

Research Article

Estimating the Sombor Index

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Abstract

Let SO and M_1 denote the Sombor index and the first Zagreb index of a graph G . Sharp estimates for the Sombor index of the form $M_1 - \Theta_1 \leq SO \leq M_1 - \Theta_2$ are derived, the parameters Θ_1 and Θ_2 are determined for various classes of graphs, and the corresponding equality cases are established.

Keywords: Sombor index; first Zagreb index; degree (of vertex); topological index; BID index.

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1. Introduction

Throughout the present paper, G denotes a simple graph whose vertex and edge sets are $V(G)$ and $E(G)$, respectively. The number of vertices (order) and the number of edges (size) of G are denoted by $n = |V(G)|$ and $m = |E(G)|$, and the degree of a vertex $u \in V(G)$ by d_u . In order to avoid trivialities, in what follows we assume that the graph G is connected and that $n \geq 3$ and $m \geq 2$.

The Sombor index is a bond incident degree (BID) topological index, introduced in 2021 [4], and defined as

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

where summation goes over all edges $uv \in E(G)$. By uv we denote the edge connecting the vertices u and v .

Another classical and much studied BID index is the first Zagreb index [1, 13], defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

In some of the earliest papers on Sombor index [5, 9], the following estimates for the Sombor index were determined

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

with equality on the left-hand side holding for regular graphs, whereas the right-hand side inequality is strict. Later these estimates were somewhat strengthened [3, 6, 7]. In the present paper, we seek other kinds of estimates, namely for

$$M_1(G) - \Theta_1 \leq SO(G) \leq M_1(G) - \Theta_2, \quad (2)$$

with appropriately chosen positive parameters Θ_1 and Θ_2 .

Remark 1.1. Whereas the upper bound in (2) is evidently better than that in (1), this is not necessarily the case with the lower bounds. For instance, as pointed out by a referee, the lower bound in Theorem 3.3 is weaker than that in (1). To see this, recall that $M_1(G) \leq 2m\Delta$. Therefore,

$$\left(1 - \frac{1}{\sqrt{2}}\right) M_1(G) \leq (2 - \sqrt{2})m\Delta \implies M_1(G) - (2 - \sqrt{2})m\Delta \leq \frac{1}{\sqrt{2}} M_1(G).$$

2. Preparations

The estimates (1) are a straightforward consequence of the well known analytical inequality stated in Lemma 2.1.

Lemma 2.1. *Let x and y be non-negative real numbers. Then*

$$\frac{1}{\sqrt{2}}(x + y) \leq \sqrt{x^2 + y^2} \leq x + y.$$

Equality on the left-hand side holds if and only if $x = y$. Equality on the right-hand side holds if and only if either $x = 0$ or $y = 0$ (or both).

Relations (1) are obtained by identifying x, y with the degrees of the vertices of the graph G , and then summing over all pairs of adjacent vertices. Of course, $1 \leq d_u, d_v \leq n - 1$ needs to be taken into account, as well as that $d_u = d_v = 1$ cannot occur in connected graphs with $n \geq 3$ vertices.

Lemma 2.1 has been much used in the recently evolving theory of Sombor-type BID indices, see for instance [8, 10, 12].

Bearing in mind Lemma 2.1, we consider an auxiliary function

$$f(x, y) = x + y - \sqrt{x^2 + y^2} \tag{3}$$

which for $x, y > 0$ is positive-valued.

Because of

$$\frac{\partial f(x, y)}{\partial x} = 1 - \frac{x}{\sqrt{x^2 + y^2}} > 0 \quad \text{and} \quad \frac{\partial f(x, y)}{\partial y} = 1 - \frac{y}{\sqrt{x^2 + y^2}} > 0,$$

we see that for any fixed value of $y > 0$, $f(x, y)$ is monotonically increasing in the variable x , and the same holds also for the variable y . Therefore, $f(d_u, d_v)$ will have its greatest (respectively, smallest) value if d_u and d_v assume their greatest (respectively, smallest) values. Denote these greatest and smallest values by θ_1 and θ_2 . Then, $\theta_2 \leq f(d_u, d_v) \leq \theta_1$, which by (3) results in

$$(d_u + d_v) - \theta_1 \leq \sqrt{(d_u)^2 + (d_v)^2} \leq (d_u + d_v) - \theta_2.$$

Summation over all edges uv of the graph G yields the estimates (2), where $\Theta_1 = m\theta_1$ and $\Theta_2 = m\theta_2$.

It remains now to determine Θ_1 and Θ_2 , which, of course, will depend on the type of graphs considered.

