

On the Symmetric Division Deg Coindex

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Abstract

Let G be a graph of minimum degree at least 1. Denote by d_i the degree of a vertex v_i in G . The notation $i \approx j$ is used to indicate that the vertices v_i and v_j are not adjacent in G . A graph of maximum degree at most 4 is known as a molecular graph. A connected graph having the same order and size is called a unicyclic graph. The symmetric division deg coindex of G is defined as $\overline{SDD}(G) = \sum_{i \approx j; v_i \neq v_j} (d_i^2 + d_j^2)(d_i d_j)^{-1}$. In this paper, new bounds for the coindex $\overline{SDD}(G)$ as well as relations between $\overline{SDD}(G)$ and some other topological indices/coindices are obtained. From one of the obtained results, it follows that the star graph (cycle graph, respectively) uniquely minimizes symmetric division deg coindex among all trees ((molecular) unicyclic graphs, respectively) of a given order.

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1 Introduction

A graph invariant is a property that remains the same under graph isomorphism. Examples of graph invariants include the order, size, and degree sequence. In chemical graph theory, real-valued graph invariants are often referred to as topological indices [17] (see also [35]). Many of the topological indices are defined as simple functions of the degrees of the vertices of a (molecular) graph. Most of the (vertex-)degree-based topological indices can be viewed as the contributions of all pairs of adjacent vertices. These types of indices are known as the bond incident degree indices (BID indices in short), see for example [5, 39]. Also, the literature contains various degree-based topological indices defined via contributions of all pairs of non-adjacent different vertices, which we refer to as the bond incident degree (BID) coindices.

Let G be a simple graph with vertex set $V = \{v_1, v_2, \dots, v_n\}$ such that $d_1 \geq d_2 \geq \dots \geq d_n > 0$, where d_i is the degree of v_i . If the vertices v_i and v_j are adjacent in G , we write $i \sim j$, while if they are nonadjacent in G , we write $i \approx j$. The set of all different vertex degrees of G is known as the degree set of G .

A bond incident degree (BID) index of the graph G is defined [24, 36, 38, 39, 41] as

$$BID(G) = \sum_{i \sim j} F(d_i, d_j),$$

where F is a symmetric real-valued function defined on the Cartesian square of the degree set of G . The BID coindex of G , corresponding to $BID(G)$, is defined [18] as

$$\overline{BID}(G) = \sum_{i \approx j; v_i \neq v_j} F(d_i, d_j).$$

The concept of coindices was introduced in [11]. Details on certain coindices can be found in [6, 13, 18, 19, 26–28, 31, 34, 42].

In the text that follows, we recall definitions of some topological indices and coindices that are of interest for our consideration.

One of the most popular and extensively studied topological indices is

the first Zagreb index that was appeared in a formula derived by Gutman and Trinajstić in [23]. This index for G is defined as

$$M_1(G) = \sum_{i=1}^n d_i^2.$$

It is known (see Exercise 10.30 in [25]) that M_1 can be also represented as

$$M_1(G) = \sum_{i \sim j} (d_i + d_j).$$

The second Zagreb index was introduced in [22] and for the graph G it is defined as

$$M_2(G) = \sum_{i \sim j} d_i d_j.$$

The corresponding coindices are defined [11] as

$$\overline{M}_1(G) = \sum_{i \not\sim j; v_i \neq v_j} (d_i + d_j) \quad \text{and} \quad \overline{M}_2(G) = \sum_{i \not\sim j; v_i \neq v_j} d_i d_j.$$

More details about the above-mentioned Zagreb indices and coindices can be found in [3, 6–8, 11, 13, 18, 19, 21–23, 26–28, 30, 34].

Multiplicative versions of the first and second Zagreb coindices were introduced in [42]. These multiplicative Zagreb coindices for G are defined as

$$\overline{\Pi}_1(G) = \prod_{i \not\sim j; v_i \neq v_j} (d_i + d_j) \quad \text{and} \quad \overline{\Pi}_2(G) = \prod_{i \not\sim j; v_i \neq v_j} d_i d_j.$$

The inverse degree index of G is defined [14] as

$$ID(G) = \sum_{i=1}^n \frac{1}{d_i}.$$

Let $TI(G)$ be the degree-based topological index of the form

$$TI(G) = \sum_{i=1}^n f(d_i),$$

where f is a real-valued function defined on the degree set of G . In [12] (see also [13]), it was proven that

$$\sum_{i \sim j} (f(d_i) + f(d_j)) = \sum_{i=1}^n d_i f(d_i). \quad (1)$$

In [18], the following identity was derived:

$$\sum_{i \rightsquigarrow j; v_i \neq v_j} (f(d_i) + f(d_j)) = \sum_{i=1}^n (n-1-d_i) f(d_i). \quad (2)$$

