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On Sombor Index

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Abstract: The concept of Sombor index (SO) was recently introduced by Gutman in the chemical graph theory. It is a vertex-degree-based topological index and is denoted by Sombor index SO: $SO = SO(G) = \sum_{v_iv_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2}$, where $d_G(v_i)$ is the degree of vertex v_i in G. Here, we present novel lower and upper bounds on the Sombor index of graphs by using some graph parameters. Moreover, we obtain several relations on Sombor index with the first and second Zagreb indices of graphs. Finally, we give some conclusions and propose future work.

Keywords: graph; sombor index; maximum degree; minimum degree; independence number

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1. Introduction

Consider a simple graph $G = (V, E)$ with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G)$, where $|V(G)| = n$ is the number of vertices and $|E(G)| = m$ is the number of edges. For $i = 1, 2, \ldots, n$ denote by $d_G(v_i)$ the degree of vertex v_i. For $v_i \in V(G)$, let $\mu_G(v_i)$ represent the *average degree* of the vertices adjacent to vertex v_i. Let δ be the *minimum vertex degree* and Δ be the *maximum vertex degree*. It is known that any vertex v of degree 1 is a *pendant vertex*. Pendant vertex is also called *leaf*. A *pendant edge* is the edge incident with a pendant vertex. We denote by $v_iv_j \in E(G)$ when vertices v_i and v_j are adjacent.

In graph theory, a number that is invariant under graph automorphisms is referred to as a graphical invariant. It is often regarded as a structural invariant relevant to a graph. The term topological index is often reserved for graphical invariant in molecular graph theory. In the mathematical and chemical literature, several dozens of vertex-degree-based graph invariants (usually referred to as "topological indices") have been introduced and extensively studied. Their general formula is

$$TI = TI(G) = \sum_{v_iv_j \in E(G)} F(d_G(v_i), d_G(v_j)), \tag{1}$$

where $F(x, y)$ is some function with the property $F(x, y) = F(y, x)$. If $F(d_G(v_i), d_G(v_j)) = d_G(v_i) + d_G(v_j)$ or $d_G(v_i)\, d_G(v_j)$, then TI is the first Zagreb index or the second Zagreb index of graph G, respectively, which are put forward in [1] by Gutman and Trinajstić. They studied the dependence of total π-electron energy related to molecular structure. Some further development can be found for example in [2]. Given a molecular graph G, we have the *first Zagreb index* $M_1(G)$ as

$$M_1(G) = \sum_{v_iv_j \in E(G)} \Big(d_G(v_i) + d_G(v_j)\Big) = \sum_{v_i \in V(G)} d_G(v_i)^2$$

and the *second Zagreb index* $M_2(G)$ as

$$M_2(G) = \sum_{v_iv_j \in E(G)} d_G(v_i)\, d_G(v_j).$$

Many fundamental mathematical properties such as lower and upper bounds involving other important graphical invariants can be bound in, e.g., [3–15]. More recent results are reported in [16–25]. Zagreb indices characterize the degree of branching in molecular carbon-atom skeleton and are regarded as powerful molecular structure-descriptors [26,27].

Gutman mentioned a list of topological indices (26 indices including two Zagreb indices) in [28]. In the same paper, Gutman presented a novel approach to the vertex-degree-based topological index of (molecular) graphs. For this we need the following definition:

Definition 1 ([28])**.** *The ordered pair* (x, y)*, where* $x = d_G(v_i)$*,* $y = d_G(v_j)$*, is the degree-coordinate (or d-coordinate) of the edge* $v_iv_j \in E(G)$*. In the (2-dimensional) coordinate system, it pertains to a point called the degree-point (or d-point) of the edge* $v_iv_j \in E(G)$*. The point with coordinates* (y, x) *is the dual-degree-point (or dd-point) of the edge* $v_iv_j \in E(G)$*. The distance between the d-point* (x, y) *and the origin of the coordinate system is the degree-radius (or d-radius) of the edge* $v_iv_j \in E(G)$*, denoted by* $r(x, y)$*. Based on elementary geometry (using Euclidean metrics), we have* $r(x, y) = \sqrt{x^2 + y^2}$*. From this, we immediately see that a d-point and the corresponding dd-point have equal degree-radii. One can easily see that for any molecular graphs* ($d_G(v) \leq 4$)*, two degree-points have equal degree-radii if and only if they coincide, that is, if and only if both have the same degree-coordinates. Unfortunately, this property is not valid for general graphs.*

