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MULTIPLICATIVE SOMBOR INDEX OF GRAPHS

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ABSTRACT. The concept of the Sombor index and the multiplicative version of the Sombor index of a graph were developed very recently. In this paper, we study the multiplicative version of the classical Sombor index and characterize the extremal graphs with respect to this graphical invariant over several classes of graphs.

1. Introduction

For molecular graphs, vertices represent the atoms of the compound, and edges correspond to chemical bonds. The topological indices of a molecular graph were developed by chemists in the process of studying the properties of chemical structures. These indices are useful to predict the physico-chemical properties in quantitative structure-property relationship and quantitative structure-activity relationship studies [41,42]. Let G be a graph with a set of vertices $V(G)$ and a set of edges $E(G)$. The degree of vertex v in G is denoted by $d_G(v)$. For two nonadjacent vertices u and v, $G+uv$ is the graph obtained by adding a new edge uv to G. If edge $uv \in E(G)$, then $G-uv$ is the graph obtained by deleting edge uv from G. The *girth* is the length of the shortest cycle contained in G. A edge uv is called a *cut edge* if $G-uv$ is disconnected. Denote by $N_G(u)$ the set that consists of all adjacent vertices of u. For vertices $u,v \in V(G)$, the *distance* $d(u,v)$ is defined as the length of the shortest path between u and v. Denote by $\mathscr{A}_{n,k}$ the class of all connected graphs of order n with k pendent vertices. Also, denote by $\mathscr{B}_{n,k}$ the class of graphs of order n with k cut edges. These classes of graphs were studied for Zagreb indices, the reduced second Zagreb indices [17,21], the augmented Zagreb index [4], the multiplicative sum Zagreb indices [23], the Randić index [40,45], and the Sombor index [22].

In 2021, a new vertex-degree-based graph invariant was introduced in [18], defined as

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

and named the *Sombor index*. This index was motivated by the geometric interpretation of the degree radius of an edge uv, which is the distance from the origin to the ordered pair $(d_G(u), d_G(v))$. Also, several variants of the Sombor index were considered in [18].

Although Sombor-type indices were introduced in 2021, dozens of articles regarding these have been published in scientific journals [1,5,7,12,14,35,37]. Chemical applications of the Sombor index

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were presented in [28, 30, 31, 36], and molecular graphs were studied in [2, 3, 6, 15]. The Sombor index has been studied for trees [8, 11, 19, 25, 39, 47], unicyclic and bicyclic graphs [7, 13], cacti [26], and graphs with integer values [14, 33]. Furthermore, bounds and extremal results related to the Sombor index and its variants can be found in [9, 10, 16, 20, 32, 34, 43, 44, 46, 47], and we suggest readers refer to a recent review [29].

The multiplicative Sombor index is defined as

$$\Pi_{SO} = \Pi_{SO}(G) = \prod_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2},$$

just as the multiplicative versions of other well-known topological indices.

Kulli [24] studied the multiplicative Sombor index of certain nanotubes, and we continue this research for certain classes of graphs. Liu [27] determined the extremal values of the multiplicative Sombor index of trees and unicyclic graphs by using some graph transformations.

The paper is organized as follows. In Section 2, we determine the extremal values of the multiplicative Sombor index over bipartite graphs with a given order. Also, we prove that a kite graph has a minimal multiplicative Sombor index in the class of graphs with a given order and clique number. In Section 3, unicyclic graphs are studied that have an extremal multiplicative Sombor index. In Section 4, we determine the graphs that have the maximum multiplicative Sombor index in $\mathscr{A}_{n,k}$ and $\mathscr{B}_{n,k}$.

2. Graphs with extremal multiplicative Sombor index

In this section, we determine the graphs with an extremal multiplicative Sombor index for some classes of graphs of order n. For this purpose, first we give the following lemmas, which are useful for characterizing graphs with an extremal multiplicative Sombor index.

Lemma 2.1. [27] *Let uv be an edge of a graph G such that $d_G(u) \geq 2$, $d_G(v) \geq 2$ and $N_G(u) \cap N_G(v) = \emptyset$. Let G' be the graph obtained from G by the contraction of uv onto u and adding a new pendent edge uv. Then $\Pi_{SO}(G) < \Pi_{SO}(G')$.*

Lemma 2.2. [27] *Let H be a connected graph and G be the graph obtained from H by attaching two paths P_1 and P_2 onto vertices u and v of H, respectively. Suppose that x is the neighbor of the vertex u on P_1 and y is the pendent vertex on P_2. Let $G' = G - ux + xy$. If $d_G(u) \geq 3$, then $\Pi_{SO}(G') < \Pi_{SO}(G)$.*

Denote by P_n, S_n, and K_n the path, the star and the complete graph of order n, respectively. Let $K_{p,q}$ be a complete bipartite graph of order n with two partite sets having p and q vertices, respectively.

