

Research Article

Relating graph energy and Sombor index*

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(Received: 29 August 2021. Accepted: 20 September 2021. Published online: 23 September 2021.)

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Abstract

The energy of a graph (ε) is the sum of absolute values of its eigenvalues, thus it is a graph-spectrum-based quantity. The Sombor index (SO) is a recently conceived vertex-degree-based topological index. We establish various relations between ε and SO , among which are lower and upper bounds. These relations improve and extend earlier results communicated in the paper [A. Ülker, A. Gürsoy, N. K. Gürsoy, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 51–58].

Keywords: energy (of graph); Sombor index; spectrum (of graph); topological index; degree (of vertex).

2020 Mathematics Subject Classification: 05C09, 05C50, 05C07.

1. Introduction

In this paper we are concerned with simple graphs, assumed to be connected. Let G be such a graph, with n vertices, m edges, vertex set $V(G)$, and edge set $E(G)$. The edge connecting the vertices u and v will be denoted by uv . The degree (= number of first neighbors) of the vertex $u \in V(G)$ is denoted by d_u . In addition, $\min_{u \in V(G)} d_u = \delta$ and $\max_{u \in V(G)} d_u = \Delta$.

Let $A(G)$ be the $(0, 1)$ -adjacency matrix of the graph G , and let $\lambda_1, \lambda_2, \dots, \lambda_n$ be its eigenvalues, forming the spectrum of G [3]. The energy of the graph G is defined as

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

This spectrum-based graph invariant has been extensively studied, both in mathematics [6–8] and in theoretical chemistry [5].

There are nowadays some 50 different bond incident degree (BID) graph invariants of the form

$$BID(G) = \sum_{uv \in E(G)} F(d_u, d_v)$$

where F is a suitably chosen function with the property $F(x, y) = F(y, x)$. Among them, a very recently introduced such invariant is the Sombor index, for which $F(x, y) = \sqrt{x^2 + y^2}$. Thus, the Sombor index is defined as [4],

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

At the first glance, there hardly could be expected that the spectrum-based graph energy ε and the vertex-degree-based indices $BID(G)$ are anyhow related. Yet, the first such relation was discovered by Arizmendi and Arizmendi [1], who showed that $\varepsilon(G) \leq 2R(G)$, where $R(G)$ is the Randić index, $F(x, y) = 1/\sqrt{xy}$. This was followed by Yan et al. [11], who proved that $\varepsilon(G) \geq (2/\Delta)R(G)$. These results motivated three of the present authors to seek for analogous connections between ε and SO [10]. They obtained lower and upper bounds between ε and SO (for details see below). In the present paper we improve and extend these bounds, and offer a few more relations of this kind.

*This paper was finalized on the day when the sad news arrived that Professor Nenad Trinajstić passed away. Let this humble article be dedicated to the memory of the Great Scholar and founder of chemical graph theory.

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2. Energy of a vertex and its properties

In what follows we will much exploit the concept of energy of a vertex, invented by Arizmendi et al. in 2018 [2]. In this section we repeat the basic facts of their theory.

Let the vertices of the graph G be labeled by v_1, v_2, \dots, v_n . Then the energy of the vertex v_i is defined as [2]

$$\varepsilon(x_i) = \left[[\mathbf{A}(G) \mathbf{A}(G)^T]^{1/2} \right]_{ii}$$

where $\mathbf{A}(G)^T$ is the transpose of $\mathbf{A}(G)$. It can be shown that [2]

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

Theorem 2.1. [2] *Let G be any graph and $v \in V(G)$. Then $\varepsilon(v) \leq \sqrt{d_v}$. Equality holds if and only if v is the central vertex of $K_{1,n-1}$.*

Proposition 2.1. *Let v be the central vertex of the star $K_{1,n-1}$. Then $SO(K_{1,n-1}) = \varepsilon(v)^2 \sqrt{\varepsilon(v)^4 + 1} > \varepsilon(v)^4$.*

Proof. $K_{1,n-1}$ has $m = n - 1$ edges, whereas $SO(K_{1,n-1}) = m \sqrt{m^2 + 1}$. The degree of the central vertex is equal to m , which by Theorem 2.1 is equal to $\varepsilon(v)^2$. \square

Theorem 2.2. [2] *Let G be a graph with $m \geq 1$ and maximum vertex degree Δ . Then for any $v \in V(G)$, $\varepsilon(v) \geq d_v/\Delta$. Equality holds if and only if $G \cong K_{a,a}$ for $a \geq 1$.*

3. First inequality between graph energy and Sombor index

In [10], the following result was obtained:

Proposition 3.1. [10] *Let G be a connected graph with minimum vertex degree $\delta \geq 2$. Then $\varepsilon(G) \leq SO(G)$.*

We now strengthen this result as follows:

Theorem 3.1. *Let G be a connected graph with n vertices. If $n = 2$, then $\varepsilon(G) > SO(G)$. If $n \geq 3$, then $\varepsilon(G) < SO(G)$.*

Proof. If $n = 2$, then $G \cong K_2$. It is easy to compute that $\varepsilon(K_2) = 2$ and $SO(K_2) = \sqrt{2}$.

