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Relations Between Sombor Index and some Degree–Based Topological Indices

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ABSTRACT

In [13] Gutman introduced a novel graph invariant called Sombor index SO, defined as $SO(G) = \sum_{e_{ij} \in E(G)} \sqrt{\deg(v_i)^2 + \deg(v_j)^2}$. In this paper we provide relations between Sombor index and some degree-based topological indices: Zagreb indices, Forgotten index and Randić index. Similar relations are established in the class of triangle-free graphs.

1. INTRODUCTION

Let $G = (V,E)$ be a simple undirected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, $|E(G)| = m$. For $i = 1, 2, \ldots, n$ the *degree* of a vertex $v_i \in V(G)$ is denoted by $\deg(v_i)$ and it is defined as the number of edges incident with v_i. If the vertices v_i and v_j are connected, then the connecting edge is labeled by e_{ij}. A *topological index* is a numerical quantity of a graph, which is invariant under graph isomorphisms. In mathematical chemistry several topological indices have been introduced and extensively studied [14, 17, 19, 20]. Vertex-degree based topological indices present an important molecular descriptor closely related with many chemical properties. Among the oldest and most studied topological indices, there are two classical vertex-degree based topological indices-the *first*

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Zagreb index and *second Zagreb index*. The Zagreb indices were introduced by Gutman et al. in [11, 12]. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a graph G are defined, respectively, as

$$M_1(G) = \sum_{v_i \in V(G)} \deg(v_i)^2 = \deg(v_1)^2 + \deg(v_2)^2 + \ldots + \deg(v_n)^2,$$

and

$$M_2(G) = \sum_{e_{ij} \in E(G)} \deg(v_i)\deg(v_j).$$

During the past decades, numerous research papers concerning Zagreb indices have been published, see [1−8, 10]. In [15,16], Li et al. introduced the generalized version of the first Zagreb index, defined as

$$Z_p(G) = M_1^p(G) = \deg(v_1)^p + \deg(v_2)^p + \ldots + \deg(v_n)^p$$

where p is a real number. This graph invariant is nowadays known under the name *general first Zagreb index*, and has also been much investigated. The case $p = 3$ was first studied by Furtula et al. [9]. They introduced the *forgotten index* of a graph G, also called as F-index, which is defined as

$$F(G) = \sum_{v_i \in V(G)} \deg(v_i)^3 = \sum_{e_{ij} \in E(G)} (\deg(v_i)^2 + \deg(v_j)^2).$$

In 2020, Gutman introduced a new vertex-degree-based topological index defined as $SO(G) = \sum_{e_{ij} \in E(G)} \sqrt{\deg(v_i)^2 + \deg(v_j)^2}$ which was named *Sombor index*, [13]. Some basic properties of the Sombor index were established in [13].

Motivated by this recent research, in this paper we provide basic relationships between the Sombor index and Zagreb/Randić indices, Section 2. In Section 3, we estimate the Sombor index for the triangle-free graphs. The results in this paper are based on elementary inequalities.

2. RELATIONS BETWEEN SOMBOR INDEX AND ZAGREB/RANDIĆ INDICES

In this section we assume that G is a simple connected graph with n vertices $v_1, v_2, \ldots, v_n$ and m edges. The corresponding vertex-degrees of G we denote by $\deg(v_1), \ldots, \deg(v_n)$.

Theorem 2.1 Let G be a graph on n vertices. Then $SO(G) \geq \frac{1}{\sqrt{2}} M_1(G)$. The equality holds if and only if G is a regular graph.

Proof. From the inequality between quadratic and arithmetic means for the positive numbers $\deg(v_i)$ and $\deg(v_j)$ we have $\sqrt{\deg(v_i)^2 + \deg(v_j)^2} \geq \frac{1}{\sqrt{2}}(\deg(v_i) + \deg(v_j))$. Thus we get $SO(G) = \sum_{e_{ij} \in E(G)} \sqrt{\deg(v_i)^2 + \deg(v_j)^2} \geq \sum_{e_{ij} \in E(G)} \frac{1}{\sqrt{2}}(\deg(v_i) + \deg(v_j)) = \frac{1}{\sqrt{2}} \sum_{v_i \in V(G)} \deg(v_i)^2 = \frac{1}{\sqrt{2}} M_1(G)$.

