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Research Article

Elliptic Sombor index of chemical graphs

Carlos Espinal[1,†], Ivan Gutman[2], Juan Rada[1,*]

[1] Instituto de Matemáticas, Universidad de Antioquia, Medellín, Colombia
[†] alejandro.espinal@udea.edu.co
[*] pablo.rada@udea.edu.co

[2] Faculty of Science, University of Kragujevac, 34000 Kragujevac, Serbia
gutman@kg.ac.rs

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Abstract: Let G be a simple graph. The elliptic Sombor index of G is defined as

$$ESO(G) = \sum_{uv} (d_u + d_v) \sqrt{d_u^2 + d_v^2},$$

where d_u denotes the degree of the vertex u, and the sum runs over the set of edges of G. In this paper we solve the extremal value problem of ESO over the set of (connected) chemical graphs and over the set of chemical trees, with equal number of vertices.

Keywords: elliptic Sombor index, chemical graph, vertex-degree-based topological index.

AMS Subject classification: 05C09, 05C35

1. Introduction

Let G be a simple graph with set of vertices V and set of edges E. The degree of the vertex $u \in V$ is defined as the number of vertices adjacent to u, and it is denoted by d_u. If there is an edge from vertex u to vertex v, we indicate this by writing uv (or vu). We denote by n_i the number of vertices of degree i and by $m_{i,j}$ the number of edges connecting a vertex of degree i to a vertex of degree j. We will assume that G has no isolated vertices (i.e., vertices of degree 0).
Let $\varphi(i,j)$ be a real bivariate symmetric function defined over $\mathbb{N} \times \mathbb{N}$. A vertex-degree-based (VDB, for short) topological index φ is defined on the graph G as

* *Corresponding Author*

$$\varphi(G) = \sum_{uv \in E} \varphi\left(d_u, d_v\right). \tag{1.1}$$

The general theory of VDB topological indices has been extensively studied [2, 6, 11, 12], they play an important role in chemical and pharmacological applications [5, 8, 9]. A new geometric approach to the theory was introduced in [3], and more recently in [4], where the elliptic Sombor index was invented. It is denoted by ESO and defined for the graph G as

$$\varphi(G) = \sum_{uv \in E} \left(d_u + d_v\right) \sqrt{d_u^2 + d_v^2}. \tag{1.2}$$

In other words, ESO is a VDB topological index induced by the function

$$\varphi(i, j) = (i + j) \sqrt{i^2 + j^2}.$$

We refer to [7, 10] for recent results on ESO.

Our main interest in this paper is to study the elliptic Sombor index over the set of chemical graphs. More precisely, we solve the extremal value problem for ESO over the set of (connected) graphs with equal number of vertices. Actually, our approach works for a general VDB topological index φ which satisfies certain properties, so it can be applied to many more VDB topological indices. Also, we solve the extremal value problem of ESO over the set of chemical trees with a fixed number of vertices.

2. Elliptic Sombor index of chemical graphs

We are particularly interested in $\varphi(G)$ when G is a chemical graph, i.e., a graph which satisfies $d_u \leq 4$ for all vertices $u \in V$. So let us assume that G is a chemical graph with n vertices. In this special situation the following well known relations hold:

$$n_1 + n_2 + n_3 + n_4 = n, \tag{2.1}$$

and

$$\begin{aligned} 2m_{1,1} + m_{1,2} + m_{1,3} + m_{1,4} &= n_1, \\ m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4} &= 2n_2, \\ m_{1,3} + m_{2,3} + 2m_{3,3} + m_{3,4} &= 3n_3, \\ m_{1,4} + m_{2,4} + m_{3,4} + 2m_{4,4} &= 4n_4. \end{aligned} \tag{2.2}$$

From (2.2) and (2.1) it easily follows that

$$\sum_{(x,y) \in P} \frac{x + y}{xy} m_{x,y} = n, \tag{2.3}$$

where

$$P = \{(x,y) \in \mathbb{N} \times \mathbb{N} \mid 1 \le x \le y \le 4\}.$$

Then from relation (1.1) we deduce that

$$\varphi(G) = \sum_{(x,y)\in P} \varphi(x,y)\, m_{x,y}. \tag{2.4}$$

Let $C = \{(x,y) \in P \mid (x,y) \neq (4,4)\}$ and consider the following property on a VDB topological index φ:

$$\frac{xy\varphi(x,y)}{x+y} < 2\varphi(4,4) \tag{2.5}$$

for all $(x,y) \in C$.