Suppose now that $n \geq 3$. Then the graph G cannot have an edge uv such that $d_u = d_v = 1$. Then the minimal value of the term $\sqrt{d_u^2 + d_v^2}$ is $\sqrt{5}$, when $d_u = 1$, $d_v = 2$. Therefore,

$$SO(G) \geq \sqrt{5} m. \quad (1)$$

Equality in (1) holds if and only if $G \cong K_{1,2}$.

The McClelland inequality is $\varepsilon(G) \leq \sqrt{2mn}$ [8,9]. For connected graphs, equality holds if and only if $G \cong K_2$.

Consider first the case that G is a tree. Then, $n = m + 1$, and $\sqrt{2mn} = \sqrt{2m(m+1)}$. It is now easy to show that $\sqrt{2m(m+1)} < \sqrt{5} m$ holds for all $m \geq 1$.

If G is a connected cycle-containing graph, then $n \geq m$, and

$$\sqrt{2mn} \leq \sqrt{2m^2} = \sqrt{2} m < \sqrt{5} m.$$

Thus, in all cases,

$$\sqrt{2mn} < \sqrt{5} m. \quad (2)$$

Bearing in mind the inequalities (1) and (2), we have

$$\varepsilon(G) \leq \sqrt{2mn} < \sqrt{5} m \leq SO(G).$$

\square

We now improve Theorem 3.1, i.e., the inequality $\varepsilon(G)^2 < SO(G)^2$.

Theorem 3.2. *Let G be a connected graph with $n \geq 3$ vertices. If $\delta \geq 2$, then*

$$\varepsilon(G) < \sqrt{\frac{\sqrt{2}}{\delta} SO(G) + n(n-1)\Delta} \quad \text{i.e.} \quad \varepsilon(G)^2 < \frac{\sqrt{2}}{\delta} SO(G) + n(n-1)\Delta.$$

If $\delta = 1$, then

$$\varepsilon(G) \leq \sqrt{\frac{2}{\sqrt{5}} SO(G) + n(n-1)\Delta} \quad \text{i.e.} \quad \varepsilon(G)^2 \leq \frac{2}{\sqrt{5}} SO(G) + n(n-1)\Delta.$$

Proof. Directly from the definition of Sombor index, he have

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

If $\delta = 1$, since $d_u = d_v$ cannot happen, the left-hand inequality can be improved by $d_u = 1, d_v = 2$ as

$$\sqrt{5} m \leq SO(G)$$

Thus,

$$m \leq \begin{cases} \frac{SO(G)}{\sqrt{2} \delta} & \text{if } \delta \geq 2 \\ \frac{SO(G)}{\sqrt{5}} & \text{if } \delta = 1. \end{cases} \quad (3)$$

Bearing in mind Theorem 2.1,

$$\begin{aligned} \varepsilon(G) &= \sum_{v \in V(G)} \varepsilon(v) < \sum_{v \in V(G)} \sqrt{d_v} = \sqrt{\left(\sum_{v \in V(G)} \sqrt{d_v} \right)^2} \\ &= \sqrt{\sum_{v \in V(G)} d_v + 2 \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \sqrt{d_u d_v}} = \sqrt{2m + 2 \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \sqrt{d_u d_v}} \leq \sqrt{2m + 2 \binom{n}{2} \Delta} \end{aligned}$$

resulting in

$$\varepsilon(G) < \sqrt{2m + n(n-1)\Delta}. \quad (4)$$

Theorem 3.2 follows now by substituting (3) back into (4). □

4. Second inequality between graph energy and Sombor index

In [10], the following result was obtained:

Proposition 4.1. [10] *Let G be a connected graph with maximum vertex degree Δ . Then $\Delta^3 \varepsilon(G) \geq SO(G)$.*

We now establish a stronger upper bound for the Sombor index.

Theorem 4.1. *Let G be a connected graph with maximum vertex degree Δ . Then*

$$\frac{\Delta^2}{\sqrt{2}} \varepsilon(G) \geq SO(G).$$

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

Proof. By Theorem 2.2 we get

$$\varepsilon(G) = \sum_{v \in V(G)} \varepsilon(v) \geq \frac{1}{\Delta} \sum_{v \in V(G)} d_v$$

and thus

$$\varepsilon(G) \geq \frac{2m}{\Delta} \quad (5)$$

with equality if and only if $G \cong K_{a,a}$.

The term $\sqrt{d_u^2 + d_v^2}$ is maximal if $d_u = d_v = \Delta$, equal to $\sqrt{2}\Delta$. Then from the definition of Sombor index, it follows that SO is maximal if all vertex degrees are equal to Δ , i.e., if G is a regular graph. Thus

$$SO(G) \leq \sqrt{2}\Delta m \quad \text{i.e.,} \quad m \geq \frac{SO(G)}{\sqrt{2}\Delta} \quad (6)$$

with equality if and only if G is a regular graph.

Substituting (6) back into (5), we get

$$\varepsilon(G) \geq \frac{2}{\Delta} \left(\frac{SO(G)}{\sqrt{2}\Delta} \right)$$

which directly leads to Theorem 4.1. □

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