right)^{\frac{3d}{2}-7} \times \left(\sqrt{\left(n - \frac{3d}{2} + 1\right)^2 + 1}\right)^{n-\frac{3d}{2}} \times \left(\sqrt{\left(n - \frac{3d}{2} + 1\right)^2 + 4}\right)$.

Equality holds if and only if $T; T_2$ shown in Figure 5.

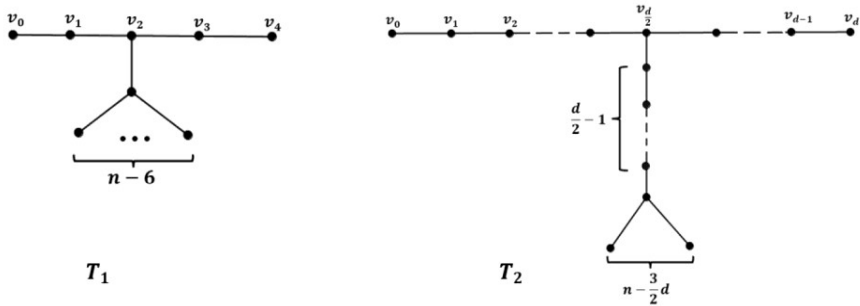


Figure 5
The trees T_1 and T_2 in Theorem 2.6.

Proof: If $d = 2$, then $T = S_n$ and consequently, $\prod_{SO}(T) = (\sqrt{(n-1)^2 + 1})^{n-2}$. If $d = 4$, then $T; T_1$ shown in Figure 5 and it is easily to check that

$$\mathfrak{M}_{SO}(T_1) = 65 \left(\sqrt{(n-5)^2 + 1} \right)^{n-6} \left(\sqrt{(n-5)^2 + 9} \right).$$

Assume that $T \in T_{n,d}$ where $d \geq 6$ is even such that T has the minimum multiplicative Sombor index among all trees in $T_{n,d}$. Suppose that $P_{d+1} = v_0 v_1 \dots v_d$ is the path of length d in T . by applying Lemmas 2.1-2.3, T contains a path $v_j x_1 x_2 \dots x_t$ such that $j \neq \frac{d}{2}$, $t < \frac{d}{2}$ and $\eta(x_1) = \dots = \eta(x_{t-2}) = 2$, $\eta(x_{t-1}) \geq 2$ and $\eta(x_t) = 1$.

Let $N(x_{t-1}) = \{x_t, z_1, z_2, \dots, z_{k-1}\}$ where $\eta(x_{t-1}) = k \geq 2$. without loss of generality, let $\frac{d}{2} < j \leq d$.

We take $T' = T - \{x_1 v_j, x_{t-1} z_1, \dots, x_{t-1} z_{k-1}\} + \{x_1 v_{\frac{d}{2}}, x_t z_1, z_1 z_2, \dots, z_{t'-1} z_{t'}, x_t z_{t'+1}, \dots, x_t z_k\}$ where $t + t' \geq \frac{d}{2}$.

Using Lemma 2.5, $\mathfrak{M}_{SO}(T') < \mathfrak{M}_{SO}(T)$ which is a contradiction. Therefore, $T; T_2$ shown in Figure 5. On the other hand for $T; T_2$, one can easily see that

$$\mathfrak{M}_{SO}(T) = 65\sqrt{13}(\sqrt{8})^{\frac{3d}{2}-7} \times \left(\sqrt{(n - \frac{3d}{2} + 1)^2 + 1} \right)^{n - \frac{3d}{2}} \times \left(\sqrt{(n - \frac{3d}{2} + 1)^2 + 4} \right).$$

Denote $T_{n,l}$ to be a family of trees with l leaves and n vertices. Assume that $\mathfrak{T}_{n,l}$ is the family of trees $T \in T_{n,l}$ where $2 \leq l \leq n-2$, formed from the path P_{n-l+1} by attaching $l-2$ new vertices to one of the end vertices in P_{n-l+1} .

Theorem 2.7: For a tree $T \in T_{n,l}$,

$$\mathfrak{M}_{SO}(T) \leq \sqrt{5} \left(\sqrt{l^2 + 1} \right)^{l-1} \left(\sqrt{l^2 + 4} \right) (\sqrt{8})^{n-l-2}.$$

Equality holds if and only if $T \in \mathfrak{T}_{n,l}$.

