

New Bounds on Sombor Index

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Abstract: The Sombor index of the graph G is a degree based topological index, defined as $SO = \sum_{uv \in \mathbf{E}(G)} \sqrt{d_u^2 + d_v^2}$, where d_u is the degree of the vertex u , and $\mathbf{E}(G)$ is the edge set of G . Bounds on SO are established in terms of graph energy, size of minimum vertex cover, matching number, and induced matching number.

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1. Introduction

The Sombor index (SO) is a recently conceived vertex-degree-based molecular structure descriptor [10], defined as

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

where d_u is the degree of the vertex u , and $\mathbf{E}(G)$ is the edge set of the underlying (molecular) graph G . Its introduction [10] and reports on its chemical applications

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[1, 12, 15], was followed by a large number of mathematical studies. Most of these were concerned with characterizing graphs with extremal SO -value (e.g., [3, 4, 7]), and several established bounds for SO and other vertex-dependent graph invariants (e.g., [6, 8, 13, 18]). However, studies of the relation between Sombor index and other (not vertex-degree-based) graph invariants were undertaken only in two paper [16, 17], in which the relations between SO and (matrix-eigenvalue-based) graph energy were investigated. In the present article we go a step forward along these directions, reporting more connections between Sombor index and graph energy, as well as a few relating SO with matchings.

The concept of graph energy ($\varepsilon(G)$) was introduced in 1978 [9], based on earlier chemical applications. In the meantime, it became a popular and much studied mathematical and multidisciplinary research area [11, 14], studied in over one thousand papers. Graph energy is a quantity defined in terms of eigenvalues of the adjacency matrix (see below), and – formally – has no relation to the vertex-degree-based Sombor index. Yet, such a connection could be established [16, 17], using the method of vertex energy by Arizmendi et al. [2].

2. Preliminaries

This section outlines some definitions and previous results that are used for the rest of the paper.

2.1. Graph theory

Let $G = (V, E)$ be a simple graph with vertex set $\mathbf{V} = \mathbf{V}(G)$ and edge set $\mathbf{E} = \mathbf{E}(G)$. Given a vertex $u \in \mathbf{V}(G)$, we denote the degree of u by d_u which is the number of vertices adjacent to u . The maximal and minimal degrees of G is denoted by Δ and δ , respectively. Given a subset $\mathbf{U} \subseteq \mathbf{V}$, the graph $G[U]$ is the *induced subgraph* of G on \mathbf{U} . If every edge of \mathbf{E} is incident with a vertex of $\mathbf{C} \subseteq \mathbf{V}$, then the set \mathbf{C} is said to be a *vertex cover* of G .

2.2. Graph energy

Definition 1. Let G be a simple graph on n vertices, and let $A(G)$ be its adjacency matrix with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ [5]. The energy of G , denoted by $\varepsilon(G)$ is defined as the sum of the absolute values of these eigenvalues [11, 14]

$$\varepsilon = \varepsilon(G) = \sum_{i=1}^n |\lambda_i|.$$

Definition 2. [2] Let G and $A(G)$ be same as in Definition 1. Let $\mathbf{V}(G) = \{v_1, v_2, \dots, v_n\}$. Then the energy of the vertex v_i , denoted by $\varepsilon_G(v_i)$, is given by

$$\varepsilon_G(v_i) = |A(G)|_{ii} \quad \text{for } i = 1, 2, \dots, n$$

where $|A(G)| = (A(G)A(G)^*)^{1/2}$.

It can be shown that [2]

$$\sum_{v \in \mathbf{V}(G)} \varepsilon_G(v) = \varepsilon(G).$$

Theorem 1. [2] *Let G be a graph with vertex covering set \mathbf{C} . Then*

$$\sum_{v_i \in \mathbf{C}} \varepsilon_G(x_i) \geq \frac{1}{2} \varepsilon(G).$$

Theorem 2. [2] (a) *Let G be a graph with $x \in \mathbf{V}(G)$. Then*

$$\varepsilon_G(x) \leq \sqrt{d_x}.$$

Equality holds if and only if G consists of one or more copies of the star graph, and x is the center of a star graph.

(b) *If G has at least one edge, and Δ is its maximum vertex degree, then*

$$\varepsilon_G(x) \geq d_x / \Delta.$$

Equality holds if and only if $G \cong K_{a,a}$, $a \geq 1$.

Theorem 3. [6] *Let G be a graph on n vertices. If Δ and δ are maximum and minimum degrees of G , then*

$$\frac{n\delta^2}{\sqrt{2}} \leq SO(G) \leq \frac{n\Delta^2}{\sqrt{2}}.$$

Equality holds if and only if G is regular.