Theorem 1. *Let φ be a VDB topological index satisfying (2.5) and let G be a chemical graph with n vertices. Then,*

$$\varphi(G) \le 2\varphi(4,4)\, n.$$

Equality occurs if and only if G is a 4-regular graph.

Proof. From relations (2.3), (2.4) and (2.5) we deduce

$$\begin{aligned}
\varphi(G) &= \varphi(4,4)\, m_{4,4} + \sum_{(x,y)\in C} \varphi(x,y)\, m_{x,y} \\
&= \varphi(4,4)\left(2n - 2\sum_{(x,y)\in C} \frac{x+y}{xy} m_{x,y}\right) + \sum_{(x,y)\in C} \varphi(x,y)\, m_{x,y} \\
&= 2\varphi(4,4)\, n + \sum_{(x,y)\in C}\left(\varphi(x,y) - 2\varphi(4,4)\frac{x+y}{xy}\right) m_{x,y} \le 2\varphi(4,4)\, n. \qquad (2.6)
\end{aligned}$$

If $\varphi(G) = 2\varphi(4,4)\, n$, then from (2.6),

$$\sum_{(x,y)\in C}\left(\varphi(x,y) - 2\varphi(4,4)\frac{x+y}{xy}\right) m_{x,y} = 0,$$

and from (2.5), $m_{x,y} = 0$ for all $(x,y) \in C$. In other words, G is a 4-regular graph. Conversely, if G is a 4-regular graph, then

$$\varphi(G) = \varphi(4,4)\, m_{4,4} = \varphi(4,4)\, m = \varphi(4,4)\frac{4n}{2} = 2\varphi(4,4)\, n.$$

□

Since $\varphi(i,j) = (i+j)\sqrt{i^2+j^2}$ satisfies property (2.5), we can apply Theorem 1 to the elliptic Sombor index,

Corollary 1. *Let G be a chemical graph with n vertices. Then*

$$ESO(G) \leq 64\sqrt{2}n.$$

Equality holds if and only G is a 4-regular graph.

Next we study lower bounds for a VDB topological index φ on chemical graphs with n vertices. Recall that two graphs are disjoint if they have no vertex in common. If G and H are disjoint, their disjoint union graph denoted by $G \cup H$, has vertex set $V(G \cup H) = V(G) \cup V(H)$ and edge set $E(G \cup H) = E(G) \cup E(H)$. The disjoint union of k copies of G is written as kG. Let $A = \{(x,y) \in P \mid (x,y) \neq (1,1)\}$ and consider the following property on φ:

$$\frac{xy\varphi(x,y)}{x+y} > \frac{1}{2}\varphi(1,1) \tag{2.7}$$

for all $(x,y) \in A$. Also, given the set $B = \{(x,y) \in A \mid (x,y) \neq (1,2)\}$, consider the following property on φ:

$$3\varphi(1,1) \leq 4\varphi(1,2) \quad \text{and} \quad \frac{xy\varphi(x,y)}{x+y} > \frac{2}{3}\varphi(1,2) \tag{2.8}$$

for all $(x,y) \in B$.

Theorem 2. *Let G be a chemical graph with n vertices.*
1. If n is even and φ satisfies (2.7), then $\varphi(G) \geq \frac{\varphi(1,1)}{2}n$. Equality occurs if and only if $G \cong \frac{n}{2}P_2$.
2. If n is odd and φ satisfies (2.8), then $\varphi(G) \geq \frac{n-3}{2}\varphi(1,1) + 2\varphi(1,2)$. Equality occurs if and only if $G \cong \frac{n-3}{2}P_2 \cup P_3$.