Theorem 2.3. *Let G be a bipartite graph of order n. Then*

$$\Pi_{SO}(G) \leq \begin{cases} \left(\frac{n^2}{2}\right)^{\frac{n^2}{8}} & \text{if } n \text{ is even,} \\ \left(\frac{n^2+1}{2}\right)^{\frac{n^2-1}{8}} & \text{if } n \text{ is odd} \end{cases}$$

with equality if and only if G is isomorphic to $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

Proof. Let p and q be the number of vertices of parts in G, where $p+q=n$ and $p \geq q$. Then by the definition of Π_{SO}, one can easily obtain that $\Pi_{SO}(G)^2 \leq (p^2+q^2)^{pq}$ with equality if and only if G is isomorphic to $K_{p,q}$. Let us consider the following functions

$$f(x) = [x^2+(n-x)^2]^{x(n-x)}, \quad \left\lceil \frac{n}{2} \right\rceil \leq x \leq n-1$$

and

$$g(x) = \ln(2x^2-2nx+n^2) - \frac{2x(n-x)}{2x^2-2nx+n^2}, \quad \left\lceil \frac{n}{2} \right\rceil \leq x \leq n-1. \tag{1}$$

Then, we have

$$\begin{aligned} f'(x) &= f(x)\left[(n-2x)\ln(2x^2-2nx+n^2) + \frac{2(nx-x^2)(2x-n)}{2x^2-2nx+n^2}\right] \\ &= (n-2x)f(x)\left[\ln(2x^2-2nx+n^2) - \frac{2x(n-x)}{2x^2-2nx+n^2}\right] \end{aligned} \tag{2}$$

and

$$g'(x) = \frac{4x-2n}{2x^2-2nx+n^2} - \frac{2(n-2x)n^2}{(2x^2-2nx+n^2)^2} = \frac{4(2x-n)(x^2-nx+n^2)}{(2x^2-2nx+n^2)^2}.$$

On the other hand, since $2x-n \geq 0$, we have $g'(x) \geq 0$ which means that $g(x)$ is an increasing function. Thus, $g(x) \geq g\left(\lceil \frac{n}{2} \rceil\right) \geq 0$ for $\left\lceil \frac{n}{2} \right\rceil \leq x \leq n-1$ and from (1), we obtain

$$(n-2x)\ln(2x^2-2nx+n^2) \leq \frac{2x(n-x)(n-2x)}{2x^2-2nx+n^2} \tag{3}$$

as $2x-n \geq 0$. Hence, from (2) and (3), we get $f'(x) \leq 0$ for $\left\lceil \frac{n}{2} \right\rceil \leq x \leq n-1$. Therefore, $f(x)$ is a decreasing function for $\left\lceil \frac{n}{2} \right\rceil \leq x \leq n-1$ and one can easily see that

$$\Pi_{SO}(G)^2 \leq (p^2+q^2)^{pq} = (p^2+(n-p)^2)^{p(n-p)} \leq f\left(\left\lceil \frac{n}{2} \right\rceil\right) \leq \left(\left\lfloor \frac{n}{2} \right\rfloor^2 + \left\lceil \frac{n}{2} \right\rceil^2\right)^{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}$$

with equality if and only if G is isomorphic to $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$. □

The *kite graph* $Ki_{n,\omega}$ is the graph of order n obtained by identifying a pendent vertex of $P_{n-\omega+1}$ with a vertex of K_ω. In particular, $Ki_{n,n} \cong K_n$, and $Ki_{n,2} \cong P_n$.

Theorem 2.4. *Let G be a connected graph of order n with clique number ω. Then $\Pi_{SO}(G) \geq \Pi_{SO}(Ki_{n,\omega})$ with equality if and only if G is isomorphic to $Ki_{n,\omega}$.*

Proof. If $\omega = n$, then $G \cong K_n$ and hence the equality holds. Otherwise, $2 \leq \omega \leq n-1$. We consider the following three cases:

Case 1. $\omega = 2$. In this case the girth of G is greater than 3 or $G \cong T$, where T is any tree of order n. First we assume that $G \cong T$. Let Δ be the maximum degree in T. If $\Delta = 2$, then $T \cong P_n$ and hence

$\Pi_{SO}(G) = \Pi_{SO}(T) = \Pi_{SO}(P_n) = \Pi_{SO}(Ki_{n,2})$, the equality holds. Otherwise, $\Delta \geq 3$. Using Lemma 2.2 several times (if exists) on tree T, we obtain

$$\Pi_{SO}(G) = \Pi_{SO}(T) > \cdots > \Pi_{SO}(Ki_{n,2}) = \Pi_{SO}(P_n),$$

the inequality strictly holds.

Next we assume that the girth of G is greater than 3. Then, by deleting the edges on the cycles of G, we arrive at a tree. Similarly, as above, we prove that $\Pi_{SO}(G) > \Pi_{SO}(P_n)$. The inequality strictly holds.

Case 2. $3 \leq \omega \leq n-2$. Suppose that $\Pi_{SO}(G)$ is the minimum in the class of graphs of order n with clique number ω and G is not isomorphic to $Ki_{n,\omega}$. By the definition of Π_{SO}, we have $\Pi_{SO}(G-e) < \Pi_{SO}(G)$, where e is any edge in G. Using this, we conclude that G is isomorphic to a graph such that $G - E(K_\omega)$ is a forest of order n. Since $G \not\cong Ki_{n,\omega}$, then there are at least two pendent paths P_1 and P_2 with origins u and v, respectively. Let x be the neighbor of u on P_1 and y be the pendent vertex on P_2. Then, by Lemma 2.2, we get $\Pi_{SO}(G-ux+xy) < \Pi_{SO}(G)$, which is a contradiction.

