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On Sombor Index and Some Topological Indices

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ABSTRACT

Gutman recently introduced a new vertex-degree-based topological index called the Sombor index. In this paper, we present some new results relating the Sombor index and some well-studied topological indices: Zagreb indices, forgotten index, harmonic index, (general) sum-connectivity index and symmetric division deg index.

1. INTRODUCTION

We consider only finite simple graph in this paper. Let G be a finite simple graph on n vertices and m edges. We denote the vertex set and the edge set of G by $V(G)$ and $E(G)$, respectively. The degree of a vertex $v_i \in V(G)$ is denoted by d_i and it is defined as the number of edges incident with v_i. Let Δ and δ denote the maximum vertex degree and the minimum vertex degree of the graph G, respectively.

In chemical graph theory, one generally considers various graph-theoretical invariants of molecular graphs (also known as topological indices or molecular descriptors)

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and study their correlation with various properties of the corresponding molecules. The first such topological index was introduced in 1947 by Harry Wiener and used for correlation with boiling points of alkanes. Wiener's index is related to the distances in molecular graphs. Historically, the first vertex-degree-based topological indices were the graph invariants that are now known as Zagreb indices. Numerous graph invariants have been (and continue to be) explored with varying degree of success in QSAR (quantitative structure-activity relationship) and QSPR (quantitative structure-property relationship) studies.

The Zagreb indices are amongst the most studied invariants [11] and they are defined as sums of contributions dependent on the degrees of adjacent vertices over all edges of a graph. The Zagreb indices of a graph G, i.e., the *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$, were originally defined [9] as follows.

$$M_1(G) = \sum_{v_i \in V(G)} d_i^2, \quad M_2(G) = \sum_{v_i v_j \in E(G)} d_i\, d_j.$$

The first Zagreb index of G can also be expressed as $M_1(G) = \sum_{v_i v_j \in E(G)} [d_i + d_j]$.

Generalised version of the first Zagreb index has also been introduced [10], known as the *general first Zagreb index,* and is defined as $M_1^p(G) = \sum_{v_i \in V(G)} d_i^p$.
When $p = 3$, $M_1^3(G) = \sum_{v_i \in V(G)} d_i^3$ is known as the *forgotten index* $F(G)$ and is also equal to $F(G) = \sum_{v_i v_j \in E(G)} [d_i^2 + d_j^2]$.

Owing to its reasonable prediction ability, the *symmetric division deg index* $SDD(G)$ has attracted considerable attention recently [1], [6]. It is defined as

$$SDD(G) = \sum_{v_i v_j \in E(G)} \left[\frac{d_i}{d_j} + \frac{d_j}{d_i}\right].$$

Another important topological index is the *harmonic index* $H(G)$ whose chemical applicability was tested and found to be at par in correlation to the well-known Randić index [8]. It is defined as $H(G) = \sum_{v_i v_j \in E(G)} \frac{2}{d_i + d_j}$.

Motivated by Randić, Zagreb and harmonic indices, Zhou and Trinajstić defined *sum-connectivity index* $\chi(G)$ [14] and *general sum-connectivity index* $\chi_\alpha(G)$ [15], α *is real*, which are defined as follows:

$$\chi(G) = \sum_{v_i v_j \in E(G)} \frac{1}{\sqrt{d_i + d_j}}; \ \chi_\alpha(G) = \sum_{v_i v_j \in E(G)} [d_i + d_j]^\alpha.$$

Gutman recently introduced [7] a new vertex-degree-based topological index called the *Sombor index*, which is defined as $SO(G) = \sum_{v_i, v_j \in E(G)} \sqrt{d_i^2 + d_j^2}$. The Sombor index has shown good predictive potential in its application to chemical graph theory [12]. Computations of Sombor index of various graphs have been carried out, for example chemical graphs [2]. Basic properties of the Sombor index have been presented and its relations with other topological indices: the Zagreb indices, are investigated in [3]. In [5] and [13], in addition to Zagreb indices, relations between Sombor index and other topological indices are carried out. Motivated by such results, in this paper we present some new relations of Sombor index with other topological indices.

2. RELATIONS BETWEEN SOMBOR INDEX AND OTHER TOPOLOGICAL INDICES

In this section, we present some new results relating the Sombor index with some other topological indices: Zagreb indices, forgotten index, harmonic index, (general) sum-connectivity index and symmetric division deg index. We first recall the following well-known inequalities which are needed for our results in this section.