Since the function $F(x, y) = \sqrt{x^2 + y^2}$ has not been used before in the theory of vertex-degree-based topological indices, from the above considerations motivated by the author in [28], introduce a new such index defined as

$$SO = SO(G) = \sum_{v_iv_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2}$$

and called the Sombor index. In the same paper, several mathematical properties have been discussed.

Given $W \subseteq E(G)$, we denote by $G - W$ the subgraph of G which is obtained by removing any edge within W. If $W = \{v_iv_j\}$, we will write $G - v_iv_j$ instead of the subgraph $G - W$ for ease of expression. For a pair of nonadjacent vertices v_i and v_j in G, we write $G + v_iv_j$ for the graph obtained by adding the edge v_iv_j to G. Let $G[S]$ be the induced subgraph of G by $S \subseteq V(G)$. S is said to be an independent set of G if $G[S]$ is formed by $|S|$ isolated vertices. The number of vertices in the largest independent set is called the *independence number* of a given graph, which is denoted conventionally by α. If a graph on n vertices contains a clique of $n - \alpha$ vertices and the rest α vertices is a stable set, where every vertex within the clique is linked to every vertex in the stable set, then the graph is called a complete split graph and is denoted by $CS(n, \alpha)$, $1 \leq \alpha \leq n - 1$. Another interesting graph class is called (Δ, δ)-semiregular bipartite graph, where G is a bipartite graph with a bipartition U and W. Here, each vertex v_i in U admits constant degree Δ while each vertex v_j in W admits constant degree δ. Clearly, if $\Delta = \delta$, G becomes regular. As usual, K_n is a complete graph and $K_{a,b}$ with $(a + b = n)$ is a complete bipartite graph over n vertices. We refer the reader to the book [29] for other standard graph theoretical notations.

The rest of the paper is organized as follows. In Section 2, we obtain some lower and upper bounds on $SO(G)$ in terms of graph parameters. In Section 3, we present some relations between $SO(G)$ and the Zagreb indices $M_1(G)$ and $M_2(G)$. In Section 4, we give some conclusions and future work.

2. Bounds on Sombor Index of Graphs

In this section, we give several lower and upper bounds on $SO(G)$ building on some useful graph parameters. From the definition of Sombor index, the following result can be summarized.

Lemma 1. *For a graph G, we have*
(i) $SO(G) > SO(G-e)$, *where* $e = v_i v_j$ *is any edge in G,*
(ii) $SO(G+e) > SO(G)$, *where* $e = v_i v_j$ *and vertices* v_i *&* v_j *are non-adjacent in G.*

First we give the uppper and lower bounds on $SO(G)$ building on n, Δ and δ.

Theorem 1. *Suppose that G is a graph over n vertices. If G has maximum degree* Δ *and minimum degree* δ,

$$\frac{n\,\delta^2}{\sqrt{2}} \le SO(G) \le \frac{n\,\Delta^2}{\sqrt{2}}$$

with equality (left and right) if and only if G becomes a regular graph.

Proof. Recall that Δ is the maximum degree of G and δ is the minimum degree of G. By employing the Handshaking lemma, we obtain

$$n\,\delta \le \sum_{v_i \in V(G)} d_G(v_i) = 2m \le n\,\Delta$$

with equality holding (left and right) if and only if $d_G(v_i) = \Delta$ for any $v_i \in V(G)$. It follows from the definition of the Sombor index, we obtain

$$\begin{aligned} SO(G) &= \sum_{v_i v_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} \\ &\le \sqrt{2}\,\Delta\,m \le \frac{n\,\Delta^2}{\sqrt{2}}. \end{aligned}$$

Moreover, the equality herein holds if and only if $d_G(v_i) = \Delta$ for any $v_i \in V(G)$, i.e., G is regular. Similarly, we get the lower bound on Sombor index and equality holds if and only if G becomes regular. □

Since $\Delta \le n-1$, we get the following corollary.