Proof. 1. Assume that n is even. From relations (2.3), (2.4) and (2.7) we deduce that

$$\begin{aligned}
\varphi(G) &= \varphi(1,1)\, m_{1,1} + \sum_{(x,y)\in A} \varphi(x,y)\, m_{x,y} \\
&= \varphi(1,1)\left(\frac{1}{2}n - \frac{1}{2}\sum_{(x,y)\in A} \frac{x+y}{xy} m_{x,y}\right) + \sum_{(x,y)\in A} \varphi(x,y)\, m_{x,y} \\
&= \frac{\varphi(1,1)}{2}n + \sum_{(x,y)\in A}\left(\varphi(x,y) - \frac{1}{2}\varphi(1,1)\frac{x+y}{xy}\right) m_{x,y} \geq \frac{\varphi(1,1)}{2}n.
\end{aligned} \tag{2.9}$$

If $\varphi(G) = \frac{\varphi(1,1)}{2}n$, then from the inequality (2.9),

$$\sum_{(x,y)\in A}\left(\varphi\left(x,y\right)-\frac{1}{2}\varphi\left(1,1\right)\frac{x+y}{xy}\right)m_{x,y}=0$$

and from property (2.7), it follows that $m_{x,y} = 0$ for all $(x, y) \in A$. In other words, G is a disjoint union of copies of P_2, that is, $G \cong \frac{n}{2}P_2$. Conversely, if $G \cong \frac{n}{2}P_2$ then $\varphi(G) = \frac{n}{2}\varphi(P_2) = \frac{n}{2}\varphi\left(1,1\right)$.

2. Assume that n is odd. Since G has no isolated vertices, $m_{1,1} \leq \frac{n-3}{2}$. Then, from relation (2.3),

$$2m_{1,1}+\frac{3}{2}m_{1,2}+\sum_{(x,y)\in B}\frac{x+y}{xy}m_{x,y}=n,$$

and so

$$m_{1,2}=\frac{2}{3}n-\frac{4}{3}m_{1,1}-\frac{2}{3}\sum_{(x,y)\in B}\frac{x+y}{xy}m_{x,y}. \tag{2.10}$$

Consequently, bearing in mind (2.10), (2.4) and (2.8),

$$\begin{aligned}
\varphi(G) &= \varphi\left(1,1\right)m_{1,1}+\varphi\left(1,2\right)m_{1,2}+\sum_{(x,y)\in B}\varphi\left(x,y\right)m_{x,y}\\
&= \varphi\left(1,1\right)m_{1,1}+\varphi\left(1,2\right)\left(\frac{2}{3}n-\frac{4}{3}m_{1,1}-\frac{2}{3}\sum_{(x,y)\in B}\frac{x+y}{xy}m_{x,y}\right)\\
&+\sum_{(x,y)\in B}\varphi\left(x,y\right)m_{x,y}\\
&= \left(\varphi\left(1,1\right)-\frac{4}{3}\varphi\left(1,2\right)\right)m_{1,1}+\frac{2}{3}\varphi\left(1,2\right)n\\
&+\sum_{(x,y)\in B}\left(\varphi\left(x,y\right)-\frac{2}{3}\varphi\left(1,2\right)\frac{x+y}{xy}\right)m_{x,y}\\
&\geq \left(\varphi\left(1,1\right)-\frac{4}{3}\varphi\left(1,2\right)\right)m_{1,1}+\frac{2}{3}\varphi\left(1,2\right)n\\
&\geq \left(\varphi\left(1,1\right)-\frac{4}{3}\varphi\left(1,2\right)\right)\frac{n-3}{2}+\frac{2}{3}\varphi\left(1,2\right)n\\
&= \frac{n-3}{2}\varphi\left(1,1\right)+2\varphi\left(1,2\right).
\end{aligned} \tag{2.11}$$