From (1) and (2), it is concluded that the following identities are valid:

$$ID(G) = \sum_{i \sim j} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right) \quad \text{and} \quad \overline{ID}(G) = \sum_{i=1}^n \frac{(n-1-d_i)}{d_i^2}.$$

For the graph G , the geometric–arithmetic index [40] and its corresponding coindex are defined, respectively, as

$$GA(G) = \sum_{i \sim j} \frac{2\sqrt{d_i d_j}}{d_i + d_j} \quad \text{and} \quad \overline{GA}(G) = \sum_{i \rightsquigarrow j; v_i \neq v_j} \frac{2\sqrt{d_i d_j}}{d_i + d_j}.$$

Albertson [1] introduced the following topological index, which was later referred to as the *Albertson index* [20] and also the *third Zagreb index* [15]:

$$Alb(G) = \sum_{i \sim j} |d_i - d_j|.$$

We call that the Albertson coindex satisfies the identity

$$\overline{Alb}(G) = \sum_{i \rightsquigarrow j; v_i \neq v_j} |d_i - d_j| = Alb(\overline{G}),$$

where \overline{G} is the complement of G .

A family of 148 topological indices was introduced and analyzed in [41] (see also [38]). An especially interesting subclass of these indices consists of 20 indices which are useful for predicting certain physicochemical prop-

erties of chemical compounds. Two of them are the inverse sum indeg (ISI) index and the symmetric division deg (SDD) index, which are defined as

$$ISI(G) = \sum_{i \sim j} \frac{d_i d_j}{d_i + d_j} \quad \text{and} \quad SDD(G) = \sum_{i \sim j} \frac{d_i^2 + d_j^2}{d_i d_j}.$$

The ISI index is a significant predictor of the total surface area for octane isomers, while the SDD index is a significant predictor of the total surface area of polychlorobiphenyls, see [41]. For the graph G , the ISI coindex and the SDD coindex [31] are defined as

$$\overline{ISI}(G) = \sum_{i \not\sim j; v_i \neq v_j} \frac{d_i d_j}{d_i + d_j} \quad \text{and} \quad \overline{SDD}(G) = \sum_{i \not\sim j; v_i \neq v_j} \frac{d_i^2 + d_j^2}{d_i d_j}.$$

For details about most of the topological indices defined above, see the surveys [2–4, 7, 9, 17, 32] and references listed therein. In this paper, we prove a number of inequalities, which give upper and lower bounds for $\overline{SDD}(G)$ and its relationship with other topological indices/coindices.

2 Main results

We start this section by establishing a relationship between $\overline{SDD}(G)$ and $\overline{GA}(G)$.

Theorem 1. *Let G be a simple graph of order n , size m , and minimum degree at least 1. Then,*

$$2(\overline{SDD}(G) + n(n-1) - 2m) [\overline{GA}(G)]^2 \geq (n(n-1) - 2m)^3. \quad (3)$$

Equality in (3) holds if and only if either G is the complete graph or there exists a positive real number ℓ such that

$$\frac{d_i}{d_j} + \frac{d_j}{d_i} = \ell$$

for every pair of nonadjacent different vertices v_i and v_j of G .

Proof. Certainly, the equality in (3) holds for the case where $G \cong K_n$. In

what follows, we assume that $G \not\cong K_n$. Let v_1, v_2, \dots, v_n be the vertices of G . First, we notice that the following equality holds:

$$\begin{aligned} \sum_{i \sim j; v_i \neq v_j} \frac{(d_i + d_j)^2}{d_i d_j} &= \sum_{i \sim j; v_i \neq v_j} \left(\frac{d_i^2 + d_j^2}{d_i d_j} + 2 \right) \\ &= \overline{SDD}(G) + 2\overline{m}, \end{aligned} \quad (4)$$

where

$$\overline{m} = \frac{n(n-1) - 2m}{2}.$$

On the other hand, by using Cauchy–Bunyakovsky–Schwarzs inequality, we have

$$\overline{m} \sum_{i \sim j; v_i \neq v_j} \frac{(d_i + d_j)^2}{4d_i d_j} \geq \left(\sum_{i \sim j; v_i \neq v_j} \frac{d_i + d_j}{2\sqrt{d_i d_j}} \right)^2, \quad (5)$$