Corollary 1 ([28]). *Let G be a graph of order n. Then*

$$SO(G) \le \frac{n\,(n-1)^2}{\sqrt{2}}$$

with equality if and only if $G \cong K_n$.

For triangle-free graph G, we obtain an upper bound on $SO(G)$ based on n, m, Δ and δ.

Theorem 2. *Let G be a triangle-free graph of order n with m edges and maximum degree* Δ, *minimum degree* δ. *Then*

$$SO(G) \le \begin{cases} m\,\sqrt{\delta^2 + (n-\delta)^2} & \text{if } \Delta + \delta \le n, \\ m\,\sqrt{\Delta^2 + (n-\Delta)^2} & \text{if } \Delta + \delta \ge n. \end{cases}$$

Proof. Let $d_G(v_i)$ be the degree of the vertex v_i in G. Since G is triangle-free graph, we have $d_G(v_i) + d_G(v_j) \le n$ for any edge $v_i v_j \in E(G)$. Let us consider a function

$h(x) = x^2 + (n-x)^2$ for $\delta \le x \le \Delta$. Then one can easily see that $h(x)$ is an increasing function on $n/2 \le x \le \Delta$ and a decreasing function on $\delta \le x \le n/2$. Hence

$$d_G(v_i)^2 + (n - d_G(v_i))^2 \le \begin{cases} \sqrt{\delta^2 + (n-\delta)^2} & \text{if } \Delta + \delta \le n, \\ \sqrt{\Delta^2 + (n-\Delta)^2} & \text{if } \Delta + \delta \ge n. \end{cases}$$

With the results obtained above, we derive

$$\begin{aligned} SO(G) &= \sum_{v_i v_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} \\ &\le \sum_{v_i v_j \in E(G)} \sqrt{d_G(v_i)^2 + (n - d_G(v_i))^2} \\ &\le \begin{cases} m\sqrt{\delta^2 + (n-\delta)^2} & \text{if } \Delta + \delta \le n, \\ m\sqrt{\Delta^2 + (n-\Delta)^2} & \text{if } \Delta + \delta \ge n. \end{cases} \end{aligned}$$

□

Gutman [28] proved that the path P_n gives the minimum value of Sombor index for any connected graph of order n. Therefore, the path P_n gives the minimum value of Sombor index for any connected bipartite graph of order n. We now give an upper bound on the Sombor index of bipartite graphs.

Theorem 3. *Let G be a bipartite graph over n vertices. Then*

$$SO(G) \le \begin{cases} \dfrac{n^3}{4\sqrt{2}} & \text{if } n \text{ is even}, \\ \dfrac{(n^2-1)\sqrt{n^2+1}}{4\sqrt{2}} & \text{if } n \text{ is odd}, \end{cases}$$

with equality if and only if $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

Proof. Let G be a bipartite graph of order n $(n = p + q,\ p \ge q)$ with two partite sets having p and q vertices, respectively. Since G is bipartite graph, by Lemma 1, we obtain $SO(G) \le SO(K_{p,q})$ with equality if and only if $G \cong K_{p,q}$. Hence

$$SO(G) \le S(K_{p,q}) = pq\sqrt{p^2+q^2} = p(n-p)\sqrt{p^2+(n-p)^2}.$$

Let us consider a function

$$f(x) = x(n-x)\sqrt{x^2+(n-x)^2}, \quad \left\lceil \frac{n}{2} \right\rceil \le x \le n-1.$$

Then

$$f'(x) = -\frac{(2x-n)\,[x^2+(n-x)^2-1]}{\sqrt{x^2+(n-x)^2}} \le 0 \ \text{ for } \left\lceil \frac{n}{2} \right\rceil \le x \le n-1.$$

Thus $f(x)$ is a decreasing function on $\lceil \frac{n}{2} \rceil \le x \le n-1$, and hence

$$SO(G) \le p(n-p)\sqrt{p^2+(n-p)^2} \le \left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor \sqrt{\left\lceil \frac{n}{2} \right\rceil^2 + \left\lfloor \frac{n}{2} \right\rfloor^2}.$$

The required inequality has been proved. Besides, the equality holds if and only if $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$. □

Next, we present an upper bound on $SO(G)$ by using n and independence number α.