If $\varphi(G) = \frac{n-3}{2}\varphi\left(1,1\right) + 2\varphi\left(1,2\right)$, then from inequality (2.11) and property (2.8), $m_{1,1} = \frac{n-3}{2}$, $m_{1,2} = 2$ and $m_{x,y} = 0$ for all $(x, y) \in B$. Therefore, $G \cong \frac{n-3}{2}P_2 \cup P_3$. Conversely, if $G \cong \frac{n-3}{2}P_2 \cup P_3$, then $\varphi(G) = \frac{n-3}{2}\varphi(P_2) + \varphi(P_3) = \frac{n-3}{2}\varphi\left(1,1\right) + 2\varphi\left(1,2\right)$. □

Since $\varphi(i,j) = (i+j)\sqrt{i^2+j^2}$ satisfies properties (2.7) and (2.8), we can apply Theorem 2 to the elliptic Sombor index.

Corollary 2. *Let G be a chemical graph with n vertices.*

1. *If n is even, then $ESO(G) \geq \sqrt{2}n$. Equality occurs if and only if $G \cong \frac{n}{2}P_2$.*
2. *If n is odd, then $ESO(G) \geq (n-3)\sqrt{2}+6\sqrt{5}$. Equality occurs if and only if $G \cong \frac{n-3}{2}P_2 \cup P_3$.*

For connected chemical graphs we have the following result.

Corollary 3. *Let G be a connected chemical graph with n vertices. Then,*

$$8\sqrt{2}(n-3)+6\sqrt{5} \leq ESO(G) \leq 64\sqrt{2}n.$$

The equality in the left occurs if and only if $G \cong P_n$. The equality on the right occurs if and only if G is a connected 4-regular graph.

Proof. This result is a consequence of [4, Theorem 4] together with Corollary 1. □

Note that minimal value of ESO over connected graphs was already determined in [4, Theorem 4]. It is noteworthy to state that many of the well-known VDB topological indices satisfy conditions given in (2.5), (2.7) and (2.8). Consequently, Theorems 1 and 2 can be used to recover in a unified form known results on extremal values of VDB topological indices over chemical graphs, and can also be applied to study new VDB topological indices.

3. Elliptic Sombor index of chemical trees

Next we consider the elliptic Sombor index among chemical trees. Let $\mathcal{C}_n$ denote the set of all chemical trees with n vertices. In [4, Theorem 5], it was shown that P_n has the minimal ESO-value among all n-vertex trees. Evidently, then P_n has minimal ESO-value also among all n-vertex chemical trees. In spite of this, in order that the present paper be self-contained, we state it for chemical trees.

Theorem 3. *Let n be a positive integer. Among all chemical trees in $\mathcal{C}_n$, the minimal value of ESO is attained in the unique path tree P_n.*

Next we consider the maximal value problem of ESO among chemical trees with n vertices. Let $\varphi(i,j) = (i+j)\sqrt{i^2+j^2}$ and consider the following functions:

$$f(p,q) = [\varphi(2,p) - \varphi(3,p)] + [\varphi(2,q) - \varphi(3,q)],$$

$$g(p,q,r) = [\varphi(2,p) - \varphi(4,p)] + [\varphi(3,q) - \varphi(4,q)] + [\varphi(3,r) - \varphi(4,r)],$$

and

$$h(p,q,r,s) = [\varphi(3,p) - \varphi(4,p)] + [\varphi(3,q) - \varphi(2,q)] + [\varphi(3,r) - \varphi(4,r)] + [\varphi(3,s) - \varphi(4,s)],$$

where p, q, r, s are integers such that $4 \geq p, q, r, s \geq 1$. Let us consider the following subsets of $\mathcal{C}_n$:

$$\mathcal{C}_{00}(n) = \{T \in \mathcal{C}_n \mid n_2(T) = n_3(T) = 0\},$$

$$\mathcal{C}_{10}(n) = \{T \in \mathcal{C}_n \mid n_2(T) = 1,\ n_3(T) = 0\},$$

and

$$\mathcal{C}_{01}(n) = \{T \in \mathcal{C}_n \mid n_2(T) = 0,\ n_3(T) = 1\}.$$

It was shown in [1] that exactly one of the sets $\mathcal{C}_{00}(n)$, $\mathcal{C}_{10}(n)$, or $\mathcal{C}_{01}(n)$ is non-empty for each positive integer n (see Figures 1, 2, and 3).