Case 3. $\omega = n-1$. Let δ be the minimum degree in G. Since G is connected, $\delta \geq 1$. If $\delta = 1$, then $G \cong Ki_{n,n-1}$ as $\omega = n-1$. Otherwise, $\delta \geq 2$. We can assume that $d_G(v_1) \geq d_G(v_2) \geq \cdots \geq d_G(v_n)$, where $d_G(v_i)$ is the degree of the vertex v_i. Let $H \cong Ki_{n,n-1}$. Then $d_H(v_1) = n-1$, $d_H(v_i) = n-2\,(2 \leq i \leq n-1)$, $d_H(v_n) = 1$. Again since G is connected and $\omega = n-1$ with $\delta \geq 2$, we have that H is a strictly subgraph of G with $V(G) = V(H)$ and $d_G(u) \geq d_H(u)$ for all $u \in V(G)$. Thus we have $d_G(v_1) = d_G(v_2) = n-1$, $d_G(v_i) \geq n-2\,(3 \leq i \leq n-1)$ and $d_G(v_n) = \delta \geq 2$. From the above, one can easily see that

$$\Pi_{SO}(Ki_{n,n-1}) = \Pi_{SO}(H) = \prod_{uv\in E(H)} \sqrt{d_H(u)^2 + d_H(v)^2} < \prod_{uv\in E(H)} \sqrt{d_G(u)^2 + d_G(v)^2}$$
$$< \prod_{uv\in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} = \Pi_{SO}(G).$$

The inequality strictly holds. This completes the proof of the theorem. □

3. Unicyclic graphs with extremal multiplicative Sombor index

Denote by $\mathscr{U}_{n,g}$ the class of all unicyclic graphs of order n with girth g. Let $C_{n,g}$ be the unicyclic graph obtained by identifying a pendent vertex of P_{n-g+1} with a vertex of the cycle of order g. Also, let C_n^g be the unicyclic graph obtained by attaching $n-g$ pendent edges to a vertex of the cycle with length g. Liu [27] proved that $C_{n,g}$ has the minimum value in $\mathscr{U}_{n,g}$. Now, we prove that C_n^g has the maximum value in $\mathscr{U}_{n,g}$.

Theorem 3.1. *Let n and g be positive integers with $3 \leq g \leq n-2$. If $G \in \mathscr{U}_{n,g}$, then*

$$5^{\frac{1}{2}} \cdot 8^{\frac{n-4}{2}} 13^{\frac{3}{2}} \leq \Pi_{SO}(G) \leq 8^{\frac{g-2}{2}}[(n-g+2)^2+4][(n-g+2)^2+1]^{\frac{n-g}{2}}$$

with left-hand side of equality if and only if G is isomorphic to $C_{n,g}$, and with right-hand side of equality if and only if G is isomorphic to C_n^g.

Proof. **Lower Bound:** Suppose that G has a minimum Π_{SO}-value in $\mathscr{U}_{n,g}$ and it is not isomorphic to $C_{n,g}$. Then there are two pendent paths P_1 and P_2 with origins u and v, respectively. Let x be the neighbor of u on P_1 and y be the pendent vertex on P_2. Then, by Lemma 2.2, we get $\Pi_{SO}(G') < \Pi_{SO}(G)$, where $G' = G - ux + xy$. Clearly, $G' \in \mathscr{U}_{n,g}$ and a contradiction. Hence, G is isomorphic to $C_{n,g}$ and $\Pi_{SO}(C_{n,g}) = 5^{\frac{1}{2}} \cdot 8^{\frac{n-4}{2}} 13^{\frac{3}{2}}$.

Upper Bound: Now suppose that G has a maximum Π_{SO}-value in $\mathscr{U}_{n,g}$ and it is not isomorphic to C_n^g. Let C_g be the cycle of G, and $u_1, u_2, \ldots, u_g$ be the vertices on the cycle. By Lemma 2.1, one can easily conclude that all cut edges of G are pendent, and it follows that each cut edge of G is incident to a vertex of C_g. Let n_i denote the number of pendent edges incident to u_i. Then $n_i = d_G(u_i) - 2$ for $1 \le i \le g$. Without loss of generality, we assume that $n_1 = \max\{n_j \mid 1 \le j \le g\}$, $n_k = \min\{n_j \mid n_j \ge 1,\ 1 \le j \le g\}$. Let now $x_1, x_2, \ldots, x_{n_k}$ be the pendent vertices that are adjacent to u_k. Since $G \ncong C_n^g$, u_k is different from u_1. Then one can construct a new graph $G' = G - \{u_k x_1, \ldots, u_k x_{n_k}\} + \{u_1 x_1, \ldots, u_1 x_{n_k}\}$. We distinguish the following two cases.

