On a conjecture regarding the exponential reduced Sombor index of chemical trees

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Abstract

Let \( G \) be a graph and denote by \( d_u \) the degree of a vertex \( u \) of \( G \). The sum of the numbers \( e^\sqrt{(d_u-1)^2+(d_v-1)^2} \) over all edges \( uv \) of \( G \) is known as the exponential reduced Sombor index. A chemical tree is a tree with the maximum degree at most 4. In this paper, a conjecture posed by Liu et al. [MATCH Commun. Math. Comput. Chem. 86 (2021) 729–753] is disproved and its corrected version is proved.

Keywords: topological index; chemical graph theory; Sombor index; reduced Sombor index; exponential reduced Sombor index.

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1. Introduction

Let \( G \) be a graph. The sets of edges and vertices of \( G \) are represented by \( E(G) \) and \( V(G) \), respectively. For the vertex \( v \in V(G) \), the degree of \( v \) is denoted by \( d_G(v) \) (or simply by \( d_v \) if only one graph is under consideration). A vertex \( u \in V(G) \) is said to be a pendant vertex if \( d_u = 1 \). The degree set of \( G \) is the set of all unequal degrees of vertices of \( G \). The set \( N_G(u) \) consists of the vertices of the graph \( G \) that are adjacent to the vertex \( u \). The members of \( N_G(u) \) are known as neighbors of \( u \). A chemical tree is the tree of maximum degree at most 4. The (chemical-)graph-theoretical terminology and notation that are used in this study without explaining here can be found in the books [1, 2, 11].

For the graph \( G \), the Sombor index and reduced Sombor index abbreviated as \( SO \) and \( SO_{red} \), respectively, are defined [5] as

\[
SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \quad \text{and} \quad SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d_u-1)^2 + (d_v-1)^2}.
\]

These degree-based graph invariants, introduced recently in [5], have attained a lot of attention from researchers in a very short time, which resulted in many publications; for example, see the review papers [4, 9], and the papers listed therein.

The following exponential version of the reduced Sombor index was considered in [10]:

\[
e^{SO_{red}(G)} = \sum_{uv \in E(G)} e^{\sqrt{(d_u-1)^2+(d_v-1)^2}}.
\]

Let \( n_i \) denote the number of vertices in the graph \( G \) with degree \( i \). The cardinality of the set consisting of the edges joining the vertices of degrees \( i \) and \( j \) in the graph \( G \) is denoted by \( m_{i,j} \). Denote by \( \mathbb{T}_n \) the class of chemical trees of order \( n \) such that \( n_2 + n_3 \leq 1 \) and \( m_{1,3} = m_{1,2} = 0 \). Deng et al. [3] proved that the members of the class \( \mathbb{T}_n \) are the only trees possessing the maximum value of the reduced Sombor index for every \( n \geq 11 \). Keeping in mind this result of Deng et al. [3], Liu et al. [10] posed the following conjecture concerning the exponential reduced Sombor index for chemical trees.

Conjecture 1.1. [10] Among all chemical trees of a fixed order \( n \), the members of the class \( \mathbb{T}_n \) are the only trees possessing the maximum value of the exponential reduced Sombor index for every \( n \geq 11 \).

Conjecture 1.1 was also discussed in [12] and was left open. In fact, there exist counter examples to Conjecture 1.1; for instance, for the trees \( T_1 \) and \( T_2 \) depicted in Figure 1, it holds that

\[
278 \approx e^{SO_{red}(T_1)} = 8e^3 + e^{3\sqrt{7}} + 2e^{\sqrt{11}} < e + 7e^3 + 2e^{3\sqrt{7}} + e^{\sqrt{11}} = e^{SO_{red}(T_2)} \approx 306.
\]

The next theorem gives a corrected statement of Conjecture 1.1.