Lemma 2.1 (Pólya-Szegö inequality [4]) Let $a_1, a_2, \dots, a_m$ and $b_1, b_2, \dots, b_m$ be two sequences of positive real numbers. If there exist real numbers A, a, B and b such that $0 < a \leq a_k \leq A < \infty$ and $0 < b \leq b_k \leq B < \infty$ for $k = 1,2, \dots, m$, then

$$\frac{\sum_{k=1}^{m} a_k^2 \sum_{k=1}^{m} b_k^2}{\left(\sum_{k=1}^{m} a_k b_k\right)^2} \leq \frac{(ab+AB)^2}{4abAB}.$$

Equality holds if and only if $p = m\frac{A}{a} / \left(\frac{A}{a} + \frac{B}{b}\right), q = m\frac{B}{b} / \left(\frac{A}{a} + \frac{B}{b}\right)$ are integers and if p of the numbers $a_1, a_2, \dots, a_m$ are equal to a and q of these numbers are equal to A, and if the corresponding numbers b_k are equal to B and b, respectively.

Lemma 2.2 (Radon's inequality [3]) If $a_k, b_k > 0$ for $k = 1,2, \dots, m$ and $p > 0$, then

$$\sum_{k=1}^{m} \frac{a_k^{p+1}}{b_k^p} \geq \frac{\left(\sum_{k=1}^{m} a_k\right)^{p+1}}{\left(\sum_{k=1}^{m} b_k\right)^p}$$

Equality holds if $\frac{a_1}{b_1} = \frac{a_2}{b_2} = \cdots = \frac{a_m}{b_m}$.

In [5] and [13], the upper bound of Sombor index involving forgotten index is presented which is an easy consequence of Cauchy-Schwarz inequality. More precisely, they found that for a graph with m edges $SO(G) \leq \sqrt{mF(G)}$, where the equality holds if and only if G is a regular graph. In [13], a lower bound for the same is also obtained in addition to a new upper bound $SO(G) \leq \frac{F(G)}{\delta\sqrt{2}}$. Here, we present a new lower bound for $SO(G)$ involving the forgotten index which is still tight for regular graphs.

Theorem 2.3. Let G be a graph on n vertices and m edges. Then

$$\sqrt{mF(G)} \leq \frac{1}{2}\left(\frac{\delta}{\Delta} + \frac{\Delta}{\delta}\right) SO(G).$$

Proof. Let $V(G) = \{v_1, v_2, \dots, v_n\}$. Letting $a_k \to \sqrt{d_i^2 + d_j^2}$ and $b_k = \sqrt{2}\delta$ in Lemma 2.1 and choosing $a = \sqrt{2}\delta = b$ and $A = \sqrt{2}\Delta = \mathrm{B}$, we have $0 < a \leq a_k \leq A < \infty$ and

$0 < b \leq b_k \leq B < \infty$ for $k = 1,2, \dots, m$. Notice that $\frac{(ab+AB)^2}{4abAB} = \frac{1}{4}\left(\frac{\delta}{\Delta} + \frac{\Delta}{\delta}\right)^2$. Applying the Lemma 2.1 with the sums running over the edges in G, we have

$$\frac{\sum_{v_iv_j\in E(G)}[d_i^2 + d_j^2]\sum_{v_iv_j\in E(G)} 2\delta^2}{\left(\sum_{v_iv_j\in E(G)} \sqrt{2}\delta\sqrt{d_i^2 + d_j^2}\right)^2} \leq \frac{1}{4}\left(\frac{\delta}{\Delta} + \frac{\Delta}{\delta}\right)^2.$$

So, $\frac{F(G)m}{SO(G)^2} \leq \frac{1}{4}\left(\frac{\delta}{\Delta} + \frac{\Delta}{\delta}\right)^2$. Hence $\sqrt{mF(G)} \leq \frac{1}{2}\left(\frac{\delta}{\Delta} + \frac{\Delta}{\delta}\right)SO(G)$. ■

In [5] and [13] bounds of Sombor index involving first Zagreb index were reported. More precisely, $\frac{1}{\sqrt{2}}M_1(G) \leq SO(G)$, where the equality is attained when the graph is regular. Here we present a new lower bound of Sombor index involving first Zagreb index, m, δ and Δ.

