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On the product of Sombor and modified Sombor indices

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Abstract: The Sombor index (SO) and the modified Sombor index (${}^{m}SO$) are two closely related vertex-degree-based graph invariants. Both were introduced in the 2020s, and have already found a variety of chemical, physicochemical, and network-theoretical applications. In this paper, we examine the product $SO \cdot {}^{m}SO$ and determine its main properties. It is found that the structure-dependence of this product is fully different from that of either SO or ${}^{m}SO$. Lower and upper bounds for $SO \cdot {}^{m}SO$ are established and the extremal graphs are characterized. For connected graphs, the minimum value of the product $SO \cdot {}^{m}SO$ is the square of the number of edges. In the case of trees, the maximum value pertains to a special type of eclipsed sun graph, trees with a single branching point.

Keywords: Sombor index; modified Sombor index; topological index; degree (of vertex).

MSC: 05C07, 05C09.

1. Introduction

In this paper, we are concerned with simple graphs. In order to avoid unnecessary complications, the graphs considered will be assumed to be connected. Let G be such a graph with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$, with $|\mathbf{V}(G)| = n$ vertices and $|\mathbf{E}(G)| = m$ edges. By $e = uv \in \mathbf{E}(G)$ we denote the edge of G, connecting the vertices u and v. The degree of the vertex u (= the number of first neighbors of u) will be denoted by $d(u)$. For other graph-theoretical notions, the readers are referred to [1].

In contemporary discrete mathematics and mathematical chemistry, a class of graph invariants of the form

$$TI = TI(G) = \sum_{uv \in \mathbf{E}(G)} F\big(d(u), d(v)\big)$$

attracted much attention and is studied in detail [2–4]. Here F is a suitably chosen function with properties $F(x,y) = F(y,x)$ and $F(x,y) \geq 0$. These invariants are usually referred to as "vertex-degree-based topological indices", or shorter: VDB indices. Nowadays, several dozens of VDB indices are being examined in the literature, and their number is increasing.

A few years ago, based on geometric considerations, a new vertex-degree-based graph invariant was introduced [5–7], named Sombor index, defined as

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

where, of course, $d(u)^2$ denotes the square of the degree of the vertex u. In a short time, this index gained much popularity, and its applicability in chemistry and network science was soon recognized. The mathematical properties [6,8–18] and the various applications [19–25] of the Sombor index have been studied in detail.

A short time after the invention of the Sombor index, its modified version

$${}^{m}SO = {}^{m}SO(G) = \sum_{uv \in \mathbf{E}(G)} \frac{1}{\sqrt{d(u)^2 + d(v)^2}}$$

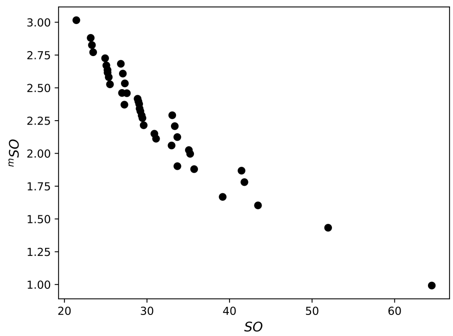

Figure 1. Correlation between Sombor and modified Sombor indices for the 47 nine-vertex trees.

was put forward [26], and studied in a few consecutive papers [27–29].

The Sombor and modified Sombor indices have a number of analogous (opposite) properties. For instance,

$$SO(G+e) > SO(G) \quad ; \quad {}^mSO(G+e) < {}^mSO(G)$$

where $G+e$ is the graph obtained by inserting a new edge to G;

$$SO(G) \leq SO(K_n) \quad ; \quad {}^mSO(G) \geq {}^mSO(K_n)$$

where K_n is the complete graph and where the equalities hold if and only if $G \cong K_n$;

$$SO(P_n) < SO(T_n) < SO(S_n) \quad ; \quad {}^mSO(P_n) > {}^mSO(T_n) > {}^mSO(S_n)$$

where P_n and S_n are the n-vertex path and star, respectively, and T_n is any n-vertex tree different from P_n and S_n.

The close correlation between SO and ${}^mSO$ is seen in the example depicted in Figure 1.

Bearing in mind the close analogy between Sombor and modified Sombor indices, we got interested in their product,

$$\pi SO = \pi SO(G) = SO(G) \cdot {}^mSO(G)$$

i.e.,

$$\pi SO = \pi SO(G) = \left(\sum_{uv \in \mathbf{E}(G)} \sqrt{d(u)^2 + d(v)^2} \right) \left(\sum_{uv \in \mathbf{E}(G)} \frac{1}{\sqrt{d(u)^2 + d(v)^2}} \right) \tag{1}$$

which we will refer to as the π-Sombor index.