with equality if and only if $\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}}$ is constant (and hence the square of $\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}}$ is constant) for every pair of nonadjacent different vertices v_i and v_j of G . From the inequality between the arithmetic and harmonic means, that is the AM–HM inequality (see e.g. [29]), we have

$$\sum_{i \sim j; v_i \neq v_j} \frac{d_i + d_j}{2\sqrt{d_i d_j}} \sum_{i \sim j; v_i \neq v_j} \frac{2\sqrt{d_i d_j}}{d_i + d_j} \geq \overline{m}^2,$$

which yields

$$\sum_{i \sim j; v_i \neq v_j} \frac{d_i + d_j}{2\sqrt{d_i d_j}} \geq \frac{\overline{m}^2}{\overline{GA}(G)}, \quad (6)$$

with equality if and only if $\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}}$ is a constant for every pair of nonadjacent different vertices v_i and v_j of G . Now, from (5), (6) and (4) we obtain

$$(\overline{SDD}(G) + 2\overline{m}) [\overline{GA}(G)]^2 \geq 4\overline{m}^3. \quad (7)$$

Since $\overline{m} = \frac{n(n-1)-2m}{2}$, from (7) we arrive at (3). ■

Corollary 1. *Let G be a simple graph of order n , size m , and minimum*

degree at least 1. Then,

$$\overline{SDD}(G) \geq n(n-1) - 2m, \quad (8)$$

with equality if and only if $d_i = d_j$ for every pair of nonadjacent different vertices v_i and v_j of G .

Proof. Let v_1, v_2, \dots, v_n be the vertices of G . From the inequality between the arithmetic and geometric means, that is the AM–GM inequality (see e.g. [29]), we have

$$\overline{GA}(G) = \sum_{i \not\sim j; v_i \neq v_j} \frac{2\sqrt{d_i d_j}}{d_i + d_j} \leq \sum_{i \not\sim j; v_i \neq v_j} 1 = \frac{n(n-1) - 2m}{2}, \quad (9)$$

with equality if and only if $d_i = d_j$ for every pair of nonadjacent different vertices v_i and v_j of G . Now, (8) follows from (3) and (9). ■

The next two results are direct consequences of Corollary 1.

Corollary 2. *If T is a tree with $n \geq 2$ vertices, then*

$$\overline{SDD}(T) \geq (n-1)(n-2),$$

with equality if and only if T is isomorphic to the star $K_{1,n-1}$.

By a unicyclic graph, we mean a connected graph having the same order and size.

Corollary 3. *If U is a unicyclic graph of order n , then*

$$\overline{SDD}(U) \geq n(n-3),$$

with equality if and only if U is isomorphic to the cycle C_n .

Remark. A graph of maximum degree at most 4 is known as a molecular graph. From Corollary 1 (or particularly, from Corollaries 2 and 3) it follows that the star $K_{1,n-1}$ (cycle C_n , respectively) uniquely minimizes the SDD coindex among all trees ((molecular) unicyclic graphs, respectively) of order $n \geq 4$.

Corollary 4. *Let G be a simple graph of order n and minimum degree at least 1. Then,*

$$SDD(G) + \overline{SDD}(G) \geq n(n-1), \quad (10)$$

with equality if and only if G is regular.

Proof. In [37], it was shown that $SDD(G) \geq 2m$, with equality if and only if G is regular. Hence, from (8), we obtain (10). ■

The next two results follow directly from (9).

Corollary 5. *Let T be a tree with $n \geq 2$ vertices. Then*

$$\overline{GA}(T) \leq \frac{(n-1)(n-2)}{2},$$

with equality if and only if $T \cong K_{1,n-1}$.

Corollary 6. *Let U be a unicyclic graph of order n . Then*

$$\overline{GA}(U) \leq \frac{n(n-3)}{2},$$

with equality if and only if $U \cong C_n$.

Corollary 7. *Let G be a simple graph of order n and minimum degree at least 1. Then,*

$$GA(G) + \overline{GA}(G) \leq \frac{n(n-1)}{2}. \quad (11)$$

Equality in (11) holds if and only if G is regular.

Proof. Note that $GA(G) \leq m$, with equality if and only if G is regular (see for example [9]). Hence, from (9), we obtain (11). ■

Next, we establish an inequality involving $\overline{SDD}(G)$, $M_1(G)$ and $M_2(G)$ for a given graph G .