If G is a k-regular graph, then we have $SO(G)=\frac{nk^2}{\sqrt{2}}=\frac{1}{\sqrt{2}}M_1(G)$. □

Remark 2.2 It is well known that for a simple connected graph with n vertices and m edges occurs $M_1 \geq \frac{4m^2}{n}$. From Theorem 2.1, we conclude that $SO(G)\geq \frac{2\sqrt{2}m^2}{n}$.

Theorem 2.3 Let G be a graph on n vertices. Then $SO(G)\geq \frac{\sqrt{2}}{n-1}M_2(G)$. The equality holds if and only if G is a complete graph on n vertices.

Proof. Clearly $\deg(v_i)+\deg(v_j)\leq 2n-2$ for each $i,j\in\{1,\ldots,n\}$. The inequality between quadratic and harmonic means for the numbers $\deg(v_i)$ and $\deg(v_j)$ yields

$$\sqrt{\frac{\deg(v_i)^2+\deg(v_j)^2}{2}} \geq \frac{2}{\frac{1}{\deg(v_i)}+\frac{1}{\deg(v_j)}} = \frac{2\deg(v_i)\deg(v_j)}{\deg(v_i)+\deg(v_j)} \geq \frac{1}{n-1}\deg(v_i)\deg(v_j). \quad (1)$$

From (1) we obtain the following lower bound for the Sombor index

$$SO(G)=\sum_{e_{ij}\in E(G)}\sqrt{\deg(v_i)^2+\deg(v_j)^2} \geq \frac{\sqrt{2}}{n-1}\sum_{e_{ij}\in E(G)}\deg(v_i)\deg(v_j)=\frac{\sqrt{2}}{n-1}M_2(G).$$

If G is a complete graph on n vertices, then $\frac{\sqrt{2}}{n-1}M_2(K_n)=\frac{n(n-1)^2}{\sqrt{2}}=SO(K_n)$, see in [13]. □

Theorem 2.4 Let G be a graph on n vertices and m edges. Then $SO(G)\leq\sqrt{mF(G)}$. The equality holds if and only if G is a regular graph.

Proof. We apply the inequality between arithmetic and quadratic means to the m numbers $\sqrt{\deg(v_i)^2+\deg(v_j)^2}$ determined by the edges $e_{ij}\in E(G)$. Hence

$$SO(G)=\sum_{e_{ij}\in E(G)}\sqrt{\deg(v_i)^2+\deg(v_j)^2}\leq\sqrt{m}\sqrt{\sum_{e_{ij}\in E(G)}(\deg(v_i)^2+\deg(v_j)^2)}=$$

$$=\sqrt{m}\cdot\sqrt{\sum_{v_i\in V(G)}\deg(v_i)^3}=\sqrt{m\cdot F(G)}.$$

If G is a k-regular graph, then $m\cdot F(G)=\frac{n^2k^4}{2}=SO^2(G)$. □

Theorem 2.5 Let G be a graph with n vertices and m edges. If $Z_5(G)$ is a general Zagreb index of G, then

$$SO(G)\leq\sqrt[4]{2m^3Z_5(G)}\,.$$

The equality holds if and only if G is a regular graph.