Theorem 4. *Let G be a connected graph of order n with independence number α. Then $SO(G) \leq \sqrt{2}\binom{n-\alpha}{2}(n-1) + \alpha(n-\alpha)\sqrt{(n-1)^2 + (n-\alpha)^2}$ with equality if and only if $G \cong CS(n, \alpha)$.*

Proof. We obtain

$$SO(CS(n, \alpha)) = \sqrt{2}\binom{n-\alpha}{2}(n-1) + \alpha(n-\alpha)\sqrt{(n-1)^2 + (n-\alpha)^2}.$$

Since G has order n and independence number α, by Lemma 1, we obtain

$$SO(G) \leq SO(CS(n, \alpha)) = \sqrt{2}\binom{n-\alpha}{2}(n-1) + \alpha(n-\alpha)\sqrt{(n-1)^2 + (n-\alpha)^2}$$

with equality if and only if $G \cong CS(n, \alpha)$. □

We now offer an additional upper bound on $SO(G)$ in terms of m, δ and $M_1(G)$.

Theorem 5. *Let G be a graph of size m and minimum degree δ. Then*

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

where $M_1(G)$ is the first Zagreb index of graph G. Moreover, the equality holds if and only if G is a regular graph.

Proof. For any edge $v_iv_j \in E(G)$ $(d_G(v_i) \geq d_G(v_j))$, one can easily check that

$$\sqrt{d_G(v_i)^2 + d_G(v_j)^2} \leq d_G(v_i) + (\sqrt{2} - 1)\,d_G(v_j)$$

with equality if and only if $d_G(v_i) = d_G(v_j)$. Now,

$$\begin{aligned}
SO(G) &= \sum_{v_iv_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} \\
&\leq \sum_{\substack{v_iv_j \in E(G) \\ d_G(v_i) \geq d_G(v_j)}} \Big(d_G(v_i) + (\sqrt{2} - 1)\,d_G(v_j)\Big) \\
&= \sum_{v_iv_j \in E(G)} \Big(d_G(v_i) + d_G(v_j)\Big) - \sum_{\substack{v_iv_j \in E(G) \\ d_G(v_i) \geq d_G(v_j)}} (2 - \sqrt{2})\,d_G(v_j) \\
&\leq M_1(G) - (2 - \sqrt{2})\,\delta\, m.
\end{aligned}$$

Moreover, the above two inequalities are equalities if and only if G is a regular graph. □

We give an upper bound on $SO(G) + SO(\overline{G})$ by employing the number n only.

Theorem 6. *Let G be a graph over n vertices. We have*

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

with equality if and only if $G \cong K_n$ or $G \cong \overline{K}_n$.

Proof. Since $\Delta \leq n-1$, it can be easily checked that

$$\sqrt{d_G(v_i)^2 + d_G(v_j)^2} \leq \sqrt{2}\,(n-1) \quad \text{for any edge } v_iv_j \in E(G).$$

Since $|E(G)| + |E(\overline{G})| = \frac{n\,(n-1)}{2}$, we obtain

$$\begin{aligned} SO(G) + SO(\overline{G}) &= \sum_{v_iv_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2} + \sum_{v_iv_j \in E(\overline{G})} \sqrt{d_{\overline{G}}(v_i)^2 + d_{\overline{G}}(v_j)^2} \\ &\leq \frac{n\,(n-1)}{2} \times \sqrt{2}\,(n-1) = \frac{n(n-1)^2}{\sqrt{2}}. \end{aligned}$$