Theorem 2. *Let G be a simple graph of order n , size m , and minimum degree at least 1. Then*

$$\begin{aligned} & \left(4m^2 - M_1(G) - 2M_2(G)\right) \left(\overline{SDD}(G) + n(n-1) - 2m\right) \\ & \geq 2 \left(2m(n-1) - M_1(G)\right)^2. \end{aligned} \quad (12)$$

Equality in (12) holds if and only if either G is the complete graph or there exists a positive real number ℓ such that $\frac{1}{d_i} + \frac{1}{d_j} = \ell$ for every pair of nonadjacent different vertices v_i and v_j of G .

Proof. Certainly, the equality in (23) holds for the case where $G \cong K_n$. In what follows, we assume that $G \not\cong K_n$. Let v_1, v_2, \dots, v_n be the vertices of G . By using Cauchy–Bunyakovsky–Schwarzs inequality, we have

$$\sum_{i \sim j; v_i \neq v_j} d_i d_j \sum_{i \sim j; v_i \neq v_j} \frac{(d_i + d_j)^2}{d_i d_j} \geq \left(\sum_{i \sim j; v_i \neq v_j} (d_i + d_j) \right)^2,$$

that is

$$\overline{M}_2(G) \sum_{i \sim j; v_i \neq v_j} \frac{(d_i + d_j)^2}{d_i d_j} \geq [\overline{M}_1(G)]^2, \quad (13)$$

where the equality in (13) holds if and only if there exists a positive real number ℓ such that $\frac{1}{d_i} + \frac{1}{d_j} = \ell$ for every pair of nonadjacent different vertices v_i and v_j of G . In [8] (see also [6, 19, 26]), it was proven that

$$\overline{M}_1(G) = 2m(n-1) - M_1(G). \quad (14)$$

Also, it holds [8] that

$$\overline{M}_2(G) = 2m^2 - \frac{1}{2}M_1(G) - M_2(G). \quad (15)$$

Now, by using (4), (14) and (15) in (13), we arrive at (12). ■

Next, we establish a relationship between $\overline{SDD}(G)$, $\overline{\Pi}_1(G)$ and $\overline{\Pi}_2(G)$ for a given graph G .

Theorem 3. *Let G be a simple graph of order n , size m , and minimum degree at least 1, such that $G \not\cong K_n$. Then,*

$$\overline{SDD}(G) \geq 2m - n(n-1) + \frac{n(n-1) - 2m}{2} \left(\frac{[\overline{\Pi}_1(G)]^2}{\overline{\Pi}_2(G)} \right)^{\frac{2}{n(n-1) - 2m}}. \quad (16)$$

Equality in (16) holds if and only if there exists a positive real number ℓ

such that

$$\frac{d_i}{d_j} + \frac{d_j}{d_i} = \ell$$

for every pair of nonadjacent different vertices v_i and v_j of G .

Proof. Let $\{v_1, v_2, \dots, v_n\}$ be the vertex set of G . Let $\bar{m} = \frac{n(n-1)-2m}{2}$. From the AM–GM inequality we have

$$\sum_{i \not\sim j; v_i \neq v_j} \frac{(d_i + d_j)^2}{d_i d_j} \geq \bar{m} \left(\prod_{i \not\sim j; v_i \neq v_j} \frac{(d_i + d_j)^2}{d_i d_j} \right)^{1/\bar{m}},$$

which yields

$$\sum_{i \not\sim j; v_i \neq v_j} \frac{(d_i + d_j)^2}{d_i d_j} \geq \frac{n(n-1) - 2m}{2} \left(\frac{[\bar{\Pi}_1(G)]^2}{\bar{\Pi}_2(G)} \right)^{\frac{2}{n(n-1)-2m}}. \quad (17)$$

The equality in (17) holds if and only if $\frac{(d_i + d_j)^2}{d_i d_j}$ (that is, $\frac{d_i}{d_j} + \frac{d_j}{d_i} + 2$) is constant for every pair of nonadjacent different vertices v_i and v_j of G . Now, by using (4) in (17), we obtain (16). ■

If G is a connected graph of order n and size m , then it holds [42] that

$$[\bar{\Pi}_1(G)]^2 \geq 2^{n(n-1)-2m} \bar{\Pi}_2(G). \quad (18)$$

Motivated by (18), we now establish an inequality involving the coindices $\bar{\Pi}_1$ and $\bar{\Pi}_2$.

Theorem 4. *Let G be a simple graph of order n , size m , and minimum degree at least 1, such that $G \not\cong K_n$. Then,*

$$\bar{\Pi}_1(G) \leq \bar{\Pi}_2(G) \left(\frac{2((n-1)ID(G) - n)}{n(n-1) - 2m} \right)^{\frac{n(n-1)-2m}{2}}. \quad (19)$$

Equality in (19) holds if and only if there exists a positive real number ℓ such that

$$\frac{1}{d_i} + \frac{1}{d_j} = \ell$$

for every pair of nonadjacent different vertices v_i and v_j of G .

