

NEW BOUNDS ON SOMBOR AND ELLIPTIC SOMBOR INDEX

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ABSTRACT. The Sombor index (SO) is a vertex-degree-based graph invariant, equal to the sum of the terms $\sqrt{d(u)^2 + d(v)^2}$ over all pairs of adjacent vertices u, v of the underlying graph, where $d(u)$ is the degree of the vertex u . The elliptic Sombor index (ESO) is a recently introduced variant of SO , equal to the sum of terms $[d(u) + d(v)] \sqrt{d(u)^2 + d(v)^2}$. In this paper, we establish new lower and upper bounds for SO and ESO , as well as bounds involving their coindices.

1. Introduction

In this paper we are concerned with simple graphs, i.e., graphs without directed, multiple or weighted edges, and without self-loops [2, 14]. Let G be such a graph, with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. The number of vertices and edges of G are $n = |\mathbf{V}(G)|$ and $m = |\mathbf{E}(G)|$, respectively. An edge connecting the vertices $u, v \in \mathbf{V}(G)$ will be denoted by uv . The degree (= number of first neighbors) of a vertex $u \in \mathbf{V}(G)$ is denoted by $d(u)$. For other graph theoretic notations and terminology see [2, 14].

In contemporary mathematics and mathematical chemistry, a large number of graph invariants are studied, aimed at modeling structural properties of chemical compounds [17, 28]. A large group of such invariants is of the form

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

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where $\varphi(x, y)$ is a conveniently chosen function with property $\varphi(x, y) = \varphi(y, x)$. These are usually referred to as vertex-degree-based (VDB) topological indices.

The coindex of the invariant TI is defined as

$$\overline{TI} = \overline{TI}(G) = \sum_{uv \notin \mathbf{E}(G)} \varphi(d(u), d(v))$$

where it is assumed that the vertices $u, v \in \mathbf{V}(G)$ are distinct, i.e., $u \neq v$.

Two recently introduced VDB graph invariants are the Sombor index (SO) [7] and the elliptic Sombor index (ESO) [11], both conceived by using geometric considerations. These are defined as

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

and

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

Of their several noteworthy applications we mention here just a few [1, 15, 25, 26]. Their mathematical properties are found in the review [18] and in the recent papers [6, 23, 24, 27]. For researches on Sombor coindex see in [3, 4, 19, 22].

Several lower and upper bounds for Sombor and elliptic Sombor indices were earlier communicated [8, 9, 12, 16, 20]. In the present paper we offer a few more such results.

In order to present our findings, we need some preparations.

2. Preparations

In the below considerations, the following well-known VDB topological indices will be applied [5, 13, 21]: the first Zagreb index (M_1), the second Zagreb index (M_2), and the forgotten index (F). These are defined as

$$M_1(G) = \sum_{uv \in \mathbf{E}(G)} [d(u) + d(v)] = \sum_{u \in \mathbf{V}(G)} d(u)^2$$

$$M_2(G) = \sum_{uv \in \mathbf{E}(G)} d(u) d(v)$$

$$F(G) = \sum_{uv \in \mathbf{E}(G)} [d(u)^2 + d(v)^2] = \sum_{u \in \mathbf{V}(G)} d(u)^3.$$

The respective coindices are

$$\begin{aligned}\overline{M}_1(G) &= \sum_{uv \notin \mathbf{E}(G)} [d(u) + d(v)] \\ \overline{M}_2(G) &= \sum_{uv \notin \mathbf{E}(G)} d(u) d(v) \\ \overline{F}(G) &= \sum_{uv \notin \mathbf{E}(G)} [d(u)^2 + d(v)^2].\end{aligned}$$