Interestingly, the π-Sombor and the Sombor indices are completely uncorrelated, as shown by the example depicted in Figure 2.

In what follows we establish a few basic properties of πSO. First, however, we prove a pair of more general results.

2. Two general properties of product-topological indices

As before, G is a connected simple graph possessing n vertices and m edges.

Theorem 1. *Let $f(u)$ be any quantity, defined for a vertex $u \in \mathbf{V}(G)$, such that $f(u) > 0$ for all $u \in \mathbf{V}(G)$. Then,*

$$\left(\sum_{u \in \mathbf{V}(G)} f(u) \right) \left(\sum_{u \in \mathbf{V}(G)} \frac{1}{f(u)} \right) \geq n^2 . \tag{2}$$

Equality holds if and only if $f(u)$ are mutually equal for all $u \in \mathbf{V}(G)$.

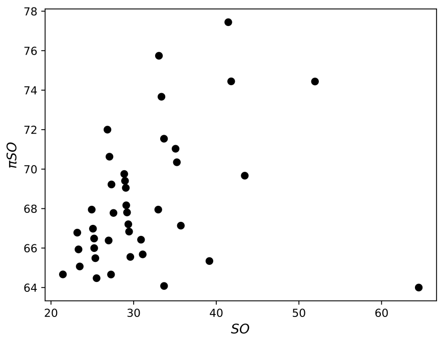

Figure 2. The absence of any correlation between the Sombor and π-Sombor indices, in the case of 9-vertex trees.

Theorem 2. *Let $g(e)$ be any quantity, defined for an edge $e \in \mathbf{E}(G)$, such that $g(e) > 0$ for all $e \in \mathbf{E}(G)$. Then,*

$$\left(\sum_{e\in\mathbf{E}(G)} g(e)\right)\left(\sum_{e\in\mathbf{E}(G)} \frac{1}{g(e)}\right) \geq m^2\,. \tag{3}$$

Equality holds if and only if $g(e)$ are mutually equal for all $e \in \mathbf{E}(G)$.

Proof. According to the Cauchy–Schwarz inequality,

$$\left(\sum_{i=1}^{p} a_i\, b_i\right)^2 \leq \sum_{i=1}^{p} a_i^2 \,\sum_{i=1}^{p} b_i^2 \tag{4}$$

holds for any positive-valued a_i and b_i, with equality if and only if

$$a_1 = a_2 = \cdots = a_p \qquad \text{and} \qquad b_1 = b_2 = \cdots = b_p\,.$$

Setting in (4), $a_i = \sqrt{f(u)}$ and $b_i = 1/\sqrt{f(u)}$, after summation over all $u \in \mathbf{V}(G)$, we arrive at inequality (2). For $a_i = \sqrt{g(e)}$ and $b_i = 1/\sqrt{g(e)}$, after summation over all $e \in \mathbf{E}(G)$, we arrive at inequality (3). □

3. Estimating the π-Sombor index

Setting $g(e) = \sqrt{d(u)^2 + d(v)^2}$ into Theorem 2, we immediately arrive at:

Theorem 3. *Let G be a connected graph with $n \geq 2$ vertices and m edges, and let its π-Sombor index be defined via Eq. (1). Then,*

$$\pi SO(G) \geq m^2\,. \tag{5}$$

Equality holds if G is either a regular graph or a complete bipartite graph $K_{p,q}$.

Remark 1. Inequality (5) holds also for non-connected graphs. However, the equality case is somewhat more complicated. First of all, in a trivial manner, if equality holds for a graph G, then equality holds also for the graph obtained by adding to G any number of isolated vertices.

Because of $1^2 + 7^2 = 5^2 + 5^2$, equality in (3) will hold for a graph whose components are the 8-vertex star and any regular graph of degree 5. Examples of this kind can be constructed ad libitum.

Theorem 3 has a number of noteworthy consequences.

Corollary 4. *For $n = 1, 2, 3$, there exists a single n-vertex tree. For all $n \geq 4$, the unique n-vertex tree with minimum π-Sombor index is the star S_n (identical to the complete bipartite graph $K_{1,n-1}$).*

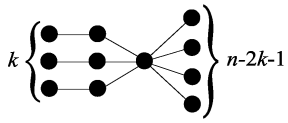

Figure 3. The eclipsed sun graph $ES(n,k)$ with $n = 11$ and $k = 3$.

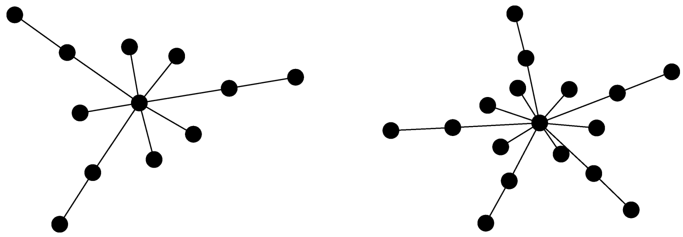

Figure 4. The 12- and 17-vertex trees with maximum π-Sombor index; these are the eclipsed sun graphs $ES(12,3)$ and $E(17,5)$.

