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 pendent 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 \(v\). 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 \(T_n\) 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 \(T_n\) 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 \(T_n\) 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

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

The next theorem gives a corrected statement of Conjecture 1.1.

*This paper is dedicated to the memory of Professor Nenad Trinajstić (one of the pioneers of chemical graph theory).
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Figure 1: The trees $T_1$ and $T_2$ providing a counterexample to Conjecture 1.1.

**Theorem 1.1.** For $n \geq 7$, if $T$ is a chemical tree of order $n$, then

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

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 $n_3 = m_{1,4} = 1$ 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

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

$$n_1 + n_2 + n_3 + n_4 = n, \quad n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1), \quad \sum_{1 \leq i,j \leq 4 \atop i \neq j} m_{i,j} + 2m_{j,j} = j \cdot n_j \text{ for } j = 1, 2, 3, 4.$$  \hspace{1cm} (1)

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

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

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

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

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

We take

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

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

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

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

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

$$- 29.4651m_{2,4} - 41.6713m_{3,3} - 27.2888m_{3,4}. \quad (7)$$
Then, Equation (5) can be written as

\[
e^{-\lambda T}(T) = \frac{1}{3} \left(2e^3 + 3\sqrt{2}\right) n + \frac{1}{3} \left(2e^3 - 5\sqrt{2}\right) + \Gamma(T).
\]

(8)

For any given integer \( n \) greater than 4, it is evident from Equation (8) that a tree \( T \) attains the greatest value of \( e^{-\lambda T}(T) \) 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 \( e^{-\lambda T}(T) \) in the next lemma.

**Lemma 2.1.** Let \( T \) be a chemical tree of order \( n \), where \( n \geq 7 \). The inequality

\[
\Gamma(T) < \frac{1}{3} \left(6e^2 - 7e^3 - 2e^{3\sqrt{2}} + 3e^{3\sqrt{3}}\right) (\approx -41.6804),
\]

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

\[
e^{-\lambda T}(T) < \frac{1}{3} \left(2e^3 + 3\sqrt{2}\right) n + \frac{1}{3} \left(2e^3 - 5\sqrt{2}\right) + \frac{1}{3} \left(6e^2 - 7e^3 - 2e^{3\sqrt{2}} + 3e^{3\sqrt{3}}\right)
\]

\[
< \frac{1}{3} \left(2e^3 + 3\sqrt{2}\right) n + \frac{1}{3} \left(2e^3 - 5\sqrt{2}\right) + \frac{1}{3} \left(6e^2 - 7e^3 - 2e^{3\sqrt{2}} + 3e^{3\sqrt{3}}\right)
\]

\[
< \frac{1}{3} \left(2e^3 + 3\sqrt{2}\right) n + \frac{1}{3} \left(2e^3 - 5\sqrt{2}\right),
\]

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 \( (n_2, n_3) = \{(0, 0), (1, 0), (0, 1)\} \). From Equations (2) and (3), it follows that \( n_2 + 2n_3 \equiv n - 2 \) (mod 3), which gives

\[
(n_2, n_3) = \begin{cases} (1, 0) & \text{if } n \equiv 0 \text{ (mod 3)}, \\ (0, 1) & \text{if } n \equiv 1 \text{ (mod 3)}, \\ (0, 0) & \text{if } n \equiv 2 \text{ (mod 3)}, 
\end{cases}
\]

this together with the system of equations (4) implies that

\[
(m_{1,2}, m_{1,3}, m_{2,4}, m_{3,4}) = \begin{cases} (1, 0, 1, 0) & \text{if } n \equiv 0 \text{ (mod 3)}, \\ (0, 2, 0, 1) & \text{if } n \equiv 1 \text{ (mod 3)}, \\ (0, 0, 0, 0) & \text{if } n \equiv 2 \text{ (mod 3)}. 
\end{cases}
\]

Now, from Equation (5) the required result follows.\[\square\]
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

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

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 $T_n^\star$ 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 $T_n^\star$ 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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