Moreover, the equality holds if and only if $d_G(v_i)^2 + d_G(v_j)^2 = 2\,(n-1)^2$ for any edge $v_iv_j \in E(G)$ or $d_{\overline{G}}(v_i)^2 + d_{\overline{G}}(v_j)^2 = 2(n-1)^2$ for any edge $v_iv_j \in E(\overline{G})$, that is, $G \cong K_n$ or $G \cong \overline{K}_n$. □

3. Relation between Sombor Index with Zagreb Indices of Graphs

Topological indices in mathematical chemistry are well studied in the literature. In particular we have seen several mathematical and chemical properties on topological indices of graphs, some of them are very similar, but some of them are totally different. So it is natural to ask how two topological indices are related or to find some relations between two topological indices of graphs. In last 10 years several papers have been published on this topic in the literature, see [23,25,30–37]. In this section we try to find some relations between Sombor index and the (first & second) Zagreb indices of graphs. For this we need the following result:

Lemma 2. [38] *Let $a_1, a_2, \ldots, a_k$ and $b_1, b_2, \ldots, b_k$ be real numbers so that there are constants s and t satisfying for any i, $i = 1, 2, \ldots, k$ we have $s\,a_i \leq b_i \leq t\,a_i$. Then*

$$\sum_{i=1}^{k} b_i^2 + s\,t \sum_{i=1}^{k} a_i^2 \leq (s+t) \sum_{i=1}^{k} a_i\,b_i \tag{2}$$

with equality if and only if for at least one i, $1 \leq i \leq k$ holds $s\,a_i = b_i = t\,a_i$.

Next, we investigate the relation between Sombor index $SO(G)$ and the first Zagreb index $M_1(G)$ of graph G.

Theorem 7. *Let G be a graph containing n vertices and m edges. The maximum degree is denoted by Δ and its minimum degree is $\delta > 0$. Then*

$$\left(\sqrt{2(\Delta^2 + \delta^2)} + \Delta + \delta\right) SO(G) \geq \sqrt{\Delta^2 + \delta^2}\, M_1(G) + \sqrt{2}\,(\Delta + \delta)\,\delta\,m, \tag{3}$$

where $M_1(G)$ is the first Zagreb index of graph G. Moreover, the equality holds if and only if G is a regular graph.

Proof. One can easily see that

$$\frac{\sqrt{d_G(v_i)^2 + d_G(v_j)^2}}{d_G(v_i) + d_G(v_j)} \geq \frac{1}{\sqrt{2}}, \quad \text{that is,} \quad \Big(d_G(v_i) - d_G(v_j)\Big)^2 \geq 0$$

with equality if and only if $d_G(v_i) = d_G(v_j)$. Since $0 < \delta \leq d_G(v_i) \leq \Delta$, for any $v_i \in V(G)$, we have

$$\frac{\delta}{\Delta} \leq \frac{d_G(v_i)}{d_G(v_j)} \leq \frac{\Delta}{\delta} \tag{4}$$

with right (left) equality if and only if $d_G(v_i) = \Delta$ and $d_G(v_j) = \delta$ ($d_G(v_i) = \delta$ and $d_G(v_j) = \Delta$). Let $f(x) = \dfrac{\sqrt{1+x^2}}{1+x}$, $x \geq 1$. Then we have

$$f'(x) = \frac{x-1}{\sqrt{1+x^2}\,(1+x)^2},\ x \geq 1.$$

Thus $f(x)$ is an increasing function on $x \geq 1$. Using the above results, we obtain

$$\frac{1}{\sqrt{2}} \leq \frac{\sqrt{d_G(v_i)^2 + d_G(v_j)^2}}{d_G(v_i) + d_G(v_j)} = \frac{\sqrt{1 + \dfrac{d_G(v_i)^2}{d_G(v_j)^2}}}{1 + \dfrac{d_G(v_i)}{d_G(v_j)}} \leq \frac{\sqrt{\Delta^2 + \delta^2}}{\Delta + \delta}.$$