Theorem 4. *Let n be a positive integer. Among all trees in $\mathcal{C}_n$, the maximal value of ESO is attained by any of the trees U, V, W, satisfying the conditions:*

1. *$U \in \mathcal{C}_{10}(n)$ such that $m_{1,2}(U) = 1$ if $n \equiv 0 \mod 3$ and $n \geq 6$;*
2. *$V \in \mathcal{C}_{01}(n)$ such that $m_{1,3}(V) = 2$ if $n \equiv 1 \mod 3$ and $n \geq 7$;*
3. *$W \in \mathcal{C}_{00}(n)$ if $n \equiv 2 \mod 3$ and $n \geq 5$.*

Proof. As we can see in Tables below, the following relations hold:

$$f(p,q) + \varphi(2,2) - \varphi(1,3) < 0 \tag{3.1}$$

and

$$f(p,q) + 2\varphi(2,4) - \varphi(1,4) - \varphi(3,4) < 0, \tag{3.2}$$

for all $1 \leq p \leq q \leq 4$;

$$g(p,q,r) + \varphi(2,3) - \varphi(1,4) < 0 \tag{3.3}$$

and

$$g(p,q,r) + \varphi(2,4) - \varphi(1,4) + \varphi(3,4) - \varphi(4,4) < 0, \tag{3.4}$$

for all $1 \leq p \leq 4$ and $1 \leq q \leq r \leq 4$;

$$h(p,q,r,s) + \varphi(3,3) - \varphi(2,4) < 0 \tag{3.5}$$

and

$$h(p,q,r,s) + 2\varphi(3,4) - \varphi(2,4) - \varphi(4,4) < 0, \tag{3.6}$$

in any of the following situations, where $p \neq 2$, $q \neq 2$, $r \neq 2$ and $s \neq 2$:

$$\begin{aligned} p = r = 1 \ &;\ 1 \leq q \leq s \leq 4; \\ 3 \leq p \leq q \leq 4 \ &;\ 1 \leq r \leq s \leq 4. \end{aligned}$$

Moreover,

$$\varphi(1,2) - \varphi(1,4) + \varphi(4,4) - \varphi(2,4) > 0 \tag{3.7}$$

and

$$\varphi(4,4) - \varphi(1,4) + \varphi(1,3) - \varphi(3,4) > 0. \tag{3.8}$$

Now the result follows from [1, Theorem 3.2]. □

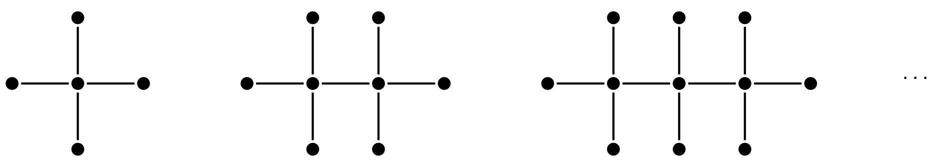

Figure 1. **Trees in $\mathcal{C}_{00}(n)$ when $n \equiv 2 \mod 3$.**

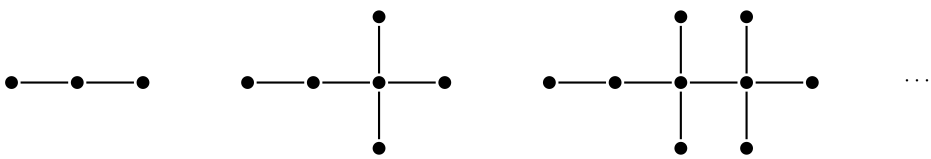

Figure 2. **Trees in $\mathcal{C}_{10}(n)$ when $n \equiv 0 \mod 3$**

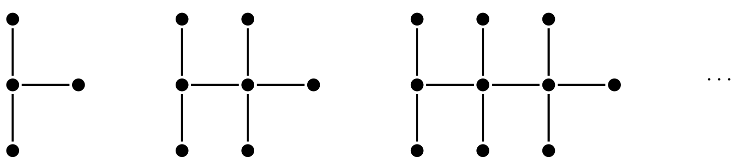

Figure 3. **Trees in $\mathcal{C}_{01}(n)$ when $n \equiv 1 \mod 3$.**

Table 1. Approximate values of the left hand side of conditions (3.1) and (3.2).