Case 1. $d(u_1, u_k) \ge 2$. By the definition of Π_{SO}, we obtain

$$\frac{\Pi_{SO}(G')^2}{\Pi_{SO}(G)^2} = \frac{(n_1+n_k+2)^2+(n_2+2)^2}{(n_1+2)^2+(n_2+2)^2} \cdot \frac{(n_1+n_k+2)^2+(n_g+2)^2}{(n_1+2)^2+(n_g+2)^2}$$

$$\times \frac{2^2+(n_{k-1}+2)^2}{(n_k+2)^2+(n_{k-1}+2)^2} \cdot \frac{2^2+(n_{k+1}+2)^2}{(n_k+2)^2+(n_{k+1}+2)^2} \times \frac{\left[(n_1+n_k+2)^2+1\right]^{n_1+n_k}}{\left[(n_1+2)^2+1\right]^{n_1}\left[(n_k+2)^2+1\right]^{n_k}}$$

$$> \left[\frac{8}{(n_k+2)^2+4}\right]^2 \cdot \left[1+\frac{n_k(2n_1+n_k+4)}{(n_1+2)^2+1}\right]^{n_1}\left[1+\frac{n_1(n_1+2n_k+4)}{(n_k+2)^2+1}\right]^{n_k}. \tag{4}$$

First we can assume that $n_k = 1$. Then by (4) and Bernoulli's inequality,

$$\begin{aligned}
\frac{\Pi_{SO}(G')^2}{\Pi_{SO}(G)^2} &> \left(\frac{8}{13}\right)^2 \cdot \left[1+\frac{2n_1+5}{(n_1+2)^2+1}\right]^{n_1}\left[1+\frac{n_1(n_1+6)}{10}\right] \\
&\ge \frac{64}{169} \cdot \frac{(n_1+2)^2+1+n_1(2n_1+5)}{(n_1+2)^2+1} \cdot \frac{n_1^2+6n_1+10}{10} \\
&= \frac{192n_1^4+1728n_1^3+5696n_1^2+7680n_1+3200}{1690n_1^2+6760n_1+8450} \\
&\ge \frac{1728n_1^3+7680n_1+5696n_1^2+3200}{1690n_1^2+6760n_1+8450} > 1. \qquad (5)
\end{aligned}$$

Next we can assume that $n_k \ge 2$. Then $n_1 \ge n_k \ge 2$ and

$$(2n_1+n_k+4)^2 > 2\left[(n_1+2)^2+1\right] \text{ and } (2n_k+n_1+4)^2 > 2\left[(n_k+2)^2+1\right]. \tag{6}$$

On the other hand, by Taylor's theorem, we have $(1+x)^\alpha \geq 1+\alpha x+\frac{\alpha(\alpha-1)}{2}x^2$ for $\alpha \geq 2$ and $x>0$. Therefore, by using inequality (6) in (4), we obtain

$$\begin{aligned}
\frac{\Pi_{SO}(G')^2}{\Pi_{SO}(G)^2} &> \left[\frac{8}{(n_k+2)^2+4}\right]^2 \cdot \left(1+\frac{n_1 n_k(2n_1+n_k+4)}{(n_1+2)^2+1}+\frac{n_1(n_1-1)n_k^2(2n_1+n_k+4)^2}{2\left[(n_1+2)^2+1\right]^2}\right) \\
&\quad \times \left(1+\frac{n_1 n_k(2n_k+n_1+4)}{(n_k+2)^2+1}+\frac{n_k(n_k-1)n_1^2(2n_k+n_1+4)^2}{2\left[(n_k+2)^2+1\right]^2}\right) \\
&\geq \left[\frac{8}{(n_k+2)^2+4}\right]^2 \cdot \left[1+\frac{n_1 n_k^2+2n_1 n_k(n_1+2)}{(n_1+2)^2+1}+\frac{n_1(n_1-1)n_k^2}{(n_1+2)^2+1}\right] \\
&\quad \times \left[1+\frac{n_1^2 n_k+2n_1 n_k(n_k+2)}{(n_1+2)^2+1}+\frac{n_k(n_k-1)n_1^2}{(n_1+2)^2+1}\right] \\
&\geq \left[\frac{8}{(n_k+2)^2+4}\right]^2 \cdot \left[1+\frac{n_1^2 n_k^2+2n_1 n_k(n_k+2)}{(n_1+2)^2+1}\right]^2 \\
&= \left[\frac{8}{(n_k+2)^2+4}\right]^2 \cdot \left[\frac{(n_1+2)^2+1+n_1^2 n_k^2+2n_1 n_k(n_k+2)}{(n_1+2)^2+1}\right]^2 \\
&= \left(\frac{n_1^2 n_k^2+7n_1^2 n_k^2+4n_1 n_k^2+12n_1 n_k^2+8n_1^2+16n_1 n_k+32n_1+16n_1 n_k+40}{n_1^2 n_k^2+4n_1^2 n_k+4n_1 n_k^2+5n_k^2+8n_1^2+16n_1 n_k+32n_1+20n_k+40}\right)^2 > 1
\end{aligned}$$

as $7n_1^2 n_k^2 > 4n_1^2 n_k$, $12n_1 n_k^2 > 5n_k^2$ and $16n_1 n_k > 20n_k$.