Corollary 5. *For $n = 3$, there exists a single n-vertex connected unicyclic graph. For all $n \geq 4$, the unique n-vertex connected unicyclic graph with minimum π-Sombor index is the cycle C_n (the regular graph of degree 2).*

Corollary 6. *Among connected bicyclic graphs, equality in (5) holds only if $n = 5$ and $G \cong K_{3,2}$.*

Corollary 7. *Among connected tricyclic graphs, equality in (5) holds only if either $n = 4$ and $G \cong K_4$ or $n = 6$ and $G \cong K_{4,2}$.*

Corollary 8. *Among connected tetracyclic graphs, equality in (5) holds only if either $n = 6$ and G is one of the two regular graphs of degree 3 (of which one is $K_{3,3}$) or $n = 7$ and $G \cong K_{5,2}$.*

Corollary 9. *Among connected pentacyclic graphs, equality in (5) holds only if $n = 8$ and either $G \cong K_{6,2}$ or G is a regular graph of degree 3.*

Corollary 10. *Among connected hexacyclic graphs, equality in (5) holds only if either $n = 5$ and $G \cong K_5$ or $n = 9$ and $G \cong K_{7,2}$ or $n = 10$ and G is a regular graph of degree 3.*

Because of the absence of correlation between Sombor and π-Sombor indices (cf. Figure 2), characterizing the graphs with maximum πSO-value appears to be a much more difficult task. We tried to shed some light on this problem in the case of trees. For this end, we made a computer search of all trees up to $n = 17$ vertices.

In order to describe our findings, we need some preparation.

Definition 11. The sun graph is a tree having a central vertex to which 2-vertex branches are attached. The eclipsed sun graph is a tree having a central vertex to which 2-vertex branches and pendent vertices are attached. The eclipsed sun graph with n vertices and k 2-vertex branches will be denoted by $ES(n,k)$, see Figure 3.

Recall that if $k = 0$, then $ES(n,k)$ coincides with the star S_n. If n is odd and $k = (n-1)/2$, then $ES(n,k)$ coincides with the ordinary sun graph.

All calculations (up to $n = 17$) showed that the tree with maximum πSO-value is an eclipsed sun graph. Two characteristic examples are depicted in Figure 4.

Moreover, we found that the respective eclipsed sun graphs are:

- $ES(n,1)$ for $n = 5,6,7$
- $ES(n,2)$ for $n = 8,9,10$
- $ES(n,3)$ for $n = 11,12,13$

- $ES(n,4)$ for $n = 14, 15, 16$
- $ES(n,5)$ for $n = 17$.

This encourage us to state the following:

Conjecture 12. *For $n \geq 5$, the n-vertex tree with maximum π-Sombor index is the eclipsed sun graph $E(n,k)$ for $k = \lfloor (n-2)/3 \rfloor$.*

Bearing in mind that

$$\begin{aligned} SO\big(ES(n,k)\big) &= \sqrt{5}\,k + k\sqrt{4+d^2} + (n-2k-1)\sqrt{1+d^2} \\ {}^{m}SO\big(ES(n,k)\big) &= \frac{k}{\sqrt{5}} + \frac{k}{\sqrt{4+d^2}} + \frac{n-2k-1}{\sqrt{1+d^2}} \end{aligned}$$

we can re-formulate Conjecture 12 as

Conjecture 13. *Let T_n be an n-vertex tree, $n \geq 5$. Then,*

$$\pi SO(T_n) \leq \left[\sqrt{5}\,k + k\sqrt{4+d^2} + (n-2k-1)\sqrt{1+d^2}\right]\left[\frac{k}{\sqrt{5}} + \frac{k}{\sqrt{4+d^2}} + \frac{n-2k-1}{\sqrt{1+d^2}}\right]$$

for $k = \lfloor (n-2)/3 \rfloor$. Equality holds if and only if $T_n \cong ES(n, \lfloor (n-2)/3 \rfloor)$.

4. Conclusion

The result stated as Conjectures 12 and 13 were verified by direct calculation up to $n = 17$. Establishing if these are generally valid (or are violated for some larger value of n) remains a task for the future. Bearing in mind the structure of the eclipsed sun graph, this task appears to be difficult. It will stay as a challenge to mathematicians better than the present authors.

What also remains to be done is to study additional properties of the π-Sombor index, especially of its correlating properties with regard to physicochemical parameters of chemical substances, first of all of alkanes. Results along these lines are expected to be achieved in a reasonable future.

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