p	q	Value (3.1)	Value (3.2)
1	1	-13.217	-13.831
1	2	-13.990	-14.604
1	3	-14.704	-15.318
1	4	-15.443	-16.057
2	2	-14.763	-15.377
2	3	-15.477	-16.092
2	4	-16.216	-16.831
3	3	-16.191	-16.806
3	4	-16.930	-17.545
4	4	-17.669	-18.284

Table 2. Approximate values of the left hand side of conditions (3.3) and (3.4).

p	q	r	Value (3.3)	Value (3.4)
1	1	1	-32.427	-33.877
1	1	2	-33.266	-34.716
1	1	3	-34.005	-35.455
1	1	4	-34.716	-36.166
1	2	2	-34.105	-35.554
1	2	3	-34.844	-36.294
1	2	4	-35.554	-37.004
1	3	3	-35.583	-37.033
1	3	4	-36.294	-37.743
1	4	4	-37.004	-38.454
2	1	1	-34.039	-35.489
2	1	2	-34.878	-36.328
2	1	3	-35.617	-37.067
2	1	4	-36.328	-37.777
2	2	2	-35.716	-37.166
2	2	3	-36.456	-37.905
2	2	4	-37.166	-38.616
2	3	3	-37.195	-38.644
2	3	4	-37.905	-39.355
2	4	4	-38.616	-40.066
3	1	1	-35.492	-36.942
3	1	2	-36.331	-37.781
3	1	3	-37.070	-38.520
3	1	4	-37.781	-39.231
3	2	2	-37.170	-38.619
3	2	3	-37.909	-39.359
3	2	4	-38.619	-40.069
3	3	3	-38.648	-40.098
3	3	4	-39.359	-40.808
3	4	4	-40.069	-41.519
4	1	1	-36.942	-38.392
4	1	2	-37.781	-39.231
4	1	3	-38.520	-39.970
4	1	4	-39.231	-40.680
4	2	2	-38.619	-40.069
4	2	3	-39.359	-40.808
4	2	4	-40.069	-41.519
4	3	3	-40.098	-41.547
4	3	4	-40.808	-42.258
4	4	4	-41.519	-42.969

Table 3. Approximate values of the left hand side of conditions (3.5) and (3.6).

p	q	r	s	Value (3.5)	Value (3.6)
1	1	1	1	-19.335	-20.045
1	1	1	3	-20.913	-21.623
1	1	1	4	-21.623	-22.334
1	3	1	3	-19.425	-20.136
1	3	1	4	-20.136	-20.847
1	4	1	4	-19.397	-20.108
3	3	1	1	-19.425	-20.136
3	3	1	3	-21.003	-21.714
3	3	1	4	-21.714	-22.424
3	3	3	3	-22.581	-23.292
3	3	3	4	-23.292	-24.002
3	3	4	4	-24.002	-24.713
3	4	1	1	-18.686	-19.397
3	4	1	3	-20.264	-20.975
3	4	1	4	-20.975	-21.685
3	4	3	3	-21.842	-22.552
3	4	3	4	-22.552	-23.263
3	4	4	4	-23.263	-23.974
4	4	1	1	-19.397	-20.108
4	4	1	3	-20.975	-21.685
4	4	1	4	-21.685	-22.396
4	4	3	3	-22.552	-23.263
4	4	3	4	-23.263	-23.974
4	4	4	4	-23.974	-24.684

Table 4. Approximate values of the left hand side of conditions (3.7) and (3.8).

Value (3.7)	Value (3.8)
4.514	2.288

Conflict of Interest: The authors declare that they have no conflict of interest.

Data Availability: Data sharing is not applicable to this article as no data sets were generated or analyzed during the current study.

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