3. Energy and Sombor index

In [17] it was demonstrated that for any connected graph G with 3 or more vertices, $\varepsilon(G) < SO(G)$. If G is a bipartite graph, then this bound can be improved as follows.

Theorem 4. *Let G be a bipartite graph and δ its minimum vertex degree. Then*

$$\varepsilon(G) \leq \sqrt{\frac{2}{\delta^3}} SO(G).$$

Proof. Let the bipartite sets of G be \mathbf{U} and \mathbf{W} . We observe now that

$$\sum_{i \in \mathbf{U}} \sqrt{d_i} \leq \sum_{ij \in \mathbf{E}(G)} \frac{\sqrt{d_i}}{d_i}$$

or, more generally,

$$\sum_{i \in \mathbf{U}} \sqrt{F_i} \leq \sum_{ij \in \mathbf{E}(G)} \frac{\sqrt{F_i}}{d_i}$$

for arbitrary F . Now,

$$\sum_{ij \in \mathbf{E}(G)} \frac{\sqrt{d_i}}{d_i} \leq \sum_{ij \in \mathbf{E}(G)} \frac{\sqrt{d_i}}{\delta} = \frac{1}{\delta} \sum_{ij \in \mathbf{E}(G)} \sqrt{d_i}. \tag{1}$$

By Theorem 1,

$$\varepsilon(G) \leq 2 \sum_{i \in \mathbf{U}} \sqrt{d_i} \quad \text{and} \quad \varepsilon(G) \leq 2 \sum_{j \in \mathbf{W}} \sqrt{d_j}$$

since the sets \mathbf{U} and \mathbf{W} form vertex coverings. Without loss of generality assume that, \mathbf{U} is the vertex covering satisfying $\sum_{i \in \mathbf{U}} (d_i^2) \leq \sum_{j \in \mathbf{W}} (d_j^2)$. It follows that,

$$\begin{aligned} \frac{1}{2} \varepsilon(G) &\leq \sum_{i \in \mathbf{U}} \sqrt{d_i} \leq \sum_{ij \in \mathbf{E}(G)} \sqrt{d_i} \\ &= \sum_{ij \in \mathbf{E}(G)} \frac{1}{\sqrt{2}} \sqrt{2d_i} \leq \sum_{ij \in \mathbf{E}(G)} \frac{1}{\sqrt{2}} \sqrt{d_i + d_j} \end{aligned} \tag{2}$$

$$\begin{aligned} &\leq \frac{1}{\sqrt{2}} \sum_{ij \in \mathbf{E}(G)} \sqrt{\frac{d_i^2}{d_i} + \frac{d_j^2}{d_j}} \leq \frac{1}{\sqrt{2}} \sum_{ij \in \mathbf{E}(G)} \sqrt{\frac{d_i^2}{\delta} + \frac{d_j^2}{\delta}} \\ &= \frac{1}{\sqrt{2\delta}} \sum_{ij \in \mathbf{E}(G)} \sqrt{d_i^2 + d_j^2}. \end{aligned} \tag{3}$$

The inequality (2) is valid by assumption on degrees. Consequently, from Eqs. (1) and (3) we attain

$$\varepsilon(G) \leq \sqrt{\frac{2}{\delta^3}} \sum_{ij \in \mathbf{E}(G)} \sqrt{d_i^2 + d_j^2} = \sqrt{\frac{2}{\delta^3}} SO(G).$$

□

Theorem 5. *Let G be a simple graph. If \mathbf{C} is a vertex-covering set of G , then*

$$\frac{\sqrt{\delta} \varepsilon(G)}{2} + \frac{|\mathbf{C}| \Delta^2}{\sqrt{2}} \leq SO(G). \tag{4}$$

Proof. Let \mathbf{C} be a minimum vertex covering set. By Theorem 1, $\sum_{i \in \mathbf{C}} \varepsilon_G(i) \geq \frac{1}{2} \varepsilon(G)$. Since $\varepsilon(x) \leq \sqrt{d_x}$, we get $\frac{1}{2} \varepsilon(G) \leq \sum_{i \in \mathbf{C}} \sqrt{d_i}$. Then,

$$\begin{aligned} \sum_{i \in \mathbf{C}} \sqrt{d_i} &\leq \sum_{i \in \mathbf{C}, j \in \mathbf{V} \setminus \mathbf{C}} \sqrt{d_i + d_j} = \sum_{i \in \mathbf{C}, j \in \mathbf{V} \setminus \mathbf{C}} \sqrt{\frac{d_i^2}{d_i} + \frac{d_j^2}{d_j}} \leq \sum_{i \in \mathbf{C}, j \in \mathbf{V} \setminus \mathbf{C}} \sqrt{\frac{d_i^2}{\delta} + \frac{d_j^2}{\delta}} \\ &= \sum_{ij \in \mathbf{E}(G)} \left(\sqrt{\frac{d_i^2}{\delta} + \frac{d_j^2}{\delta}} \right) - \sum_{i, j \in \mathbf{C}} \left(\sqrt{\frac{d_i^2}{\delta} + \frac{d_j^2}{\delta}} \right) \end{aligned}$$