Proof: If $l = 2$, then $T; P_n$ and $\mathfrak{M}_{SO}(T) = 5(\sqrt{8})^{n-3} = g(n, l)$. To simplify the computations, we consider

$$g(n, l) = \sqrt{5} \left(\sqrt{l^2 + 1} \right)^{l-1} \left(\sqrt{l^2 + 4} \right) (\sqrt{8})^{n-l-2}.$$

Suppose that $3 \leq l \leq n-2$ and T is a tree with the maximum multiplicative Sombor index among all trees in $T_{n,l}$. We investigate the following cases.

Case 1: The tree T has a pendant path of length at least one. Suppose that $x_0 x_1 \dots x_k$ is the pendant path in T rooted at x_0 where $\eta(x_0) \geq 3$ and $k \geq 2$. We take $T_1 = \{x_0, x_1, \dots, x_k\}$. Let T_1 be a nonempty graph. By applying Lemma 2.5 and by putting $x_0 = y$ and $x_{k-1} = x$, we construct a tree $T^* \in T_{n,l}$ where $\mathfrak{M}_{SO}(T^*) > \mathfrak{M}_{SO}(T)$. It is a contradiction.

Therefore, T_1 is an empty graph and consequently, $T \in \mathfrak{T}_{n,l}$.

Case 2: The length of any pendant path in T is one. In such a case, $l \geq 3$. Let $x_0x_1 \dots x_k$ be a path of length $k \geq 2$. Since all pendant paths in T are length one, thus $\eta(x_1), \eta(x_{k-1}) \geq 3$. Let for some vertices x_h , $\eta_T(x_h) \geq 3$ where $2 \leq h \leq k-2$. Among such vertices, we suppose that x_j is the closest one to x_1 . By applying Lemma 2.5 and by putting $x = x_1$ and $y = x_j$, we obtain a tree $T^* \in \mathcal{T}_{n,l}$. Then $\mathfrak{M}_{SO}(T^*) > \mathfrak{M}_{SO}(T)$ where is a contradiction. Using Lemma 2.7 in [23], we can reach a tree T' with $\mathfrak{M}_{SO}(T') > \mathfrak{M}_{SO}(T)$ such that $T' \in \mathcal{T}_{n,l}$. Therefore, either $\eta_T(x_1) = 2$ or $\eta_T(x_{k-1}) = 2$ where shown there is only a pendant path in T with length $n - l - 1$. Consequently, $T \in \mathcal{T}_{n,l}$.

Suppose that m_{ij} is the number of edges $e = wz$ that $\{\eta(w), \eta(z)\} = \{i, j\}$. Therefore, for a tree $T \in \mathcal{T}_{n,l}$, we have $m_{12} = 1$, $m_{1l} = l - 1$, $m_{2l} = 1$ and $m_{22} = n - l - 2$. Therefore, we get

$$\begin{aligned} \mathfrak{M}_{SO}(T) &= \prod_{wz \in E(T)} \sqrt{\eta(w)^2 + \eta(z)^2} \\ &= (\sqrt{5})^{m_{12}} \times (\sqrt{l^2 + 1})^{m_{1l}} \times (\sqrt{8})^{m_{22}} \times (\sqrt{l^2 + 4})^{m_{2l}} \\ &= \sqrt{5}(\sqrt{l^2 + 4}) \times (\sqrt{l^2 + 1})^{l-1} \times (\sqrt{8})^{n-l-2}. \end{aligned}$$

Next, we determine sharp bounds on $\mathfrak{M}_{SO}$ of simple graphs in terms of some graph parameters. We establish the relationship between this index and the Sombor index.

Theorem 2.8: For a simple graph $\mathcal{A}$ of order n and size m ,

$$\mathfrak{M}_{SO}(\mathcal{A}) \leq (2(n-1)^2)^{\frac{m}{2}}.$$

Equality holds if and only if $\mathcal{A}; K_n$.

Proof: Obviously, for any vertex $w \in V_{\mathcal{A}}$, $\eta(w) \leq n - 1$. Therefore,

$$\begin{aligned} \mathfrak{M}_{SO}(\mathcal{A}) &= \prod_{wz \in E_{\mathcal{A}}} \sqrt{\eta(w)^2 + \eta(z)^2} \\ &\leq \prod_{wz \in E_{\mathcal{A}}} \sqrt{(n-1)^2 + (n-1)^2} \\ &= \prod_{wz \in E_{\mathcal{A}}} \sqrt{2(n-1)^2} \\ &= (\sqrt{2(n-1)^2})^m. \end{aligned}$$

Equality holds if and only if $\eta(w) = n - 1$ for any $w \in V_{\mathcal{A}}$. This holds if and only if $\mathcal{A}$ is a complete graph.