Bearing in mind that

$$TI(G) + \overline{TI}(G) = \frac{1}{2} \left[\sum_{u \in \mathbf{V}(G)} \sum_{v \in \mathbf{V}(G)} \varphi(d(u), d(v)) - \sum_{u \in \mathbf{V}(G)} \varphi(d(u), d(u)) \right]$$

and therefore

$$M_1(G) + \overline{M}_1(G) = \frac{1}{2} \left[\sum_{u \in \mathbf{V}(G)} \sum_{v \in \mathbf{V}(G)} [d(u) + d(v)] - \sum_{u \in \mathbf{V}(G)} [d(u) + d(u)] \right]$$

and recalling that

$$\sum_{u \in \mathbf{V}(G)} d(u) = 2m$$

we get

$$M_1(G) + \overline{M}_1(G) = \frac{1}{2} [2mn + 2mn - 4m]$$

and thus arrive at:

LEMMA 2.1. [10] *Let G be a graph with n vertices and m edges. Then*

$$M_1(G) + \overline{M}_1(G) = 2m(n - 1).$$

In an analogous manner, we have:

LEMMA 2.2. [10] *Let G be a graph with m edges. Then*

$$M_2(G) + \overline{M}_2(G) = 2m^2 - \frac{1}{2} M_1(G).$$

LEMMA 2.3. *Let G be a graph with n vertices. Then*

$$F(G) + \overline{F}(G) = (n - 1)M_1(G).$$

3. Main results

The starting point in several earlier studies of estimates of Sombor-type indices [8, 9, 20] were the inequalities

$$(3.1) \quad \frac{1}{\sqrt{2}} (a + b) \leq \sqrt{a^2 + b^2} < a + b.$$

When applying (3.1) to vertex degrees, one must take into account that a and b are positive integers not greater than $n - 1$. Therefore, the left-hand side equality holds whenever $a = b$, whereas the right-hand inequality is strict (i.e., equality would hold if either $a = 0$ or $b = 0$).

Applying (3.1) to the definitions of Sombor and elliptic Sombor indices, one immediately obtains the many-times reported relations:

$$(3.2) \quad \frac{1}{\sqrt{2}} M_1(G) \leq SO(G) < M_1(G)$$

and

$$(3.3) \quad \frac{1}{\sqrt{2}} [F(G) + 2 M_2(G)] \leq ESO(G) < F(G) + 2 M_2(G).$$

In (3.3) we have used the fact that

$$\sum_{uv \in \mathbf{E}(G)} [d(u) + d(v)]^2 = F(G) + 2 M_2(G).$$

Equality on the left-hand side of (3.2) and (3.3) holds if and only if the graph G is regular.

We are now going to improve the bounds (3.2) and (3.3). From now on, without losing generality, it will be assumed that $a \geq b$.

Denote by Δ and δ the maximal and minimal vertex degree in the considered graph G . Then Δ is the greatest possible value of the parameter a , whereas δ is the smallest possible value of the parameter b .

Introduce the auxiliary functions

$$Q_1 = Q_1(a, b) = a + b - \sqrt{a^2 + b^2}$$

and

$$Q_2 = Q_2(a, b) = \sqrt{a^2 + b^2} - \frac{1}{\sqrt{2}} (a + b)$$

and note that that (3.1) is equivalent to the conditions $Q_1 > 0$ and $Q_2 \geq 0$.

Since

$$\frac{\partial Q_1}{\partial a} = 1 - \frac{a}{\sqrt{a^2 + b^2}}$$

is positive-valued for any $a > 0$, the function Q_1 is monotonically increasing in the variable a . By symmetry, the same holds also for the variable b . Therefore, the maximal value of Q_1 is $Q_1(\Delta, \Delta)$. This implies

$$a + b - \sqrt{a^2 + b^2} \leq \Delta + \Delta - \sqrt{\Delta^2 + \Delta^2} = (2 - \sqrt{2}) \Delta$$

and by summation over all pairs of adjacent vertices of the graph G , we obtain:

$$(3.4) \quad M_1(G) - SO(G) \leq (2 - \sqrt{2}) \Delta m.$$

The case of the function Q_2 is somewhat different. The derivative

$$\frac{\partial Q_2}{\partial a} = \frac{a}{\sqrt{a^2 + b^2}} - \frac{1}{\sqrt{2}}$$