Proof. From the power inequality of order 4 and 1 for m numbers $\sqrt{\deg(v_i)^2+\deg(v_j)^2}$ determined by the edges $e_{ij}\in E(G)$ we obtain

$$\sqrt[4]{\frac{\sum_{e_{ij}\in E(G)}\left(\sqrt{\deg(v_i)^2+\deg(v_j)^2}\right)^4}{m}}\geq\frac{\sum_{e_{ij}\in E(G)}\sqrt{\deg(v_i)^2+\deg(v_j)^2}}{m}=\frac{SO(G)}{m}. \qquad (2)$$

From $\deg(v_i)^4+\deg(v_j)^4\geq 2\deg(v_i)^2\cdot\deg(v_j)^2$ and from the inequality in (2) we get

$$\sqrt[4]{\frac{2\sum_{e_{ij}\in E(G)}(\deg(v_i)^4+\deg(v_j)^4)}{m}}\geq\frac{SO(G)}{m}\Leftrightarrow$$

$$\sqrt[4]{2}\cdot\sqrt[4]{\frac{\sum_{v_i\in V(G)}\deg(v_i)^5}{m}}\geq\frac{SO(G)}{m}\Leftrightarrow\sqrt[4]{2}\cdot\sqrt[4]{\frac{Z_5(G)}{m}}\geq\frac{SO(G)}{m}\Leftrightarrow SO(G)\leq\sqrt[4]{2m^3Z_5(G)}.$$

If G is a k - regular graph, then $2m^3Z_5(G)=\frac{n^4k^8}{4}=SO^4(G)$. □

In the last two results of this section we establish relationships between Sombor and Randić index (reduced reciprocal Randić index). The Randić index $R(G)$ was introduced in 1975 by Randić [18] as follows:

$$R(G)=\sum_{e_{ij}\in E(G)}\frac{1}{\sqrt{\deg(v_i)\deg(v_j)}}.$$

It is a measure of branching of the carbon-atom skeleton and has been closely correlated with many chemical properties.

Theorem 2.6 Let G be a graph on n vertices and m edges. Then $SO(G)\geq\frac{\sqrt{2}m^2}{R(G)}$. The equality holds if and only if G is a regular graph.

Proof. Since $\deg(v_i)^2+\deg(v_j)^2\geq 2\deg(v_i)\deg(v_j)$ we obtain

$$SO(G)=\sum_{e_{ij}\in E(G)}\sqrt{\deg(v_i)^2+\deg(v_j)^2}\geq\sqrt{2}\sum_{e_{ij}\in E(G)}\sqrt{\deg(v_i)\deg(v_j)}.$$

From the inequality between arithmetic and harmonic means for the numbers $\sqrt{\deg(v_i)\deg(v_j)}$, where $v_iv_j=e_{ij}$, we have

$$SO(G)\geq\sqrt{2}\sum_{e_{ij}\in E(G)}\sqrt{\deg(v_i)\deg(v_j)}\geq\sqrt{2}\frac{m^2}{\sum_{e_{ij}\in E(G)}\frac{1}{\sqrt{\deg(v_i)\deg(v_j)}}}=\frac{m^2\sqrt{2}}{R(G)}.$$

If G is a k-regular graph, then $R(G)=\frac{n}{2}$. Thus, $\frac{\sqrt{2}m^2}{R(G)}=\frac{nk^2}{\sqrt{2}}=SO(G)$. □

Theorem 2.7 Let G be a graph with n vertices and m edges and let $\deg(v_i)>1$ for every vertex $v_i\in V(G)$. If $RRR(G)$ is reduced reciprocal Randić index of G, then

$$SO(G)\geq\sqrt{2}(RRR(G)+m).$$

The equality holds if and only if G is a regular graph.

Proof. Using the inequality between geometric and arithmetic means for the numbers $\deg(v_i)-1$ and $\deg(v_j)-1$ we have

$$\sqrt{(\deg(v_i)-1)(\deg(v_j)-1)}\leq\frac{\deg(v_i)+\deg(v_j)-2}{2}=\frac{\deg(v_i)+\deg(v_j)}{2}-1\leq \\ \leq\sqrt{\frac{\deg(v_i)^2+\deg(v_j)^2}{2}}-1. \tag{3}$$