3. Main Results: Lower Bounds

Consider first a general connected graph G of order n . Then for $u, v \in V(G)$, $f(d_u, d_v)$ will be maximal if both vertex degrees are as large as possible, i.e., if $d_u = d_v = n - 1$. Therefore,

$$\theta_1 = [(n-1) + (n-1)] - \sqrt{(n-1)^2 + (n-1)^2} = (2 - \sqrt{2})(n-1).$$

This gives the following result.

Theorem 3.1. *Denote by K_n the complete graph of order n . Let G be a connected graph of order n and size m . Then*

$$M_1(G) - (2 - \sqrt{2})m(n-1) \leq SO(G).$$

Equality holds if and only if $G \cong K_n$.

Since $m \leq n(n-1)/2$, as a special case of Theorem 3.1, we have the following corollary.

Corollary 3.2. *Let G be a connected graph of order n . Then*

$$M_1(G) - \frac{2 - \sqrt{2}}{2} n(n-1)^2 \leq SO(G)$$

which is equivalent to

$$M_1(G) + SO(K_n) - M_1(K_n) \leq SO(G). \quad (4)$$

Equality holds if and only if $G \cong K_n$.

Denote by Δ the greatest vertex degree of the graph G . Then in a fully analogous manner, we obtain the next result.

Theorem 3.3. *Let G be a connected graph of size m and let Δ be its greatest vertex degree. Then*

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

Equality holds if and only if G is a regular graph of degree Δ .

Bearing in mind that the star is the tree with the greatest Sombor and first Zagreb indices, by analogy to inequality (4), we would expect the following claim.

Claim 3.4. *Denote by S_n the star graph of order n . Let T be a tree of order n . Then*

$$M_1(T) + SO(S_n) - M_1(S_n) \leq SO(T)$$

which is equivalent to

$$M_1(T) - (n-1) \left[n - \sqrt{(n-1)^2 + 1} \right] \leq SO(T).$$

Equality holds if and only if $T \cong S_n$.

Unfortunately, as demonstrated by a referee, not only is Claim 3.4 invalid, but its opposite

$$M_1(T) - (n-1) \left[n - \sqrt{(n-1)^2 + 1} \right] \geq SO(T) \quad (5)$$

holds. In order to see this, notice that

$$f(x, y) = \frac{(x + y - \sqrt{x^2 + y^2})(x + y + \sqrt{x^2 + y^2})}{x + y + \sqrt{x^2 + y^2}} = \frac{2xy}{x + y + \sqrt{x^2 + y^2}} = \frac{2(x + y)}{x + y + \sqrt{x^2 + y^2}} \cdot \frac{xy}{x + y}.$$

Therefore,

$$\begin{aligned} \sum_{uv \in \mathbf{E}(T)} f(d_u, d_v) &= \sum_{uv \in \mathbf{E}(T)} \frac{2(d_u + d_v)}{d_u + d_v + \sqrt{(d_u)^2 + (d_v)^2}} \cdot \frac{d_u d_v}{d_u + d_v} \geq \sum_{uv \in \mathbf{E}(T)} \frac{2n}{\sqrt{(n-1)^2 + 1} + n} \cdot \frac{d_u d_v}{d_u + d_v} \\ &= \frac{2n}{\sqrt{(n-1)^2 + 1} + n} \sum_{uv \in \mathbf{E}(T)} \frac{d_u d_v}{d_u + d_v} \end{aligned}$$

because, as shown in [11],

$$\frac{\sqrt{(d_u)^2 + (d_v)^2}}{d_u + d_v} \leq \frac{\sqrt{(n-1)^2 + 1}}{n}.$$

Using Cauchy's inequality, we further have

$$\sum_{uv \in \mathbf{E}(T)} \frac{d_u d_v}{d_u + d_v} = \sum_{uv \in \mathbf{E}(T)} \frac{1}{1/d_u + 1/d_v} \geq \frac{(n-1)^2}{\sum_{uv \in \mathbf{E}(T)} (1/d_u + 1/d_v)} = \frac{(n-1)^2}{n}$$

which implies (5). Equality in (5) holds if and only if every edge of T has degree pair $\{1, n-1\}$, that is, $T \cong S_n$.

4. Main Results: Upper Bounds

If G is any connected graph, then the smallest possible value of $f(d_u, d_v)$ is attained for $d_u = 2$, $d_v = 1$ or vice versa. Recall that in connected graphs with more than two vertices, $d_u = d_v = 1$ cannot occur.