since

$$\frac{1}{\sqrt{\delta}} SO(G) = \sum_{ij \in \mathbf{E}(G)} \sqrt{\frac{d_i^2}{\delta} + \frac{d_j^2}{\delta}}$$

and

$$\frac{1}{\sqrt{\delta}} SO(G[\mathbf{C}]) = \sum_{i, j \in \mathbf{C}} \sqrt{\frac{d_i^2}{\delta} + \frac{d_j^2}{\delta}}$$

where δ is the minimum degree of G . Then we get,

$$\varepsilon(G) \leq \frac{2}{\sqrt{\delta}} [SO(G) - SO(G[\mathbf{C}])]. \quad (5)$$

By Theorem 3, $SO(G[\mathbf{C}]) \leq \frac{|\mathbf{C}| \Delta^2}{\sqrt{2}}$. Combining this bound with (5) we arrive at Eq. (4). \square

4. Sombor index and matchings

In this section, we give a lower bound for Sombor index in terms of matching and induced matching number.

Definition 3. Let $G = (\mathbf{V}, \mathbf{E})$ be a graph. A subset $M \subseteq E(G)$ is called *matching* if no two edges of M share a common vertex. An *induced matching* is a matching $\mathbf{M} \subseteq \mathbf{E}(G)$, such that no edge $e \in \mathbf{E}(G)$, $e \notin \mathbf{M}$, is incident to two distinct edges of \mathbf{M} . The maximum number of edges in a matching and induced matching are called *matching number* and *induced matching number*, respectively, and are denoted by $\mu(G)$ and $\mu_i(G)$, respectively.

Theorem 6. Let G be a connected graph on $n \geq 3$ vertices and $\mu(G)$ be its matching number. Then $SO(G) \geq \sqrt{8}(\mu(G) - 1) + \sqrt{5} \mu(G)$.

Proof. Let \mathbf{M} be a maximum matching set. Suppose that $|\mathbf{M}| = \mu(G) \geq 2$. If $e_1, e_2 \in \mathbf{M}$, then there exists at least one edge $e \notin \mathbf{M}$ which has one endpoint is in e_1 and other endpoint is in e_2 . It follows that there are at least $|\mathbf{M}| - 1$ edges in $\mathbf{E}(G) \setminus \mathbf{M}$ that contribute to $SO(G)$ by at least $\sqrt{8}$, since G is connected. On the other hand, the edges belonging to \mathbf{M} contribute by at least $\sqrt{5}$. Theorem 6 follows.

By direct checking one can verify that the claim of Theorem 6 holds also if $|\mathbf{M}| = 1$. \square

Theorem 7. *Let G be a connected graph on $n \geq 4$ vertices with m edges. Then $SO(G) \geq \sqrt{5}m - (\sqrt{8} - \sqrt{5})\mu(G)$. Equality holds if and only if $G \cong P_4$ and $G \cong P_5$.*

Proof. Let $e \in \mathbf{M}$. Then the contribution of the edge e to $SO(G)$ is at least $\sqrt{5}$. Let $f \notin \mathbf{M}$. If f is not a pendent edge, then its contribution to $SO(G)$ is at least $\sqrt{8}$. If f is a pendent edge, then there must exist another incident pendent edge, belonging to \mathbf{M} . Therefore one end-vertex of f must have degree 3 or greater. Therefore, the contribution of f to $SO(G)$ is at least $\sqrt{10} > \sqrt{8}$. Therefore $SO(G) \geq \sqrt{5}\mu(G) + \sqrt{8}(m - \mu(G))$, from which the claim of Theorem 7 follows.

P_4 and P_5 are the only graphs in which all elements of a maximum matching are pendent edges, and all other edges of $(2, 2)$ -type. \square

Theorem 8. *Let G be a connected graph on $n \geq 3$ vertices and $\mu_i(G)$ be its induced matching number. Then $SO(G) \geq 2\sqrt{5}\mu_i(G)$.*

Proof. Notice that an edge of a connected graph G contributes to its Sombor index by at least $\sqrt{5}$, since G has at least 3 vertices. Let \mathbf{M}_i be a maximal induced matching set. Since G is connected, if $e \in \mathbf{M}_i$, then there is at least one edge $e' \in \mathbf{E}(G) \setminus \mathbf{M}_i$, such that e' is adjacent only to e . The fact that each edge contributes to $SO(G)$ by at least $\sqrt{5}$ implies $SO(G) \geq 2\sqrt{5}\mu_i(G)$. \square

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