is positive-valued if and only if $a > b$. On the other hand, in view of $b \leq a$, $\delta Q_2/\delta b$ is negative valued, i.e., Q_2 is monotonically decreasing in the variable b . Therefore, the maximal value of Q_2 is $Q_2(\Delta, \delta)$. This implies

$$\sqrt{a^2 + b^2} - \frac{1}{\sqrt{2}}(a + b) \leq \sqrt{\Delta^2 + \delta^2} - \frac{1}{\sqrt{2}}(\Delta + \delta)$$

and by summation over all pairs of adjacent vertices of the graph G , we obtain:

$$(3.5) \quad SO(G) - \frac{1}{\sqrt{2}} M_1(G) \leq \left[\sqrt{\Delta^2 + \delta^2} - \frac{1}{\sqrt{2}}(\Delta + \delta) \right] m.$$

Combining relations (3.4) and (3.5) we arrive at our first main result.

THEOREM 3.1. *Let G be a graph with m edges, maximum vertex degree Δ , and minimum vertex degree δ . Then its Sombor index is bounded as:*

$$M_1(G) - (2 - \sqrt{2}) \Delta m \leq SO(G) \leq \frac{1}{\sqrt{2}} M_1(G) + \left[\sqrt{\Delta^2 + \delta^2} - \frac{1}{\sqrt{2}}(\Delta + \delta) \right] m.$$

Equality on the left-hand side holds if and only if G is regular. Equality on the right-hand side holds if and only if all edges of G connect a vertex of degree Δ with a vertex of degree δ (which includes regular graphs when $\Delta = \delta$).

In order to obtain analogous estimates for the elliptic Sombor index, we consider the auxiliary functions

$$\begin{aligned} R_1 &= R_1(a, b) = (a + b)^2 - (a + b) \sqrt{a^2 + b^2} \\ R_2 &= R_2(a, b) = (a + b) \sqrt{a^2 + b^2} - \frac{1}{\sqrt{2}}(a + b)^2. \end{aligned}$$

Since $R_1 = (a + b) Q_1$, and since Q_1 is monotonically increasing in both variables a and b , this must be the case also with R_1 . Thus

$$(a + b)^2 - (a + b) \sqrt{a^2 + b^2} \leq (\Delta + \Delta)^2 - (\Delta + \Delta) \sqrt{\Delta^2 + \Delta^2} = 2(2 - \sqrt{2}) \Delta^2$$

and by summation over all pairs of adjacent vertices of the graph G , we get

$$(3.6) \quad F(G) + 2 M_2(G) - ESO(G) \leq 2(2 - \sqrt{2}) \Delta^2 m.$$

From $R_2 = (a + b) Q_2$ we conclude that provided $a > b$, R_2 monotonically increases in the variable a . In order to resolve the case of variable b , rewrite R_2 as

$$R_2 = a^2 \left[(1 + \gamma) \sqrt{1 + \gamma^2} - \frac{1}{\sqrt{2}}(1 + \gamma)^2 \right]$$

where $\gamma = b/a$.

By numerical testing it can be shown that $(1 + \gamma) \sqrt{1 + \gamma^2} - \frac{1}{\sqrt{2}}(1 + \gamma)^2$ monotonically decreases in the interval $(0, 1)$. This implies that R_2 attains its greatest value for minimal γ , which must be $\gamma = \delta/\Delta$, that is $a = \Delta$ and $b = \delta$, that is at $R_2(\Delta, \delta)$. We thus have

$$(a + b) \sqrt{a^2 + b^2} - \frac{1}{\sqrt{2}}(a + b)^2 \leq (\Delta + \delta) \sqrt{\Delta^2 + \delta^2} - \frac{1}{\sqrt{2}}(\Delta + \delta)^2$$

and

$$(3.7) \quad ESO(G) - \frac{1}{\sqrt{2}} [F(G) + 2 M_2(G)] \leq \left[(\Delta + \delta) \sqrt{\Delta^2 + \delta^2} - \frac{1}{\sqrt{2}} (\Delta + \delta)^2 \right] m.$$

By combining the relations (3.6) and (3.7), we obtain the second main result.