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*This paper is dedicated to the memory of Professor Nenad Trinajstić (one of the pioneers of chemical graph theory).
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Theorem 1.1. For $n \geq 7$, if $T$ is a chemical tree of order $n$, then

$$e^{SO_{red}}(T) \leq \frac{1}{3} \left( 2e^3 + e^{3\sqrt{2}} \right) n + \frac{1}{3} \left( 2e^3 - 5e^{3\sqrt{2}} \right) + \begin{cases} \frac{1}{3} \left( 3e - 5e^3 - e^{3\sqrt{2}} + 3e^{3\sqrt{2}} \right) & \text{if } n \equiv 0 \pmod{3} \\ \frac{1}{3} \left( 6e^2 - 7e^3 - 2e^{3\sqrt{2}} + 3e^{3\sqrt{2}} \right) & \text{if } n \equiv 1 \pmod{3} \\ 0 & \text{if } n \equiv 2 \pmod{3}, \end{cases}$$

with equality if and only if

- the degree set of $T$ is $\{1, 2, 4\}$ and $n_2 = m_{2,4} = m_{1,2} = 1$, whenever $n \equiv 0 \pmod{3}$;
- the degree set of $T$ is $\{1, 3, 4\}$ and $n_3 = m_{3,4} = 1$ and $m_{1,3} = 2$, whenever $n \equiv 1 \pmod{3}$;
- the degree set of $T$ is $\{1, 4\}$ whenever $n \equiv 2 \pmod{3}$.

2. Proof of Theorem 1.1

If $T$ is a chemical tree of order $n$ with $n \geq 3$, then

$$e^{SO_{red}}(T) = \sum_{1 \leq i \leq j \leq 4} m_{i,j} e\sqrt{(i-1)^2 + (j-1)^2},$$

with

$$n_1 + n_2 + n_3 + n_4 = n,$$

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n - 1),$$

and

$$\sum_{1 \leq i \leq j \leq 4, i \neq j} m_{i,j} + 2m_{i,j} = j \cdot n_j \quad \text{for } j = 1, 2, 3, 4.$$ 

By solving the system of equations (2)–(4) for the unknowns $m_{1,4}, m_{4,4}, n_1, n_2, n_3, n_4$ and then inserting the values of $m_{4,4}$ and $m_{1,4}$ (these two values are well-known, see for example [6]) in Equation (1), one gets

$$e^{SO_{red}}(T) = \frac{1}{3} \left( 2e^3 + e^{3\sqrt{2}} \right) n + \frac{1}{3} \left( 2e^3 - 5e^{3\sqrt{2}} \right) + \frac{1}{3} \left( 3e - 4e^3 + e^{3\sqrt{2}} \right) m_{1,2}$$

$$+ \frac{1}{9} \left( 9e^2 - 10e^3 + e^{3\sqrt{2}} \right) m_{1,3} + \frac{1}{3} \left( 3e\sqrt{2} - 2e^3 - e^{3\sqrt{2}} \right) m_{2,2}$$

$$+ \frac{1}{9} \left( 9e\sqrt{2} - 4e^3 - 5e^{3\sqrt{2}} \right) m_{2,3} + \frac{1}{3} \left( 3e\sqrt{3} - 2e^3 - 2e^{3\sqrt{2}} \right) m_{2,4}$$

$$+ \frac{1}{9} \left( 9e\sqrt{2} - 2e^3 - 7e^{3\sqrt{2}} \right) m_{3,3} + \frac{1}{9} \left( 9e\sqrt{2} - 3 - 8e^{3\sqrt{2}} \right) m_{3,4}. \quad (5)$$