For any edge $v_iv_j \in E(G)$, one can easily check that

$$\frac{d_G(v_i)^2 + d_G(v_j)^2}{d_G(v_i) + d_G(v_j)} \geq \delta$$

with equality if and only if $d_G(v_i) = \delta = d_G(v_j)$, that is,

$$\sum_{v_iv_j \in E(G)} \frac{d_G(v_i)^2 + d_G(v_j)^2}{d_G(v_i) + d_G(v_j)} \geq m\,\delta \tag{5}$$

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

Setting $s = \frac{1}{\sqrt{2}}$, $t = \dfrac{\sqrt{\Delta^2+\delta^2}}{\Delta+\delta}$, $a_i \to \sqrt{d_G(v_i) + d_G(v_j)}$ and $b_i \to \sqrt{\dfrac{d_G(v_i)^2 + d_G(v_j)^2}{d_G(v_i) + d_G(v_j)}}$ in Lemma 2, we obtain

$$\sum_{v_iv_j \in E(G)} \frac{d_G(v_i)^2 + d_G(v_j)^2}{d_G(v_i) + d_G(v_j)} + \frac{\sqrt{\Delta^2+\delta^2}}{\sqrt{2}(\Delta+\delta)} \sum_{v_iv_j \in E(G)} \Big(d_G(v_i) + d_G(v_j)\Big)$$
$$\leq \left(\frac{\sqrt{\Delta^2+\delta^2}}{\Delta+\delta} + \frac{1}{\sqrt{2}}\right) \sum_{v_iv_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2}, \tag{6}$$

that is,

$$m\,\delta + \frac{\sqrt{\Delta^2+\delta^2}}{\sqrt{2}(\Delta+\delta)}\,M_1(G) \leq \left(\frac{\sqrt{\Delta^2+\delta^2}}{\Delta+\delta} + \frac{1}{\sqrt{2}}\right) SO(G),$$

that is,

$$\left(\sqrt{2(\Delta^2+\delta^2)} + \Delta + \delta\right) SO(G) \geq \sqrt{\Delta^2+\delta^2}\,M_1(G) + \sqrt{2}\,(\Delta+\delta)\,\delta\,m,$$

by (5). The first part of the proof is done.

Suppose that equality holds in (3). Then all the above inequalities must be equalities. By Lemma 2, from the equality in (6), we obtain

$$\frac{1}{\sqrt{2}} = \frac{\sqrt{\Delta^2+\delta^2}}{\Delta+\delta},\ \text{ that is, }\ (\Delta-\delta)^2 = 0,\ \text{ that is, }\ \Delta = \delta.$$

Moreover, from the equality in (5), we obtain that G is a regular graph.

Conversely, let G be an r-regualr graph. Then we have

$$\left(\sqrt{2(\Delta^2+\delta^2)}+\Delta+\delta\right) SO(G) = 2\sqrt{2}\, n\Delta^3 = \sqrt{\Delta^2+\delta^2}\, M_1(G) + \sqrt{2}\,(\Delta+\delta)\,\delta\, m,$$

□

We now obtain another relation between Sombor index $SO(G)$ and the second Zagreb index $M_2(G)$ of graph G.

Theorem 8. *Let G be a graph over n vertices. Suppose it has maximum degree Δ and minimum degree $\delta > 0$. We obtain*

$$\sqrt{2}(\Delta+\delta)\, SO(G) \geq 2\, M_2(G) + n\,\Delta\,\delta^2, \tag{7}$$

where $M_2(G)$ is the second Zagreb index of graph G. Moreover, the equality holds in (7) if and only if G is a regular graph.