We present a Nordhaus-Gaddum bound for $\mathfrak{M}_{SO}$ in the following theorem.

Theorem 2.9: For a simple graph $\mathcal{A}$ with n vertices,

$$\mathfrak{M}_{SO}(\mathcal{A})\mathfrak{M}_{SO}(\bar{\mathcal{A}}) \leq (2(n-1)^2)^{\frac{n(n-1)}{4}}.$$

Equality holds if and only if $\mathcal{A}; K_n$.

Proof: Using Theorem 2.8, we get

$$\mathfrak{M}_{SO}(\mathcal{A}) \leq (\sqrt{2(n-1)^2})^m,$$

and

$$\mathfrak{M}_{SO}(\mathcal{A}) \leq \left(\sqrt{2(n-1)^2} \right)^{\binom{n}{2}-m}.$$

Therefore,

$$\begin{aligned} \mathfrak{M}_{SO}(\mathcal{A})\mathfrak{M}_{SO}(\bar{\mathcal{A}}) &\leq \left(\sqrt{2(n-1)^2} \right)^m \times \left(\sqrt{2(n-1)^2} \right)^{\binom{n}{2}-m} \\ &= \left(\sqrt{2(n-1)^2} \right)^{\binom{n}{2}} \\ &= (2(n-1)^2)^{\frac{n(n-1)}{4}}. \end{aligned}$$

Equality holds if and only if $\mathcal{A}$ is a complete graph.

Theorem 2.10: For a connected graph $\mathcal{A}$ of size m ,

$$\left(\frac{m}{SO(\mathcal{A})} \right)^m < \mathfrak{M}_{SO}(\mathcal{A}) \leq \left(\frac{SO(\mathcal{A})}{m} \right)^m.$$

Equality on the right holds if and only if $\mathcal{A}$ is regular graph.

Proof: For the lower bound, by applying geometric-harmonic mean inequality, we get

$$\begin{aligned} \mathfrak{M}_{SO}(\mathcal{A}) &\geq \left(\frac{m}{\sum_{wz \in E_{\mathcal{A}}} \frac{1}{\sqrt{\eta(w)^2 + \eta(z)^2}}} \right)^m \\ &> \left(\frac{m}{\sum_{wz \in E_{\mathcal{A}}} \sqrt{\eta(w)^2 + \eta(z)^2}} \right)^m \\ &= \left(\frac{m}{SO(\mathcal{A})} \right)^m. \end{aligned}$$

For the upper bound, we use the arithmetic-geometric mean inequality and we get

$$\begin{aligned} \mathfrak{M}_{SO}(\mathcal{A}) &= \prod_{wz \in E_{\mathcal{A}}} \sqrt{\eta(w)^2 + \eta(z)^2} \\ &\leq \left(\frac{\sum_{wz \in E_{\mathcal{A}}} \sqrt{\eta(w)^2 + \eta(z)^2}}{m} \right)^m \\ &= \left(\frac{SO(\mathcal{A})}{m} \right)^m. \end{aligned}$$

The equality holds if and only if $\eta(w) = \eta(z)$ for $e = wz \in E_{\mathcal{A}}$. Therefore, this equality holds if and only if $\mathcal{A}$ is a regular graph.

Lemma 2.11: [30] Let $a = (a_h)_{h=1}^n$ and $b = (b_h)_{h=1}^n$ be decreasing sequences where $a_h, b_h \in \mathbb{R}$. Assume that $\sum_{h=1}^t a_h \leq \sum_{h=1}^t b_h$ for each integer $1 \leq t \leq n-1$. Then $\sum_{h=1}^t f(a_h) \leq \sum_{h=1}^t f(b_h)$, for each convex function f .

Theorem 2.12: For a simple graph $\mathcal{A}$ with n vertices and size $m \leq n - 1$,

$$\mathfrak{M}_{SO}(\mathcal{A}) \leq (m^2 + 1)^{\frac{m}{2}}.$$

Equality holds if and only if $G \simeq S_{m+1} \cup (n - m + 1)K_1$.

Proof: For each edge $e = wz \in E_{\mathcal{A}}$, $\eta(w) + \eta(z) \leq m + 1$. Since,

$$\sqrt{\eta(w)^2 + \eta(z)^2} \leq \sqrt{(\eta(w) + x)^2 + \eta(z)^2},$$

in which $x = m + 1 - (\eta(w) + \eta(z))$.

