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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.

Keywords: Sombor index, degree (of vertex), graph

AMS Subject classification: 05C07, 05C09, 05C92

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 where 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 $\lambda_1, \lambda_2, \ldots, \lambda_n$ [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 $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$. Then the energy of the vertex v_i, denoted by $\varepsilon_G(v_i)$, is given by

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

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 $G \cong K_{a,a}$, $a \geq 1$.

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,

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

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,

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

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,

$$\sum_{i\in C}\sqrt{d_i} \leq \sum_{i\in\mathbf{C},j\in\mathbf{V}\setminus C}\sqrt{d_i+d_j} = \sum_{i\in\mathbf{C},j\in\mathbf{V}\setminus\mathbf{C}}\sqrt{\frac{d_i^2}{d_i}+\frac{d_j^2}{d_j}} \leq \sum_{i\in\mathbf{C},j\in\mathbf{V}\setminus\mathbf{C}}\sqrt{\frac{d_i^2}{\delta}+\frac{d_j^2}{\delta}}$$

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

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

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

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

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

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

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 $SO(G) \geq \sqrt{8}\big(\mu(G)-1\big) + \sqrt{5}\,\mu(G)$.*

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 $\mathbf{E}(G)\backslash\mathbf{M}$ 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 $|\mathbf{M}| = 1$. □

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 leat $\sqrt{5}$. 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 $SO(G) \geq \sqrt{5}\,\mu(G) + \sqrt{8}\,\big(m - \mu(G)\big)$, 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. □

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 $e' \in \mathbf{E}(G)\backslash\mathbf{M}_i$, such that e' is adjacent only to e. The fact that each edge contributes to $SO(G)$ by at least $\sqrt{5}$ implies $SO(G) \geq 2\sqrt{5}\,\mu_i(G)$. □

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