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Research Paper

Improved Estimates of Sombor Index

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(Dedicated to the memory of Professor Ali Reza Ashrafi.)

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Abstract

The Sombor index (SO) is a recently invented vertex-degree-based molecular structure-descriptor. Let M_1 be the first Zagreb index. The fact that SO is bounded from below by $M_1/\sqrt{2}$ and from above by M_1 is well-known and easy to prove. In this paper, we improve these bounds.

1 Introduction

The Sombor index is a recently introduced vertex-degree-based molecular structure descriptor, conceived on geometry-based considerations [1]. It is defined as

$$SO = SO(G) = \sum_{uv} \sqrt{d(u)^2 + d(v)^2}, \tag{1}$$

where $d(u)$ is the degree (= number of first neighbors) of the vertex u of the (molecular) graph G, and the summation goes over all pairs of adjacent vertices of G. Since its discovery in 2021 [1], the Sombor index found numerous chemical [2–7] and network-scientific [8, 9] applications. It was the subject of detailed mathematical studies, see the review [10] and the references cited therein. Relations between SO and other topological indices were also extensively investigated [11–13]. The first Zagreb index,

$$M_1 = M_1(G) = \sum_{uv} [d(u) + d(v)], \tag{2}$$

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is the oldest and most thoroughly studied vertex-degree-based topological index, see the reviews [14–16]. The fact that the Sombor index is bounded by the first Zagreb index from both below and above, namely as:

$$\frac{1}{\sqrt{2}} M_1(G) \leq SO(G) < M_1(G), \tag{3}$$

was established by numerous authors, at the very beginning of the study of mathematical properties of this graph invariant [11–13, 17, 18]. For the sake of completeness, we repeat the proof of the relations (3).

a) Let x and y be non-negative real numbers. From $(x-y)^2 \geq 0$, it follows

$$x^2 + y^2 \geq 2xy \Longleftrightarrow 2x^2 + 2y^2 \geq 2xy + x^2 + y^2 = (x+y)^2,$$

and therefore

$$2(x^2 + y^2) \geq (x+y)^2 \quad i.e., \frac{1}{\sqrt{2}}(x+y) \leq \sqrt{x^2+y^2},$$

with equality if and only if $x = y$. Applying this to degrees of adjacent vertices of a graph, we get

$$\frac{1}{\sqrt{2}}[d(u) + d(v)] \leq \sqrt{d(u)^2 + d(v)^2}. \tag{4}$$

By summation over all pairs of adjacent vertices, taking into account Equations (1) and (2), we arrive at the left-hand side of inequality (3). Equality is attained if $d(u) = d(v)$ holds for all pairs of adjacent vertices of the underlying graph G. Thus, for connected graphs, equality is attained if and only if the graph is regular.

b) For non-negative x, y it follows

$$(x+y)^2 = x^2 + y^2 + 2xy \geq x^2 + y^2 \quad i.e., x + y \geq \sqrt{x^2+y^2}, \tag{5}$$

with equality if and only if at least one among x, y is equal to zero. Applying this to degrees of adjacent vertices of a graph, we get

$$\sqrt{d(u)^2 + d(v)^2} < d(u) + d(v). \tag{6}$$

Equality is impossible, since adjacent vertices are connected by an edge and therefore their degree is at least unity. By summation over all pairs of adjacent vertices, taking into account Eqs. (1) and (2), we arrive at the right-hand side of inequality (3). Again, equality cannot occur.

2 Improving the bound $SO < M_1$

In what follows, we will assume that the graph G is connected, and has n vertices and m edges, $m \geq 1 (i.e., n \geq 2)$. The edge uv of G, whose end vertices have degrees $d(u) = i$ and $d(v) = j$ (or vice versa), will be referred to as an edge of (i, j)-type. As usual, the n-vertex path and star will be denoted by P_n and S_n, respectively. In order to improve the right-hand side of inequality (3), we note that since the difference $d(u)+d(v)-\sqrt{d(u)^2 + d(v)^2}$ is necessarily positive-valued, we need to search for its minimum value. Consider the function $\beta(x, y) = x + y - \sqrt{x^2+y^2}$. Since $x, y > 0$, we have

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

Thus, $\beta(x,y)$ is monotonically increasing in both x and y. Therefore, bearing in mind that all vertex degrees of all (connected) graphs are greater than or equal to unity, we conclude that

$$d(u)+d(v)-\sqrt{d(u)^2+d(v)^2} \geq \beta(1,1) = 2-\sqrt{2}.$$

Summation over all pairs of adjacent vertices, yields:

Theorem 2.1. *For all connected graphs with $n \geq 2$ vertices and m edges,*

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

Equality holds if and only if $G \cong P_2$, since P_2 is the only connected graph whose all edges are of $(1,1)$-type.
Let now assume that $n \geq 3$. Then edges of type $(1,1)$ cannot occur, and therefore for all edges uv of all graphs,

$$d(u)+d(v)-\sqrt{d(u)^2+d(v)^2} \geq \beta(1,2) = 3-\sqrt{5}.$$

This implies:

Theorem 2.2. *For all connected graphs with $n \geq 3$ vertices and m edges,*

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

Equality holds if and only if $G \cong P_3$, since P_3 is the only connected graph whose all edges are of $(1,2)$-type. Consider now the case $n \geq 4$. For this we need to calculate:

$$\begin{aligned}\beta(1,2) &= 3-\sqrt{5} = 0.7639,\\ \beta(1,3) &= 4-\sqrt{10} = 0.8377,\\ \beta(2,2) &= 4-\sqrt{8} = 1.1716.\end{aligned}$$

There exists a graph whose all edges are of $(1,3)$-type, namely the star S_4. In order to be able to state our next theorem, we need to compare the β-contributions of S_4 and P_4 , namely $3\beta(1,3)$ and $2\beta(1,2)+\beta(2,2)$. Direct calculation shows that the former is smaller. By this, we get:

Theorem 2.3. *For all connected graphs with $n \geq 4$ vertices and m edges,*

$$SO(G) \leq M_1(G) - (4-\sqrt{10})m.$$

Equality holds if and only if $G \cong S_4$, since S_4 is the only connected graph whose all edges are of $(1,3)$-type.

3 Improving the bound $SO \geq \dfrac{M_1}{\sqrt{2}}$

We already know that equality on the left-hand side of (3) holds for all regular graphs, i.e., that this part of the bound (3) is sharp. Therefore we have to examine the case when the graph G is non-regular. In analogy to what we did in the previous section, we now introduce the function $\gamma(x,y) = \sqrt{x^2+y62} - \frac{1}{\sqrt{2}}(x+y)$. Its minimal value is zero, whenever $x = y$. Therefore, bearing in mind that we are dealing with vertex degrees, the next-smallest value must be of the form $\gamma(x,x+1)$ or $\gamma(x,x-1)$. Since $\gamma(x,x+1)$ is a monotonically decreasing function of x, the smallest γ-value will be $\gamma(\Delta, \Delta-1)$, where Δ is the maximal vertex degree of the underlying graph. The smallest γ-contribution will be at a graph in which the degree of all vertices except one is $\Delta-1$, whereas one vertex has degree Δ. Such graphs have Δ edges of type $(\Delta, \Delta-1)$, whereas all other edges are of (Δ, Δ)-type. Bearing this in mind, we arrive at:

Theorem 3.1. *For all connected non-regular graphs with n vertices and maximum vertex degree Δ,*

$$SO(G) \geq \frac{1}{\sqrt{2}} M_1(G) + \Delta\gamma(\Delta, \Delta-1) = \frac{1}{\sqrt{2}} M_1(G) + \Delta \left[\sqrt{2\Delta^2 - 2\Delta + 1} - \frac{1}{\sqrt{2}}(2\Delta - 1) \right].$$

Equality holds if and only if G has $n-1$ vertices of degree $\Delta-1$ and one vertex of degree Δ. Note that the graphs for which equality in Theorem 3.1 holds, must have odd number of vertices whereas Δ must be even. A few examples of such graphs are depicted in Figure 1.

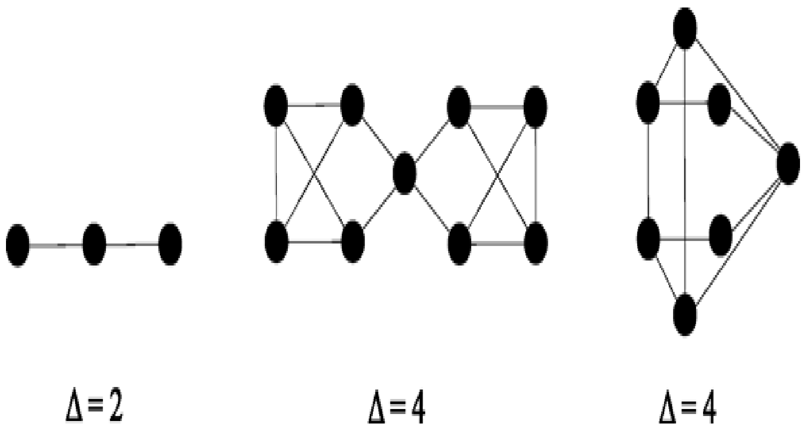

Figure 1: Examples of graphs having one vertex of degree Δ and all other vertices of degree $\Delta-1$. For such graphs equality in Theorem 3.1 holds.

4 Concluding remarks

The bounds (3) for the Sombor index are the direct consequence of the elementary analytical inequalities $\frac{1}{\sqrt{2}}(x+y) \leq \sqrt{x^2+y^2} \leq x+y$, as immediately recognized by numerous authors [11–13, 17, 18]. In this paper, by taking into account some basic structural features of graphs, we show how these bounds could be made somewhat sharper.

Conflicts of Interest. The author declares that he has no conflicts of interest regarding the publication of this article.

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