Case 2. $d(u_1,u_k)=1$. Then $k=2$ or $k=g$. Without loss of generality, we can assume that $k=2$. By the definition of Π_{SO}, we obtain

$$\begin{aligned}
\frac{\Pi_{SO}(G')^2}{\Pi_{SO}(G)^2} &= \frac{(n_1+n_2+2)^2+2^2}{(n_1+2)^2+(n_2+2)^2} \cdot \frac{(n_1+n_2+2)^2+(n_g+2)^2}{(n_1+2)^2+(n_g+2)^2} \cdot \frac{2^2+(n_3+2)^2}{(n_2+2)^2+(n_3+2)^2} \\
&\quad \times \frac{\left[(n_1+n_2+2)^2+1\right]^{n_1+n_2}}{\left[(n_1+2)^2+1\right]^{n_1}\left[(n_2+2)^2+1\right]^{n_2}} \\
&> \frac{8}{(n_2+2)^2+4} \cdot \left[1+\frac{n_2(2n_1+n_2+4)}{(n_1+2)^2+1}\right]^{n_1}\left[1+\frac{n_1(n_1+2n_2+4)}{(n_2+2)^2+1}\right]^{n_2}. \qquad (7)
\end{aligned}$$

First we can assume that $n_2=1$. Then by (7) and $n_1 \geq 1$,

$$\begin{aligned}
\frac{\Pi_{SO}(G')^2}{\Pi_{SO}(G)^2} &> \frac{8}{13} \cdot \left[1+\frac{2n_1+5}{(n_1+2)^2+1}\right]^{n_1}\left[1+\frac{n_1(n_1+6)}{10}\right] \\
&> \frac{8}{13} \cdot 1 \cdot \left[1+\frac{7}{10}\right] > 1.
\end{aligned}$$

Next we can assume that $n_2 \geq 2$. Then $n_1 \geq n_2 \geq 2$ and $(2n_1+n_2+4)^2 > 2\left[(n_1+2)^2+1\right]$. Therefore, from (7), using similar method in **Case 1**, we obtain

$$\begin{aligned}
\frac{\Pi_{SO}(G')^2}{\Pi_{SO}(G)^2} &> \frac{8}{(n_2+2)^2+4}\cdot\left[1+\frac{n_2(2n_1+n_2+4)}{(n_1+2)^2+1}\right]^{n_1}\\
&> \frac{8}{(n_2+2)^2+4}\cdot\left(1+\frac{n_1n_2(2n_1+n_2+4)}{(n_1+2)^2+1}+\frac{n_1(n_1-1)n_2^2(2n_1+n_2+4)^2}{2\left[(n_1+2)^2+1\right]^2}\right)\\
&\geq \frac{8}{(n_2+2)^2+4}\cdot\left[1+\frac{n_1n_2^2+2n_1n_2(n_1+2)}{(n_1+2)^2+1}+\frac{n_1(n_1-1)n_2^2}{(n_1+2)^2+1}\right]\\
&= \frac{8}{(n_2+2)^2+4}\cdot\left[1+\frac{n_1^2n_2^2+2n_1n_2(n_1+2)}{(n_1+2)^2+1}\right]\\
&\geq \frac{8}{(n_2+2)^2+4}\cdot\frac{(n_1+2)^2+1+n_1^2n_2^2+2n_1n_2(n_2+2)}{(n_1+2)^2+1}\\
&= \frac{n_1^2n_2^2+7n_1^2n_2^2+4n_1n_2^2+12n_1n_2^2+8n_1^2+16n_1n_2+32n_1+16n_1n_2+40}{n_1^2n_2^2+4n_1^2n_2+4n_1n_2^2+5n_2^2+8n_1^2+16n_1n_2+32n_1+20n_2+40} > 1
\end{aligned}$$

as $7n_1^2n_2^2 > 4n_1^2n_2$, $12n_1n_2^2 > 5n_2^2$ and $16n_1n_2 > 20n_2$.

In the above two cases, we have $\Pi_{SO}(G') > \Pi_{SO}(G)$ and it contradicts our assumption that G has the maximum Π_{SO}-value in $\mathscr{U}_{n,g}$. □

4. Extremal graphs in $\mathscr{A}_{n,k}$ and $\mathscr{B}_{n,k}$ with respect to the multiplicative Sombor index

In this section, we determine extremal graphs with respect to the multiplicative Sombor index for the classes of graphs of order n with k pendent vertices and of order n with k cut edges. Denote by $\mathscr{A}(n,k)$ the class of all graphs of order n with k pendent vertices in which the removal of all pendent vertices and their incident edges result in a complete graph of order $n-k$.

Lemma 4.1. *Let n and k be integers with $0 \leq k < n-1$. If $\Pi_{SO}(G)$ is maximum in $\mathscr{A}_{n,k}$, then $G \in \mathscr{A}(n,k)$.*

Proof. Assume to the contrary that $G \notin \mathscr{A}(n,k)$. Then there exist two non-adjacent vertices u and v in G whose degrees are greater than one. Consider the graph $G' = G+uv$. Then $G' \in \mathscr{A}_{n,k}$ and $\Pi_{SO}(G') > \Pi_{SO}(G)$, a contradiction as $\Pi_{SO}(G)$ is maximum in $\mathscr{A}_{n,k}$. □

Theorem 4.2. *Let n and k be integers with $0 \leq k < n-1$. If $\Pi_{SO}(G)$ is maximum in $\mathscr{A}_{n,k}$, then G is isomorphic to the graph obtained by attaching k pendent edges to a vertex of the complete graph of order $n-k$.*