Proof. Since $0 < \delta \leq d_G(v_i) \leq \Delta$ $(v_i \in V(G))$, for any edge $v_iv_j \in E(G)$, we obtain

$$\frac{\sqrt{2}}{\Delta} \leq \frac{\sqrt{d_G(v_i)^2 + d_G(v_j)^2}}{d_G(v_i)\, d_G(v_j)} = \sqrt{\frac{1}{d_G(v_i)^2} + \frac{1}{d_G(v_j)^2}} \leq \frac{\sqrt{2}}{\delta}.$$

Let $\mu_G(v_i)$ be the average degree of the adjacent vertices of vertex v_i in G. Then

$$\mu_G(v_i) = \frac{\sum\limits_{v_j:\, v_iv_j \in E(G)} d_G(v_j)}{d_G(v_i)}, \text{ that is, } d_G(v_i)\,\mu_G(v_i) = \sum_{v_j:\, v_iv_j \in E(G)} d_G(v_j).$$

From the definition of the average degree of vertex v_i, we have $\delta \leq \mu_G(v_i) \leq \Delta$. Now,

$$\begin{aligned}
\sum_{v_iv_j \in E(G)} \left(\frac{d_G(v_i)}{d_G(v_j)} + \frac{d_G(v_j)}{d_G(v_i)}\right) &= \sum_{v_i \in V(G)} \sum_{v_j: v_iv_j \in E(G)} \frac{d_G(v_j)}{d_G(v_i)} \\
&= \sum_{v_i \in V(G)} \mu_G(v_i) \\
&\geq n\,\delta
\end{aligned} \tag{8}$$

with equality holding if and only if $d_G(v_i) = \delta$ for any $v_i \in V(G)$.

Setting $s = \dfrac{\sqrt{2}}{\Delta}$, $t = \dfrac{\sqrt{2}}{\delta}$, $a_i \to \sqrt{d_G(v_i)\, d_G(v_j)}$ and $b_i \to \sqrt{\dfrac{d_G(v_i)^2 + d_G(v_j)^2}{d_G(v_i)\, d_G(v_j)}}$ in Lemma 2, we obtain

$$\begin{aligned}
&\sum_{v_iv_j \in E(G)} \frac{d_G(v_i)^2 + d_G(v_j)^2}{d_G(v_i)\, d_G(v_j)} + \frac{2}{\Delta\,\delta} \sum_{v_iv_j \in E(G)} d_G(v_i)\, d_G(v_j) \\
&\qquad \leq \frac{\sqrt{2}\,(\Delta+\delta)}{\Delta\,\delta} \sum_{v_iv_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2},
\end{aligned}$$

that is,

$$\sum_{v_iv_j\in E(G)}\left(\frac{d_G(v_i)}{d_G(v_j)}+\frac{d_G(v_j)}{d_G(v_i)}\right)+\frac{2}{\Delta\,\delta}\,M_2(G)\leq\frac{\sqrt{2}\,(\Delta+\delta)}{\Delta\,\delta}\,SO(G),$$

that is,

$$\sqrt{2}(\Delta+\delta)\,SO(G)\geq 2\,M_2(G)+n\,\Delta\,\delta^2,$$

by (8). The first part of the proof is done.

Similarly, the proof of the Theorem 7, we conclude that the equality holds in (7) if and only if G is a regular graph. □

The following inequality is due to Radon [39].

Lemma 3. (Radon's inequality) *If a_k, $x_k > 0$, $p > 0$, $k \in \{1, 2, \ldots, r\}$, then the following inequality holds:*

$$\sum_{k=1}^{r}\frac{x_k^{p+1}}{a_k^{p}}\geq\frac{\left(\sum\limits_{k=1}^{r}x_k\right)^{p+1}}{\left(\sum\limits_{k=1}^{r}a_k\right)^{p}}$$

with equality holding $\frac{x_1}{a_1}=\frac{x_2}{a_2}=\cdots=\frac{x_r}{a_r}$.

We now present a relation between Sombor index $SO(G)$ and the second Zagreb index $M_2(G)$.

Theorem 9. *Let G be a graph over n vertices. Suppose G has maximum degree Δ and minimum degree $\delta > 0$. We have*

$$SO(G)^2\leq\left(\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\right)m\,M_2(G),\tag{9}$$

with equality if and only if G is a bipartite semiregular graph or G is a regular graph.