Theorem 2.4. Let G be a graph on n vertices and m edges. Then

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

Proof. Let $V(G) = \{v_1, v_2, \dots, v_n\}$. Letting $a_k \to \sqrt{d_i + d_j}$ and $b_k \to \sqrt{\frac{d_i^2+d_j^2}{d_i+d_j}}$ in Lemma 2.1 and choosing $a = \sqrt{2\delta}$, $A = \sqrt{2\Delta}$, $b = \sqrt{\delta}$ and $B = \sqrt{\Delta}$, we have $0 < a \leq a_k \leq A < \infty$ and $0 < b \leq b_k \leq B < \infty$ for $k = 1,2, \dots, m$. Notice that $\frac{(ab+AB)^2}{4abAB} = \frac{1}{4\delta\Delta}(\Delta + \delta)^2$. Applying the Lemma 2.1 with the sums running over the edges in G, we have

$$\frac{\sum_{v_iv_j\in E(G)}[d_i+d_j]\sum_{v_iv_j\in E(G)}\frac{d_i^2+d_j^2}{d_i+d_j}}{\left(\sum_{v_iv_j\in E(G)} \sqrt{d_i^2+d_j^2}\right)^2} \leq \frac{1}{4\delta\Delta}(\Delta + \delta)^2. \tag{1}$$

Notice that $\frac{d_i^2+d_j^2}{d_i+d_j} \geq \delta$. So, $\sum_{v_iv_j\in E(G)} \frac{d_i^2+d_j^2}{d_i+d_j} \geq m\delta$. Thus Equation (1) becomes $\frac{M_1(G)m\delta}{SO(G)^2} \leq \frac{1}{4\delta\Delta}(\Delta + \delta)^2$. Hence $2\sqrt{m\Delta M_1(G)} \leq \left(1 + \frac{\Delta}{\delta}\right)SO(G)$. ■

Theorem 2.5. [13] Let G be a connected graph on n vertices and m edges. Then

$$\frac{1}{\sqrt{2}}M_1(G) \leq SO(G) \leq M_1(G) - \frac{\delta m}{2} - \frac{\delta^2 m}{2\sqrt{8\Delta^2 + \delta^2} + 4\sqrt{2}\Delta}.$$

Here we present a new upper bound of Sombor index involving first Zagreb index.

Theorem 2.6. Let G be a graph on n vertices and m edges. Then $SO(G) \leq \sqrt{m\Delta M_1(G)}$.

Proof. Let $V(G) = \{v_1, v_2, \dots, v_n\}$. Letting $a_k \to \sqrt{d_i^2 + d_j^2}$ and $b_k \to d_i + d_j$ in Lemma 2.2 with the sums running over the edges in G and $p = 1$, we have

$$\sum_{v_iv_j \in E(G)} \frac{d_i^2 + d_j^2}{d_i + d_j} \geq \frac{\left(\sum_{v_iv_j \in E(G)} \sqrt{d_i^2 + d_j^2}\right)^2}{\sum_{v_iv_j \in E(G)} [d_i + d_j]}. \tag{2}$$

Notice that $\frac{d_i^2 + d_j^2}{d_i + d_j} \leq \Delta$. So, $\sum_{v_iv_j \in E(G)} \frac{d_i^2 + d_j^2}{d_i + d_j} \leq m\Delta$. Thus Equation (2) becomes $\frac{SO(G)^2}{M_1(G)} \leq m\Delta$. Hence $SO(G) \leq \sqrt{m\Delta M_1(G)}$. ■

Next, we present a relation between Sombor index and harmonic index and general sum-connectivity index.

Theorem 2.7. Let G be a graph on n vertices and m edges. Then

$$SO(G) \leq \sqrt{\frac{\Delta}{2} H(G) \chi_2(G)}.$$

Proof. Let $V(G) = \{v_1, v_2, \dots, v_n\}$. Letting $a_k \to \sqrt{d_i^2 + d_j^2}$ and $b_k \to \frac{2}{d_i + d_j}$ in Lemma 2.2 with the sums running over the edges in G and p=1, we have

$$\frac{\left(\sum_{v_iv_j \in E(G)} \sqrt{d_i^2 + d_j^2}\right)^2}{\sum_{v_iv_j \in E(G)} \frac{2}{d_i + d_j}} \leq \sum_{v_iv_j \in E(G)} \frac{[d_i^2 + d_j^2]}{2} [d_i + d_j] = \sum_{v_iv_j \in E(G)} \frac{d_i^2 + d_j^2}{2[d_i + d_j]} [d_i + d_j]^2. \tag{3}$$

Notice that $\frac{d_i^2 + d_j^2}{d_i + d_j} \leq \Delta$. Thus Equation (3) becomes $\frac{SO(G)^2}{H(G)} \leq \frac{\Delta}{2} \chi_2(G)$. Hence $SO(G) \leq \sqrt{\frac{\Delta}{2} H(G) \chi_2(G)}$. ■

Next, we present a relation between Sombor index and (general) sum-connectivity index.