Proof. Assume to the contrary that G is not isomorphic to the graph obtained by attaching k pendent edges to a vertex of the complete graph of order $n-k$. Since $\Pi_{SO}(G)$ is maximum in $\mathscr{A}_{n,k}$, we have $G \in \mathscr{A}(n,k)$ by Lemma 4.1. Let n_i denote the number of pendent edges incident to vertex v_i of the clique of G $(1 \le i \le n-k)$. Then $n_1 + n_2 + \cdots + n_{n-k} = k$. Without loss of generality, we assume that $n_1 = \max\{n_i \mid 1 \le i \le n-k\}$. Then there exists a pendent vertex x adjacent to a vertex v_t, where v_t is different from v_1. We now construct a new $G' = G - xv_t + xv_1$. Then $d_{G'}(v_1) = d_G(v_1) + 1$, $d_G(v_t) = d_{G'}(v_t) - 1$ and $d_{G'}(v) = d_G(v)$ for $v \in V(G) \setminus \{v_1, v_t\}$. For convenience, denote $p = n-k-1$. Then

$$\begin{aligned}
\frac{\Pi_{SO}(G')^2}{\Pi_{SO}(G)^2} &= \frac{(n_1+1+p)^2+(n_t-1+p)^2}{(n_1+p)^2+(n_t+p)^2} \cdot \frac{[(n_1+1+p)^2+1]^{n_1+1}}{[(n_1+p)^2+1]^{n_1}} \cdot \frac{[(n_t-1+p)^2+1]^{n_t-1}}{[(n_t+p)^2+1]^{n_t}} \\
&\quad \times \prod_{i=2,\, i\neq t}^{p+1} \frac{[(n_1+1+p)^2+(n_i+p)^2][(n_t-1+p)^2+(n_i+p)^2]}{[(n_1+p)^2+(n_i+p)^2][(n_t+p)^2+(n_i+p)^2]} \\
&> \frac{[(n_1+1+p)^2+1]^{n_1+1}}{[(n_1+p)^2+1]^{n_1}} \cdot \frac{[(n_t-1+p)^2+1]^{n_t-1}}{[(n_t+p)^2+1]^{n_t}} \\
&\quad \times \prod_{i=2,\, i\neq t}^{p+1} \frac{[(n_1+1+p)^2+(n_i+p)^2][(n_t-1+p)^2+(n_i+p)^2]}{[(n_1+p)^2+(n_i+p)^2][(n_t+p)^2+(n_i+p)^2]}. \qquad (8)
\end{aligned}$$

Without loss of generality, we can assume that

$$\begin{aligned}
&\frac{[(n_1+1+p)^2+(n_j+p)^2][(n_t-1+p)^2+(n_j+p)^2]}{[(n_1+p)^2+(n_j+p)^2][(n_t+p)^2+(n_j+p)^2]} \\
&\le \frac{[(n_1+1+p)^2+(n_i+p)^2][(n_t-1+p)^2+(n_i+p)^2]}{[(n_1+p)^2+(n_i+p)^2][(n_t+p)^2+(n_i+p)^2]}, \qquad (9)
\end{aligned}$$

for $i = 2, \ldots, p+1, i \neq t$. Then, from (8) and (9), we get

$$\begin{aligned}
\frac{\Pi_{SO}(G')^2}{\Pi_{SO}(G)^2} &> \frac{[(n_1+1+p)^2+1]^{n_1+1}}{[(n_1+p)^2+1]^{n_1}} \cdot \frac{[(n_t-1+p)^2+1]^{n_t-1}}{[(n_t+p)^2+1]^{n_t}} \\
&\quad \times \left(\frac{[(n_1+1+p)^2+(n_j+p)^2][(n_t-1+p)^2+(n_j+p)^2]}{[(n_1+p)^2+(n_j+p)^2][(n_t+p)^2+(n_j+p)^2]} \right)^{p-1}. \qquad (10)
\end{aligned}$$

Now we consider the following functions

$$f(x) = [(x+p)^2+(n_j+p)^2]^{p-1} \cdot [(x+p)^2+1]^x, \; x \ge n_t, \qquad (11)$$

and

$$h(x) = \ln f(x) + \ln f(n_t-1) - \ln f(x-1) - \ln f(n_t), \; x \ge n_t. \qquad (12)$$

Therefore, (10) can be rewritten as

$$\frac{\Pi_{SO}(G')^2}{\Pi_{SO}(G)^2} > \frac{f(n_1+1) f(n_t-1)}{f(n_1) f(n_t)}. \qquad (13)$$

From (11), it follows that

$$\ln f(x) = (p-1)\ln[(x+p)^2+(n_j+p)^2] + x\ln[(x+p)^2+1].$$

Thus,

$$[\ln f(x)]' = \frac{2(p-1)(x+p)}{(x+p)^2+(n_j+p)^2} + \ln[(x+p)^2+1] + \frac{2x(x+p)}{(x+p)^2+1}.$$

and

$$\begin{aligned}
[\ln f(x)]'' &= 2(p-1)\frac{(x+p)^2+(n_j+p)^2-2(x+p)^2}{[(x+p)^2+(n_j+p)^2]^2} + \frac{2(x+p)}{(x+p)^2+1} \\
&\quad + \frac{(2p+4x)[(x+p)^2+1]-2(p+x)(2px+2x^2)}{[(p+x)^2+1]^2} \\
&= \frac{(2p-2)[(n_j+p)^2-(x+p)^2]}{[(x+p)^2+(n_j+p)^2]^2} + \frac{2(x+p)[(x+p)^2+1]}{[(x+p)^2+1]^2} \\
&\quad + \frac{(2p+4x)(p^2+2px+x^2+1)-(2px+2x^2)(2p+2x)}{[(x+p)^2+1]^2} \\
&= \frac{4p^3+4p+6x+2x^3+8px^2+10p^2x}{[(x+p)^2+1]^2} - (2p-2)\frac{(x+p)^2-(n_j+p)^2}{[(x+p)^2+(n_j+p)^2]^2}. \qquad (14)
\end{aligned}$$