We take

$$\Gamma(T) = \frac{1}{3} \left( 3e - 4e^3 + e^{3\sqrt{2}} \right) m_{1,2}$$

$$+ \frac{1}{9} \left( 9e^2 - 10e^3 + e^{3\sqrt{2}} \right) m_{1,3} + \frac{1}{3} \left( -2e^3 + 3e\sqrt{2} - e^{3\sqrt{2}} \right) m_{2,2}$$

$$+ \frac{1}{9} \left( -4e^3 - 5e^{3\sqrt{2}} + 9e\sqrt{2} \right) m_{2,3} + \frac{1}{3} \left( -e^3 - 2e\sqrt{2} + 3e\sqrt{3} \right) m_{2,4}$$

$$+ \frac{1}{9} \left( -2e^3 + 9e\sqrt{2} - 7e^{3\sqrt{2}} \right) m_{3,3} + \frac{1}{9} \left( -e^3 - 8e\sqrt{2} + 9e\sqrt{3} \right) m_{3,4}. \quad (6)$$

$$\approx -0.8653m_{1,2} - 7.1958m_{1,3} - 32.4742m_{2,2} - 38.2323m_{2,3}$$

$$- 29.4651m_{2,4} - 41.6713m_{3,3} - 27.2888m_{3,4}. \quad (7)$$
Then, Equation (5) can be written as
\[
e^{SO_{ext}}(T) = \frac{1}{3} \left( 2e^3 + e^{3\sqrt{2}} \right) n + \frac{1}{3} \left( 2e^3 - 5e^{3\sqrt{2}} \right) + \Gamma(T).
\] (8)

For any given integer \( n \) greater than 4, it is evident from Equation (8) that a tree \( T \) attains the greatest value of \( e^{SO_{ext}} \) over the class of all chemical trees of order \( n \) if and only if \( T \) possess the greatest value of \( \Gamma \) in the considered class. As a consequence, we consider \( \Gamma(T) \) instead of \( e^{SO_{ext}}(T) \) in the next lemma.

**Lemma 2.1.** Let \( T \) be a chemical tree of order \( n \), where \( n \geq 7 \). The inequality
\[
\Gamma(T) < \frac{1}{3} \left( 6e^2 - 7e^3 - 2e^{3\sqrt{2}} + 3e^{\sqrt{13}} \right) \approx -41.6804,
\]
holds if any of the following conditions holds:

(i) \( \max \{m_{3,3}, m_{2,2}, m_{2,3} \} \geq 1 \),

(ii) \( \max \{m_{3,4}, m_{2,4} \} \geq 2 \),

(iii) \( n_2 + n_3 \geq 2 \).

**Proof:** Take an edge \( uv \in E(T) \) with \( d_u, d_v \in \{2, 3\} \). Since \( n \geq 7 \), at least one of the two vertices \( u, v \) has at least two non-pendent neighbors. Hence, if \( \max \{m_{3,3}, m_{2,2}, m_{2,3} \} \geq 1 \) then either \( m_{3,3} + m_{2,2} + m_{2,3} \geq 2 \) or \( \max \{m_{3,4}, m_{2,4} \} \geq 1 \) and hence the required inequality follows from (6). Also, note that the desired inequality follows from (6) whenever \( \max \{m_{3,4}, m_{2,4} \} \geq 2 \). In what follows, assume that \( m_{3,3} = m_{2,2} = m_{2,3} = 0 \), \( n_2 + n_3 \geq 2 \), and \( \max \{m_{3,4}, m_{2,4} \} \leq 1 \).

Assume that \( n_3 \neq 0 \). Let \( w \in V(T) \) be a vertex of degree 3 and take \( N_T(w) = \{w_1, w_2, w_3\} \). Since \( m_{3,3} = m_{2,3} = 0 \), one has \( d_{w_i} \in \{1, 4\} \) for \( i = 1, 2, 3 \). Since \( n \geq 7 \), we have \( d_{w_i} = 4 \) for at least one \( i \in \{1, 2, 3\} \). Hence, if \( n_3 \geq t \) then \( m_{3,4} \geq t \). Similarly, if \( n_2 \geq s \) then \( m_{2,4} \geq s \). Thus, if either \( n_2 \geq 2 \) or \( n_3 \geq 2 \) then we have \( \max \{m_{3,4}, m_{2,4} \} \geq 2 \), a contradiction. Consequently, we must have \( n_2 = n_3 = 1 \), which implies that \( m_{2,4} \geq 1 \) and \( m_{3,4} \geq 1 \), and hence the required inequality follows from (6).