THEOREM 3.2. *Let G be a graph with m edges, maximum vertex degree Δ , and minimum vertex degree δ . Then its elliptic Sombor index is bounded as:*

$$\begin{aligned} & F(G) + 2 M_2(G) - 2(2 - \sqrt{2}) \Delta^2 m \leq ESO(G) \\ & \leq \frac{1}{\sqrt{2}} [F(G) + 2 M_2(G)] + \left[(\Delta + \delta) \sqrt{\Delta^2 + \delta^2} - \frac{1}{\sqrt{2}} (\Delta + \delta)^2 \right] m. \end{aligned}$$

Conditions for equality are same as in Theorem 3.1.

The coindex-version of the estimates (3.2) is

$$\frac{1}{\sqrt{2}} \overline{M}_1(G) \leq \overline{SO}(G) < \overline{M}_1(G)$$

which together with (3.2) yields

$$\frac{1}{\sqrt{2}} [M_1(G) + \overline{M}_1(G)] \leq SO(G) + \overline{SO}(G) < M_1(G) + \overline{M}_1(G).$$

Taking into account Lemma 2.1, we obtain bounds involving the Sombor index and its coindex.

THEOREM 3.3. *Let G be a graph with n vertices and m edges. Then the sum of its Sombor index and its coindex is bounded as:*

$$\sqrt{2}m(n-1) \leq SO(G) + \overline{SO}(G) < 2m(n-1).$$

Equality on the left-hand side holds if and only if the graph G is regular.

In an analogous manner, using Eq. (3.3), and Lemmas 2.2 and 2.3 we have:

THEOREM 3.4. *Let G be a graph with n vertices and m edges. Then the sum of its elliptic Sombor index and its coindex is bounded as:*

$$\frac{1}{\sqrt{2}} [(n-2) M_1(G) + 4m^2] \leq ESO(G) + \overline{ESO}(G) < (n-2) M_1(G) + 4m^2.$$

Equality on the left-hand side holds if and only if the graph G is regular.

If instead of Eqs. (3.2) and (3.3), we employ the results of Theorems 3.1 and 3.2, the following improved versions of Theorems 3.3 and 3.4 are obtained.

THEOREM 3.5. *Let G be a graph with n vertices, m edges, maximal vertex degree Δ , and minimal vertex degree δ . Then the sum of its Sombor index and its coindex is bounded as:*

$$\begin{aligned} & 2m(n-1) - (2 - \sqrt{2}) \Delta m \leq SO(G) + \overline{SO}(G) \\ & \leq \sqrt{2}m(n-1) + \left[\sqrt{\Delta^2 + \delta^2} - \frac{1}{\sqrt{2}} (\Delta + \delta) \right] m. \end{aligned}$$

Conditions for equality are same as in Theorem 3.1.

THEOREM 3.6. *Let G be a graph with n vertices, m edges, maximal vertex degree Δ , and minimal vertex degree δ . Then the sum of its elliptic Sombor index and its coindex is bounded as:*

$$\begin{aligned} & (n-2) M_1(G) + 4m^2 - 2(2 - \sqrt{2}) \Delta^2 m \leq ESO(G) + \overline{ESO}(G) \\ & \leq \frac{1}{\sqrt{2}} \left[(n-2) M_1(G) + 4m^2 \right] + \left[(\Delta + \delta) \sqrt{\Delta^2 + \delta^2} - \frac{1}{\sqrt{2}} (\Delta + \delta)^2 \right] m. \end{aligned}$$

Conditions for equality are same as in Theorem 3.1.

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