Proof. Let $\{v_1, v_2, \dots, v_n\}$ be the vertex set of G . By keeping in mind the identity (2) and the definition of $ID(G)$, we have

$$\begin{aligned} \sum_{i \not\sim j; v_i \neq v_j} \frac{d_i + d_j}{d_i d_j} &= \sum_{i=1}^n \frac{n-1-d_i}{d_i} \\ &= (n-1)ID(G) - n. \end{aligned} \quad (20)$$

Let $\bar{m} = \frac{n(n-1)-2m}{2}$. By using the AM-GM inequality, we obtain

$$\sum_{i \not\sim j; v_i \neq v_j} \frac{d_i + d_j}{d_i d_j} \geq \bar{m} \left(\prod_{i \not\sim j} \frac{d_i + d_j}{d_i d_j} \right)^{1/\bar{m}},$$

which yields

$$\sum_{i \not\sim j; v_i \neq v_j} \frac{d_i + d_j}{d_i d_j} \geq \frac{n(n-1) - 2m}{2} \left(\frac{\bar{\Pi}_1(G)}{\bar{\Pi}_2(G)} \right)^{\frac{2}{n(n-1)-2m}}. \quad (21)$$

The equality in (21) holds if and only if $\frac{d_i + d_j}{d_i d_j}$ is constant for every pair of nonadjacent different vertices v_i and v_j of G . Now, from (20) and (21) we obtain (19). ■

Let $x = (x_i)$ and $a = (a_i)$, $i = 1, 2, \dots, n$, be two sequences, where $a_i > 0$ and $x_i \geq 0$ for every i . Then, for any non-negative real number r , the following inequality holds [33]:

$$\sum_{i=1}^n \frac{x_i^{r+1}}{a_i^r} \geq \frac{\left(\sum_{i=1}^n x_i \right)^{r+1}}{\left(\sum_{i=1}^n a_i \right)^r}. \quad (22)$$

Equality in (22) holds if and only if either $r = 0$ or

$$\frac{x_1}{a_1} = \frac{x_2}{a_2} = \dots = \frac{x_n}{a_n}.$$

Theorem 5. *Let G be a simple graph of order n , size m , and minimum*

degree at least 1. Then,

$$\left(4m^2 - M_1(G) - 2M_2(G)\right) \left(\overline{SDD}(G) - n(n-1) + 2m\right) \geq 2 [\overline{Alb}(G)]^2. \quad (23)$$

Equality in (23) holds if and only if either G is the complete graph or there exists a positive real number ℓ such that

$$\left| \frac{1}{d_i} - \frac{1}{d_j} \right| = \ell$$

for every pair of nonadjacent different vertices v_i and v_j of G .

Proof. Certainly, the equality in (23) holds for the case where $G \cong K_n$. In what follows, we assume that $G \not\cong K_n$. Let $\{v_1, v_2, \dots, v_n\}$ be the vertex set of G . We note that

$$\begin{aligned} \overline{SDD}(G) &= \sum_{i \not\sim j; v_i \neq v_j} \frac{d_i^2 + d_j^2}{d_i d_j} \\ &= \sum_{i \not\sim j; v_i \neq v_j} \frac{(d_i - d_j)^2}{d_i d_j} + 2\overline{m}, \end{aligned} \quad (24)$$

where

$$\overline{m} = \frac{n(n-1) - 2m}{2}.$$

On the other hand, by taking $r = 1$, $x_i := |d_i - d_j|$, $a_i := d_i d_j$, and the summation over all edges of the complement \overline{G} of G , the inequality (22) gives

$$\sum_{i \not\sim j; v_i \neq v_j} \frac{|d_i - d_j|^2}{d_i d_j} \geq \frac{\left(\sum_{i \not\sim j; v_i \neq v_j} |d_i - d_j|\right)^2}{\sum_{i \not\sim j; v_i \neq v_j} d_i d_j},$$

that is

$$\sum_{i \not\sim j; v_i \neq v_j} \frac{(d_i - d_j)^2}{d_i d_j} \geq \frac{[\overline{Alb}(G)]^2}{\overline{M}_2(G)}. \quad (25)$$

Equality in (25) holds if and only if $\frac{|d_i - d_j|}{d_i d_j}$ (that is, $|\frac{1}{d_i} - \frac{1}{d_j}|$) is constant for every pair of nonadjacent different vertices v_i and v_j of G . Now, from (24), (25) and (15), we obtain (23). \blacksquare

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