**Proof of Theorem 1.1.** If either of the inequalities \( \max \{m_{3,3}, m_{2,2}, m_{2,3} \} \geq 1 \), \( \max \{m_{3,4}, m_{2,4} \} \geq 2 \), and \( n_2 + n_3 \geq 2 \), holds, then by using Lemma 2.1 and Equation (8), one has
\[
e^{SO_{ext}}(T) < \frac{1}{3} \left( 6e^2 - 7e^3 - 2e^{3\sqrt{2}} + 3e^{\sqrt{13}} \right) \approx -41.6804,
\]
as desired.

In the rest of the proof, assume that \( \max \{m_{3,3}, m_{2,2}, m_{2,3} \} = 0 \), \( \max \{m_{3,4}, m_{2,4} \} \leq 1 \), and \( n_2 + n_3 \leq 1 \). Then, we note that \( (n_2, n_3) \in \{(0, 0), (1, 0), (0, 1)\} \). From Equations (2) and (3), it follows that \( n_2 + 2n_3 \equiv n - 2 \pmod{3} \), which gives
\[
(n_2, n_3) = \begin{cases} (1, 0) & \text{if } n \equiv 0 \pmod{3}, \\ (0, 1) & \text{if } n \equiv 1 \pmod{3}, \\ (0, 0) & \text{if } n \equiv 2 \pmod{3}, \end{cases}
\]
this together with the system of equations (4) implies that
\[
(m_{1,2}, m_{1,3}, m_{2,4}, m_{3,4}) = \begin{cases} (1, 0, 1, 0) & \text{if } n \equiv 0 \pmod{3}, \\ (0, 2, 0, 1) & \text{if } n \equiv 1 \pmod{3}, \\ (0, 0, 0, 0) & \text{if } n \equiv 2 \pmod{3}. \end{cases}
\]
Now, from Equation (5) the required result follows. □
3. Concluding remarks

Recently, Liu [7] reported some extremal results for the multiplicative Sombor index. For a graph $G$, its multiplicative Sombor index and multiplicative reduced Sombor index are defined as

$$\Pi_{SO}(G) = \prod_{uv \in E(G)} \sqrt{d^2_u + d^2_v} \quad \text{and} \quad \Pi_{SO,\text{red}}(G) = \prod_{uv \in E(G)} \sqrt{(d_u - 1)^2 + (d_v - 1)^2}.$$  

As expected, among all chemical trees of a fixed order $n \geq 11$, the trees attaining the maximum (reduced) Sombor index (see [3]) are same as the ones possessing the maximum multiplicative (reduced) Sombor index.

**Theorem 3.1.** Among all chemical trees of a fixed order $n$, the members of the class $T_n$ are the only trees possessing the maximum value of the multiplicative (reduced) Sombor index for every $n \geq 11$.

Analogous to the definition of the exponential reduced Sombor index, the exponential Sombor index can be defined as

$$e^{SO}(G) = \sum_{uv \in E(G)} e^{\sqrt{(d_u)^2 + (d_v)^2}}.$$  

Denote by $T^*_n$ the class of chemical trees of order $n$ such that $n_2 + n_3 \leq 1$ and $m_{3,4} + m_{2,4} \leq 1$. As expected, among all chemical trees of a fixed order $n \geq 7$, the trees attaining the maximum exponential reduced Sombor index (see Theorem 1.1) are same as the ones possessing the maximum exponential Sombor index.

**Theorem 3.2.** For every $n \geq 7$, the trees of the class $T^*_n$ uniquely attain the maximum value of the exponential Sombor index among all chemical trees of a fixed order $n$.

Because the proofs of Theorems 1.1, 3.1, and 3.2 are very similar to one another, we omit the proofs of Theorems 3.1 and 3.2.

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