On the other hand, one can easily see that

$$(x+p)^2+(n_j+p)^2 > (x+p)^2+1,\ (2p-2)(x+p)^2 < 4p^3+4p+6x+2x^3+8px^2+10p^2x. \qquad (15)$$

Combining (14) and (15), we get that $[\ln f(x)]'' > 0$. Hence $[\ln f(x)]'$ is a strictly increasing function when $x \geq n_t$ and it follows that $[\ln f(x)]' > [\ln f(x-1)]'$. From this, $h'(x) = [\ln f(x) + \ln f(n_t-1) - \ln f(x-1) - \ln f(n_t)]' > 0$ for $x \geq n_t$. Thus $h(x)$ is an increasing function when $x \geq n_t$. From (12), it follows that $h(x) \geq h(n_t) = 0$. Thus, we have $\ln f(x) + \ln f(n_t-1) \geq \ln f(x-1) + \ln f(n_t)$. By setting $x = n_1+1$ in the above, we get

$$f(n_1+1)f(n_t-1) \geq f(n_1)f(n_t). \qquad (16)$$

By combining (13) and (16), we obtain $\Pi_{SO}(G') > \Pi_{SO}(G)$, which contradicts to G has the maximum Π_{SO}-value in $\mathscr{A}(n,k)$. This completes the proof of the theorem. □

The same argument as in the proof of the above theorem yields the following result.

Theorem 4.3. *Let n and k be integers with $0 \leq k < n-1$. If $\Pi_{SO}(G)$ is maximum in $\mathscr{B}_{n,k}$, then G is isomorphic to the graph obtained by attaching k pendent edges to a vertex of the complete graph of order $n-k$.*

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References

[1] A. Aashtab, S. Akbari, S. Madadinia, M. Noei, F. Salehi, *On the graphs with minimum Sombor index*, MATCH Commun. Math. Comput. Chem. **88** (2022) 553–559.

[2] S. Alikhani, N. Ghanbari, *Sombor index of polymers*, MATCH Commun. Math. Comput. Chem. **86** (2021) 715–728.

[3] A. Alsinai, B. Basavangoud, M. Sayyed, M. R. Farahani, *Sombor index of some nanostructures*, Journal of Prime Research in Math. **17** (2021) 123–133.

[4] C. Chen, M. Liu X. Gu, K.C. Das, *Extremal augmented Zagreb index of trees with given numbers of vertices and leaves*, Discrete Math. **345** (2022) 112753.

[5] H. Chen, W. Li, J. Wang, *Extremal values on the Sombor index of trees*, MATCH Commun. Math. Comput. Chem. **87** (2022) 23–49.

[6] R. Cruz, I. Gutman, J. Rada, *Sombor index of chemical graphs*, Appl. Math. Comput. **399** (2021) 126018.

[7] R. Cruz, J. Rada, *Extremal values of the Sombor index in unicyclic and bicyclic graphs*, J. Math. Chem. **59** (2021) 1098–1116.

[8] R. Cruz, J. Rada, J.M. Sigarreta, *Sombor index of trees with at most three branch vertices*, Appl. Math. Comput. **409** (2021) 126414.

[9] K.C. Das, A.S. Çevik, I.N. Cangul, Y. Shang, *On Sombor index*, Symmetry **13** (2021) 140.

[10] K.C. Das, A. Ghalavand, A.R. Ashraf, *On a conjecture about the Sombor index of graphs*, Symmetry **13** (2021) 1830.

[11] K.C. Das, I. Gutman, *On Sombor index of trees*, Appl. Math. Comput. **412** (2022) 126575.

[12] K.C. Das, Y. Shang, *Some extremal graphs with respect to Sombor index*, Mathematics **9** (2021) 1202.

[13] S. Dorjsembe, B. Horoldagva, *Reduced Sombor index of bicyclic graphs*, Asian-Europ. J. Math. **15** (2022) 2250128. https://doi.org/10.1142/S1793557122501285

[14] T. Došlić, T. Réti, A. Ali, *On the structure of graphs with integer Sombor indices*, Discr. Math. Lett. **7** (2021) 1–4.

[15] X. Fang, L. You, H. Liu, *The expected values of Sombor indices in random hexagonal chains, phenylene chains and Sombor indices of some chemical graphs*, Int. J. Quantum Chem. **121** (2021) e26740.

[16] S. Filipovski, *Relations between Sombor index and some degree-based topological indices*, Iran. J. Math. Chem. **12** (2021) 19–26.