Using Lemma 2.11,

$$\begin{aligned} \mathfrak{M}_{SO}(\mathcal{A}) &= \prod_{wz \in E_{\mathcal{A}}} \sqrt{\eta(w)^2 + \eta(z)^2} \\ &\leq \prod_{wz \in E_{\mathcal{A}}} \sqrt{(\eta(w) + x)^2 + \eta(z)^2} \\ &\leq \prod_{wz \in E_{\mathcal{A}}} \sqrt{m^2 + 1} \\ &= (m^2 + 1)^{\frac{m}{2}}. \end{aligned}$$

Equality holds if and only if $\eta(w) + \eta(z) = m + 1$ and $(\eta(w) + x, \eta(z)) = (m, 1)$ or $(\eta(w) + x)^2 + \eta(z)^2 = m^2 + 1$. Therefore, $\eta(w) = m$ and $\eta(z) = 1$ if $m \leq n - 1$. Consequently, $G \simeq S_{m+1} \cup (n - m + 1)K_1$.

Theorem 2.13: Let $\mathcal{A}$ be a simple graph of size m . Then

$$(\sqrt{2}\delta)^m \leq \mathfrak{M}_{SO}(\mathcal{A}) \leq (\sqrt{2}\Delta)^m.$$

Equality holds if and only if $\mathcal{A}$ is regular graph.

Proof: Since for any $w \in V_{\mathcal{A}}$, $\delta \leq \eta(w) \leq \Delta$, we have

$$\prod_{wz \in E_{\mathcal{A}}} \sqrt{2\delta^2} \leq \mathfrak{M}_{SO}(\mathcal{A}) = \prod_{wz \in E_{\mathcal{A}}} \sqrt{\eta(w)^2 + \eta(z)^2} \leq \prod_{wz \in E_{\mathcal{A}}} \sqrt{2\Delta^2}.$$

Hence,

$$(\sqrt{2}\delta)^m = (\sqrt{2\delta^2})^m \leq \mathfrak{M}_{SO}(\mathcal{A}) \leq (\sqrt{2\Delta^2})^m = (\sqrt{2}\Delta)^m.$$

Equality holds if and only if $\eta(w) = \delta = \Delta = \eta(z)$ for any edge $wz \in E_{\mathcal{A}}$.

Concluding remarks

The extremal problem has emerged as a critical area of research, garnering particular attention in recent times. In these problems, the extremal graphs within a given class are characterized to maximize or minimize graph invariants. Graph invariants play a crucial role in various applied sciences. Specifically, topological indices serve as potent tools in the study of chemical graph theory. These indices help characterize molecular structures, discriminate pathological structures, predict properties or bioactivity of molecules for drug discovery, and quantify intermolecular similarity.

In this work, we considered the extremal problems with respect to $\mathfrak{M}_{SO}$ among trees of order n , diameter d and l leaves. We determined a sharp upper bound for $\mathfrak{M}_{SO}$ in terms of order and given diameter and identified the extremal trees that attain this extremal value. Moreover, the trees of order n with even diameter for minimizing $\mathfrak{M}_{SO}$ among all trees are identified.

In addition, we determined the sharp upper bound for $\mathfrak{M}_{SO}$ in trees of order n and l leaves. Also, we obtained sharp bounds on Π_{SO} of simple graphs based on the order and size and established relations between $\mathfrak{M}_{SO}$ and SO .

There are extremal problems related to the $\mathfrak{M}_{SO}$ with some fixed graph parameters that remain to be solved. For instance, a future goal could be identifying trees of order n and l leaves having the minimum multiplicative Sombor index. One could also consider the extremal problem by characterizing the extremal graphs with respect to $\mathfrak{M}_{SO}$ with given degree sequence and segment sequence.

Finally, we present the following conjecture for trees of order n .

Conjecture 2.14: Let T be a tree of order n . Then

- (i) For $n \geq 3$, $5(\sqrt{8})^{n-3} \leq \mathfrak{M}_{SO}(T) \leq (\sqrt{(n-1)^2 + 1})^{n-1}$. Equality holds if and only if (in left) $T; P_n$ and (in right) $T; S_n$.
- (ii) For $n \geq 4$ and $T \neq S_n$, $\mathfrak{M}_{SO}(T) \leq \sqrt{5}(\sqrt{(n-2)^2 + 1})^{n-3} \times (\sqrt{(n-2)^2 + 4})$.

Equality holds if and only if T is a tree with n vertices and diameter 4.

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