Theorem 2.8. Let G be a graph on n vertices and m edges. Then

$$SO(G) \leq \sqrt{\Delta \chi(G) \chi_{3/2}(G)}.$$

Proof. Let $V(G) = \{v_1, v_2, \dots, v_n\}$. Letting $a_k \to \sqrt{d_i^2 + d_j^2}$ and $b_k \to \frac{1}{\sqrt{d_i + d_j}}$ in Lemma 2.2 with the sums running over the edges in G and p=1, we have

$$\frac{\left(\sum_{v_iv_j \in E(G)} \sqrt{d_i^2 + d_j^2}\right)^2}{\sum_{v_iv_j \in E(G)} \frac{1}{d_i + d_j}} \leq \sum_{v_iv_j \in E(G)} [d_i^2 + d_j^2] \sqrt{d_i + d_j} = \sum_{v_iv_j \in E(G)} \frac{d_i^2 + d_j^2}{d_i + d_j} [d_i + d_j]^{\frac{3}{2}}. \tag{4}$$

Notice that $\frac{d_i^2+d_j^2}{d_i+d_j} \leq \Delta$. Thus Equation (4) becomes $\frac{SO(G)^2}{\chi(G)} \leq \Delta\chi_{\frac{3}{2}}(G)$. Hence $SO(G) \leq \sqrt{\Delta\chi(G)\chi_{3/2}(G)}$. ■

In [13], bounds of Sombor index involving second Zagreb index is presented. Here, we present a new relation between Sombor index and second Zagreb index. Our bound and approach are different. First, we present the following relation of Sombor index involving second Zagreb index and symmetric division deg index.

Theorem 2.9. Let G be a graph on n vertices and m edges. Then

$$SO(G) \leq \sqrt{M_2(G)SDD(G)}.$$

Proof. We first recall the Cauchy-Schwarz inequality. Let $a_1, a_2, \dots, a_m$ and $b_1, b_2, \dots, b_m$ be two sequences of real numbers. Then $(\sum_{k=1}^m a_k b_k)^2 \leq \sum_{k=1}^m a_k^2 \sum_{k=1}^m b_k^2$. Let $V(G) = \{v_1, v_2, \dots, v_n\}$ and letting $b_k \to \sqrt{\frac{d_i^2+d_j^2}{d_i d_j}}$ in the Cauchy-Schwarz inequality with the sums running over the edges in G, we have

$$\begin{aligned}\left(\sum_{v_iv_j\in E(G)} \sqrt{d_i^2+d_j^2}\right)^2 &\leq \sum_{v_iv_j\in E(G)} d_i d_j \sum_{v_iv_j\in E(G)} \frac{d_i^2+d_j^2}{d_i d_j}\\ &= \sum_{v_iv_j\in E(G)} d_i d_j \sum_{v_iv_j\in E(G)} \left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)\\ &= M_2(G)SDD(G).\end{aligned}$$

Hence $SO(G) \leq \sqrt{M_2(G)SDD(G)}$. ■

As a corollary, we now present a bound of Sombor index involving second Zagreb index.

Corollary 2.10. Let G be a graph on n vertices and m edges. Then

$$SO(G) \leq \sqrt{\left(\frac{\delta}{\Delta}+\frac{\Delta}{\delta}\right) m M_2(G)}.$$

Proof. Since $0 < \delta \leq d_i \leq \Delta$ for any v_i, we have $\frac{\delta}{\Delta} \leq \frac{d_i}{d_j} \leq \frac{\Delta}{\delta}$. Now for any edge v_iv_j of G $(d_i \geq d_j)$, we have

$$\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)^2 = \left(\frac{d_i}{d_j}-\frac{d_j}{d_i}\right)^2 + 4 \leq \left(\frac{\delta}{\Delta}-\frac{\Delta}{\delta}\right)^2 + 4 = \left(\frac{\delta}{\Delta}+\frac{\Delta}{\delta}\right)^2.$$

Thus $SDD(G) \leq m\left(\frac{\delta}{\Delta}+\frac{\Delta}{\delta}\right)$. Hence from Theorem 2.9 we obtain the desired result. ■

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