From (3) we get

$$SO(G)=\sum_{e_{ij}\in E(G)}\sqrt{\deg(v_i)^2+\deg(v_j)^2}\geq\sqrt{2}\sum_{e_{ij}\in E(G)}\left(\sqrt{(\deg(v_i)-1)(\deg(v_j)-1)}+1\right) \\ =\sqrt{2}(RRR(G)+m).$$

If G is a k-regular graph, then

$$\sqrt{2}(RRR(G)+m)=\sqrt{2}(m(k-1)+m)=\sqrt{2}mk=\frac{nk^2}{\sqrt{2}}=SO(G).$$ □

3. A Sombor Index and Triangle–Free Graphs

A triangle-free graph is an undirected graph containing no triangles (3-cycles). Because of their specific structure, this family of graphs play an important role in graph theory, consequently in chemical graph theory. The topological indices of the triangle-free graphs are studied intensively in numerous research papers. We list two known results concerning Zagreb indices.

Theorem 3.1 [21] Let G be a triangle-free (n,m)-graph. Then $M_1(G)\leq mn$ and equality holds if and only if G is a complete bipartite graph.

Theorem 3.2 [21] Let G be a triangle-free graph with $m>0$ edges. Then $M_2(G)\leq m^2$ with equality if and only if G is the union of a complete bipartite graph and isolated vertices.

Similarly as in the previous section, we assume that G is a simple connected graph with n vertices $v_1, v_2, \ldots, v_n$ and corresponding vertex-degrees $\deg(v_1), \deg(v_2), \ldots, \deg(v_n)$. The next two results give a relation between the Sombor index and the second Zagreb index in the class of triangle-free graphs.

Theorem 3.3 Let G be a triangle-free graph on n vertices. If $M_2(G)$ is the second Zagreb index of G, then

$$SO(G) \geq \frac{2\sqrt{2}}{n} M_2(G).$$

The equality holds if and only if G is a complete graph on $\frac{n}{2}+1$ vertices.

Proof. The proof follows from Remark 2.2 and Theorem 3.2. □

Theorem 3.4 Let G be a triangle-free graph on n vertices and m edges. Then

$$SO(G) \leq \sqrt{m(mn^2 - 2M_2(G))}\,.$$

Proof. Recall, for $e_{ij} = v_i v_j \in E(G)$ holds $\deg(v_i) + \deg(v_j) \leq n.$ Thus

$$\sum_{e_{ij} \in E(G)} (\deg(v_i) + \deg(v_j))^2 \leq mn^2 \Leftrightarrow \sum_{v_i \in V(G)} \deg(v_i)^3 + 2 \cdot \sum_{e_{ij} \in E(G)} \deg(v_i)\deg(v_j) \leq mn^2 \Leftrightarrow$$
$$F(G) + 2M_2(G) \leq mn^2.$$

Now the required result follows directly from Theorem 2.4. □

Note that the Sombor index in Theorem 2.4 depends on the size of G and the corresponding forgotten index. We apply this result to triangle-free graphs by obtaining an upper bound for the size of G in terms of n and the maximum degree Δ.

Proposition 3.5 Let G be a triangle-free graph with n vertices, m edges and maximum degree Δ. Then, $m \leq \Delta(n-\Delta)$.

Proof. Let v be a vertex of G with maximum degree Δ. Since G is a triangle-free graph there are no edges in the neighborhood of v. Moreover, every vertex which is not in the neighborhood of v has degree at most Δ. Therefore, the maximum number of edges of G is $\Delta + (n-\Delta-1)\Delta = \Delta(n-\Delta)$. □

Remark 3.6 The above result is useful if $\Delta \geq n/2$. In this case $m \leq \Delta(n - \Delta) \leq n\Delta/2$, which is an improvement of the trivial bound $m \leq n\Delta/2$.

From Proposition 3.5 and Theorem 2.4 we derive the following result.

Corollary 3.7 Let G be a triangle-free graph with n vertices and maximum degree $\Delta \geq \frac{n}{2}$. If $F(G)$ is the forgotten index of G, then $SO(G) \leq \sqrt{\Delta(n-\Delta)F(G)}$.

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