Proof. For any edge $v_iv_j \in E(G)$ $(d_G(v_i) \geq d_G(v_j))$ and $\delta > 0$, by (4), we obtain

$$\begin{aligned}\left(\frac{d_G(v_i)}{d_G(v_j)}+\frac{d_G(v_j)}{d_G(v_i)}\right)^2&=\left(\frac{d_G(v_i)}{d_G(v_j)}-\frac{d_G(v_j)}{d_G(v_i)}\right)^2+4\\&\leq\left(\frac{\Delta}{\delta}-\frac{\delta}{\Delta}\right)^2+4=\left(\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\right)^2,\end{aligned}$$

that is,

$$\frac{d_G(v_i)}{d_G(v_j)}+\frac{d_G(v_j)}{d_G(v_i)}\leq\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\tag{10}$$

with equality if and only if $d_G(v_i) = \Delta$, $d_G(v_j) = \delta$, or $d_G(v_i) = \delta$, $d_G(v_j) = \Delta$.

Setting $p = 1$, $x_k \to \sqrt{d_G(v_i)^2 + d_G(v_j)^2}$ and $a_k \to d_G(v_j)\,d_G(v_j)$ in Lemma 3 and using the above result, we obtain

$$\frac{SO(G)^2}{M_2(G)} = \frac{\left(\sum\limits_{v_iv_j \in E(G)} \sqrt{d_G(v_i)^2 + d_G(v_j)^2}\right)^2}{\sum\limits_{v_iv_j \in E(G)} d_G(v_i)\,d_G(v_j)} \le \sum_{v_iv_j \in E(G)} \frac{d_G(v_i)^2 + d_G(v_j)^2}{d_G(v_i)\,d_G(v_j)} \tag{11}$$

$$= \sum_{v_iv_j \in E(G)} \left(\frac{d_G(v_i)}{d_G(v_j)} + \frac{d_G(v_j)}{d_G(v_i)}\right)$$

$$\le \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right) m. \tag{12}$$

The first part of the proof is done.

Suppose that equality holds in (9). Then all the above inequalities must be equalities. By Lemma 3, from the equality in (11), for any edges v_iv_j, $v_kv_\ell \in E(G)$, we obtain

$$\frac{\sqrt{d_G(v_i)^2 + d_G(v_j)^2}}{d_G(v_i)\,d_G(v_j)} = \frac{\sqrt{d_G(v_k)^2 + d_G(v_\ell)^2}}{d_G(v_k)\,d_G(v_\ell)},$$

that is,

$$\frac{1}{d_G(v_i)^2} + \frac{1}{d_G(v_j)^2} = \frac{1}{d_G(v_k)^2} + \frac{1}{d_G(v_\ell)^2}.$$

From the equality in (12), we obtain $d_G(v_i) = \Delta$, $d_G(v_j) = \delta$ for any edge $v_iv_j \in E(G)$, by (10). Using the above results, we conclude that G is a (Δ, δ)-semiregular bipartite graph (when G is bipartite) or G is a regular graph (when G is non-bipartite).

Conversely, let G be an r-regular graph. Then

$$SO(G)^2 = 2m^2r^2 = \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right) m\, M_2(G).$$

Let G be a (Δ, δ)-semiregular bipartite graph. Then

$$SO(G)^2 = m^2(\Delta^2 + \delta^2) = \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right) m\, M_2(G).$$

The proof is then complete. □

4. Conclusions

Topological indices are graph invariants and are used for quantitative structure - activity relationship $(QSAR)$ and quantitative structure - property relationship $(QSPR)$ studies. Many topological indices have been defined in the literature and several of them have found applications as a means to model physical, chemical, pharmaceutical, and other properties of molecules. Gutman introduced the SO index as a new topological index in mathematical chemistry. In this paper, we presented some upper and lower bounds on the SO index and characterized extremal graphs. Moreover, we obtained some relations between the Sombor index and the (first & second) Zagreb indices of graphs. The minimal and the maximal Sombor index (SO), in the case of unicyclic graphs and bicyclic graphs, remains an open problem. Motivation to better understand the Sombor index has been mentioned in the literature [28]. Finding the chemical applications of this Sombor index is an attractive task for the near future.

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