Theorem 4.1. Denote by P_n the path graph of order n . Let G be a connected graph of order $n \geq 3$ and of size m . Then

$$M_1(G) - (3 - \sqrt{5})m \geq SO(G).$$

Equality holds if and only if $G \cong P_3$.

Remark 4.2. Theorem 4.1 was earlier communicated in [6].

In the case of graphs without pendent vertices, we have the following variant of Theorem 4.1. Note that, in this case, $f(2, 2)$ has the smallest value.

Theorem 4.3. Denote by C_n the cycle of order n . Let G be a connected graph of order $n \geq 3$ and of size m , not possessing pendent vertices. Then

$$M_1(G) - (4 - \sqrt{8})m \geq SO(G).$$

Equality holds if and only if $G \cong C_n$.

In a manner fully analogous to that of Theorem 3.3, we obtain the following result.

Theorem 4.4. *Let G be a connected graph of size m and let δ be its smallest vertex degree. Then*

$$M_1(G) - (2 - \sqrt{2})m\delta \geq SO(G).$$

Equality holds if and only if G is a regular graph of degree δ .

Remark 4.5. *A result equivalent to Theorem 4.4 was obtained in [2]. Also, Theorem 4.3 follows from this known bound.*

Finding an upper bound applicable to trees is somewhat less straightforward. First we notice that if for an edge uv , $d_u + d_v > n$, then this edge belongs to at least one triangle. Because trees do not possess triangles, we must have $d_u + d_v \leq n$ for all edges uv of a tree.

Equation (3) can be rewritten as

$$f(x, y) = x + y - \sqrt{(x + y)^2 - 2xy}.$$

Setting $x + y = s$ and $2xy = t$, we have

$$f(x, y) \equiv g(s, t) = s - \sqrt{s^2 - t}$$

Since

$$\frac{\partial g(s, t)}{\partial s} = 1 - \frac{s}{\sqrt{s^2 - t}} < 0 \quad \text{and} \quad \frac{\partial g(s, t)}{\partial t} = \frac{1}{2\sqrt{s^2 - t}} > 0,$$

we see that for any fixed value of $t > 0$, $g(s, t)$ is monotonically decreasing in the variable s , whereas the opposite holds for the variable t . Therefore, a lower bound for $g(d_u + d_v, 2d_u d_v)$ is obtained by taking $d_u + d_v$ as large as possible and $2d_u d_v$ as small as possible. In the case of trees, we have $d_u + d_v \leq n$ and $2d_u d_v \geq 4$. This leads to the following result.

Theorem 4.6. *Let T be a tree of order n . Then*

$$M_1(T) - (n - 1)(n - \sqrt{n^2 - 4}) \geq SO(T).$$

Equality holds if and only if $T \cong P_3$.

Remark 4.7. *For $n > 3$, the upper bound in Theorem 4.6 is slightly weaker than the earlier obtained bound (5).*

Because $d_u + d_v \leq n$ holds for all edges uv of a triangle-free graph, together with Theorem 4.6, we obtain the following result.

Theorem 4.8. *Let G be a connected triangle-free graph of order n and size m . Then*

$$M_1(G) - m(n - \sqrt{n^2 - 4}) \geq SO(G).$$

Equality holds if and only if $G \cong P_3$.

The argument used to deduce Theorem 4.6 can be slightly extended, resulting in the following two theorems.

Theorem 4.9. *Let $k \geq 3$ be an integer. Let G be a connected graph of size m , such that each of its edges uv satisfies $d_u + d_v \leq k$. Then*

$$M_1(G) - m(k - \sqrt{k^2 - 4}) \geq SO(G). \quad (6)$$

If $k = 3$, equality holds if and only if $G \cong P_3$. If $k \geq 4$, the inequality (6) is strict.

Theorem 4.10. *Let k and G be the same as in Theorem 4.9, except that G has no pendent vertices. Then*

$$M_1(G) - m(k - \sqrt{k^2 - 8}) \geq SO(G). \quad (7)$$

If $k = 4$, equality holds if and only if $G \cong C_n$ for any $n \geq 3$. If $k \neq 4$, the inequality (7) is strict.

Explanation. For equality in (6), all edges uv of the underlying graph must have the property $d_u + d_v = k$. Since the bound (6) was deduced using $2d_u d_v \geq 4$, with equality only for $d_u = 1, d_v = 2$ or vice versa, i.e., $d_u + d_v = 3$, when $k > 3$, equality cannot occur. The analogous bound (7) was obtained using $2d_u d_v \geq 8$, with equality only for $d_u = d_v = 2$, i.e., $d_u + d_v = 4$. Therefore, for $k \neq 4$, equality in (7) cannot happen.

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