[17] F. Gao, K. Xu, On the reduced second Zagreb index of graphs, Rocky Mountain J. Math. **50** (3) (2020) 975–988.

[18] I. Gutman, *Geometric approach to degree-based topological indices*: *Sombor indices*, MATCH Commun. Math. Comput. Chem. **86** (2021) 11–16.

[19] I. Gutman, V.R. Kulli, I. Redžepović, *Sombor index of Kragujevac trees*, Sci. Publ. Univ. Novi Pazar Ser. A **13** (2021) 61–70.

[20] I. Gutman, J. Monsalve, J. Rada, *A relation between a vertex-degree-based topological index and its energy*, Linear Algebra Appl. **636** (2022) 134–142.

[21] B. Horoldagva, T. Selenge, L. Buyantogtokh, S. Dorjsembe, Upper bounds for the reduced second Zagreb index of graphs, Transactions on Comb. **10** (2021) 137–148.

[22] B. Horoldagva, C. Xu, *On Sombor index of graphs*, MATCH Commun. Math. Comput. Chem. **86** (2021) 703–713.

[23] B. Horoldagva, C. Xu, L. Buyantogtokh, S. Dorjsembe, *Extremal graphs with respect to the multiplicative sum Zagreb index*, MATCH Commun. Math. Comput. Chem. **84** (2020) 773–786.

[24] V.R. Kulli, *Multiplicative Sombor indices of certain nanotubes*, Int. J. Math. Arch. **12** (2021) 1–5.

[25] S. Li, Z. Wang, M. Zhang, *On the extremal Sombor index of trees with a given diameter*, Appl. Math. Comput. **416** (2022) 126731.

[26] H. Liu, *Extremal cacti with respect to Sombor index*, Iran. J. Math. Chem. **12** (2021) 197–208.

[27] H. Liu, *Multiplicative Sombor index of graphs*, Discrete Math. Lett. **9** (2022) 80–85.

[28] H. Liu, H. Chen, Q. Xiao, X. Fang, Z. Tang, *More on Sombor indices of chemical graphs and their applications to the boiling point of benzenoid hydrocarbons*, Int. J. Quantum Chem. **121** (2021) e26689.

[29] H. Liu, I. Gutman, L. You, Y. Huang, *Sombor index*: *review of extremal results and bounds*, Journal of Math. Chem. **60** (2022) 771–798.

[30] H. Liu, L. You, Y. Huang, *Ordering chemical graphs by Sombor indices and its applications*, MATCH Commun. Math. Comput. Chem. **87** (2022) 5–22.

[31] H. Liu, L. You, Z. Tang, J. B. Liu, *On the reduced Sombor index and its applications*, MATCH Commun. Math. Comput. Chem. **86** (2021) 729–753.

[32] I. Milovanović, E. Milovanović, A. Ali, M. Matejić, *Some results on the Sombor indices of graphs*, Contrib. Math. **3** (2021) 59–67.
[33] M.R. Oboudi, *Non-semiregular bipartite graphs with integer Sombor index*, Discrete Math. Lett. **8** (2022) 38–40.
[34] C. Phanjoubam, S.M. Mawiong, *On Sombor index and some topological indices*, Iran. J. Math. Chem. **12** (2021) 209–215.
[35] J. Rada, J.M. Rodriguez, J.M. Sigarreta, *General properties on Sombor indices*, Discrete Appl. Math. **299** (2021) 87–97.
[36] I. Redžepović, *Chemical applicability of Sombor indices*, J. Serb. Chem. Soc. **86** (2021) 445–457.
[37] T. Réti, T. Došlić, A. Ali, *On the Sombor index of graphs*, Contrib. Math. **3** (2021) 11–18.
[38] Ts. Selenge, B. Horoldagva, *Extremal Kragujevac trees with respect to Sombor indices*, Communications in Combinatorics and Optimization (2023) doi:10.22049/CCO.2023.28058.1430
[39] X. Sun, J. Du, *On Sombor index of trees with fixed domination number*, Appl. Math. Comput. **421** (2022) 126946.
[40] E. Swartz, T. Vetrík, *Survey on the general Randić index: extremal results and bounds*, Rocky Mountain J. Math. **52** (4) (2022) 1177–1203.
[41] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH: Weiheim, Germany, (2000).
[42] N. Trinajstić, *Chemistry Graph Theory*, CRC Press: Boca Raton, Florida, USA, (1983).
[43] A. Ülker, A. Gürsoy, *The energy and Sombor index of graphs*, MATCH Commun. Math. Comput. Chem. **87** (2022) 51–58.
[44] Z. Wang, Y. Mao, Y. Li, B. Furtula, *On relations between Sombor and other degree-based indices*, J. Appl. Math. Comput. **68** (2022) 1–17.
[45] G. Yu, L. Feng, Randić index and eigenvalues of graphs, Rocky Mountain J. Math. **40** (2) (2010) 713–721.
[46] W. Zhang, L. You, H. Liu, Y. Huang, *The expected values and variances for Sombor indices in a general random chain*, Appl. Math. Comput. **411** (2021) 126521.
[47] T. Zhou, Z. Lin, L. Miao, *The Sombor index of trees and unicyclic graphs with given maximum degree*, Discrete Math. Lett. **7** (2021) 24–29.

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