Filomat 38:14 (2024), 4805–4815
https://doi.org/10.2298/FIL2414805S

Published by Faculty of Sciences and Mathematics,
University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

On inequalities involving some renowned degree-based graph invariants

Stefan Stankov[a], Akbar Ali[b], Emina Milovanović[a], Marjan Matejić[a], Igor Milovanović[a,*]

[a]*Faculty of Electronic Engineering, University of Niš, Niš, Serbia*
[b]*Department of Mathematics, Faculty of Science, University of Ha'il, Ha'il, Saudi Arabia*

Abstract. Let G be a graph with the vertex set $V = \{v_1, \ldots, v_n\}$. We use the notation $i \sim j$ (respectively, $i \nsim j$) for indicating that the vertices v_i and v_j are adjacent (respectively, non-adjacent). Denote by d_k the degree of the vertex v_k. Most of the well–known vertex–degree–based topological indices and coindices can be represented in the forms $TI(G) = \sum_{i\sim j} F(d_i, d_j)$ and $\overline{TI}(G) = \sum_{i\nsim j} F(d_i, d_j)$, respectively, where F is a real symmetric function depending on d_i and d_j. In this paper, several novel inequalities between some well-known topological indices/coindices are presented. The graphs for which the obtained inequalities become equalities are also characterized.

1. Introduction

In this paper we consider only simple graphs, that is graphs without directed, weighted or multiple edges, and without self-loops. Let $G = (V, E)$ be a such graph, where $V = \{v_1, v_2, \ldots, v_n\}$ and $E = \{e_1, e_2, \ldots, e_m\}$, are its vertex and edge sets, respectively. The degree of vertex v_i is denoted by $d(v_i)$, or d_i if it is clear from the context. Denote by $(d_1, d_2, \cdots, d_n)$ the sequence of vertex degrees satisfying $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. The complement of G, denoted as $\overline{G}$, has the same vertex set $V(G)$, and two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent in G, that is $\overline{G} = (V, \overline{E})$. If vertices v_i and v_j are adjacent in G, we write $i \sim j$. On the other hand, if v_i and v_j are adjacent in $\overline{G}$, we write $i \nsim j$.

In graph theory, a graph invariant is a property of graphs that remains the same under graph isomorphism. Topological indices and coindices are special kinds of numerical graph invariants; these terms are often used in chemical graph theory. Various topological indices and coindices have been introduced in mathematical chemistry literature in order to predict different properties of chemical compounds (see for example [9, 26]).

Many degree–based topological indices can be viewed as the contributions of pairs of adjacent vertices. But, equally important are the degree–based topological indices that are defined over the non-adjacent pairs of vertices for computing some topological properties of graphs, and such topological indices are named as topological coindices.

2020 *Mathematics Subject Classification*. Primary 05C92; Secondary 04C50
Keywords. topological index, vertex degree, topological coindex.
Received: 23 March 2023; Accepted: 11 March 2024
Communicated by Dragan S. Djordjević
* Corresponding author: Igor Milovanović
Email addresses: stefan.stankov@elfak.ni.ac.rs (Stefan Stankov), akbarali.maths@gmail.com (Akbar Ali), ema@elfak.ni.ac.rs (Emina Milovanović), marjan.matejic@elfak.ni.ac.rs (Marjan Matejić), igor@elfak.ni.ac.rs (Igor Milovanović)

Most of the vertex–degree–based topological indices can be represented in the form

$$TI(G) = \sum_{i \sim j} F(d_i, d_j), \tag{1}$$

where F is a real symmetric function depending on d_i and d_j. In this paper, we consider the following particular cases of topological indices defined by (1):

- for $F(x, y) = x + y$, we obtain the first Zagreb index $M_1(G)$, first appeared in [13], which is defined (see for example [4]) as
$$M_1(G) = \sum_{i \sim j} (d_i + d_j) = \sum_{i=1}^{n} d_i^2,$$
- for $F(x, y) = xy$, we get the second Zagreb index $M_2(G)$, first appeared in [14], which is defined (see for example [4]) as
$$M_2(G) = \sum_{i \sim j} d_i d_j,$$
- for $F(x, y) = \frac{1}{xy}$, we obtain the modified second Zagreb index $M_2^*(G)$, defined in [22] as
$$M_2^*(G) = \sum_{i \sim j} \frac{1}{d_i d_j},$$
- for $F(x, y) = \frac{1}{x^2} + \frac{1}{y^2}$ and $F(x, y) = \frac{2}{x+y}$, the inverse degree index $ID(G)$ and the harmonic index $H(G)$ are obtained [11], respectively, as
$$ID(G) = \sum_{i \sim j} \left(\frac{1}{d_i^2} + \frac{1}{d_j^2} \right) = \sum_{i=1}^{n} \frac{1}{d_i} \quad \text{and} \quad H(G) = \sum_{i \sim j} \frac{2}{d_i + d_j},$$
- for $F(x, y) = \frac{xy}{x+y}$ and $F(x, y) = \frac{x}{y} + \frac{y}{x}$, the inverse sum indeg index $ISI(G)$ and the symmetric division deg index $SDD(G)$ are obtained [27], respectively, as
$$ISI(G) = \sum_{i \sim j} \frac{d_i d_j}{d_i + d_j} \quad \text{and} \quad SDD(G) = \sum_{i \sim j} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right) = \sum_{i \sim j} \frac{d_i^2 + d_j^2}{d_i d_j}.$$

More about these topological indices and their mathematical and chemical properties can be found, for example, in [1–4, 6, 18–21].

In [10] a concept of topological coindices was introduced. In this case the sum runs over the edges of the complement of G. In a view of (1) the corresponding coindex of G can be defined as

$$\overline{TI}(G) = \sum_{i \nsim j} F(d_i, d_j). \tag{2}$$

Here we list topological coindices which are of interest for this study:

- the first and the second Zagreb coindices, $\overline{M}_1(G)$ and $\overline{M}_2(G)$ respectively, are defined in [10] as
$$\overline{M}_1(G) = \sum_{i \nsim j} (d_i + d_j) \quad \text{and} \quad \overline{M}_2(G) = \sum_{i \nsim j} d_i d_j,$$

- the inverse sum indeg coindex $\overline{ISI}(G)$, defined as

$$\overline{ISI}(G) = \sum_{i \nsim j} \frac{d_i d_j}{d_i + d_j},$$

- the modified second Zagreb coindex, $\overline{M_2^*}(G)$, defined as

$$\overline{M_2^*}(G) = \sum_{i \nsim j} \frac{1}{d_i d_j},$$

- symmetric division deg coindex, $\overline{SDD}(G)$, defined in [23] as

$$\overline{SDD}(G) = \sum_{i \nsim j} \frac{d_i^2 + d_j^2}{d_i d_j}.$$

In [25] some bounds for linear combinations of topological indices $M_1(G)$ and $M_2(G)$ were established. In this paper we present some novel inequalities between various topological indices/coindices and characterize graphs for which equalities in these inequalities are attained.

2. Some Known Results

In this section, we recall some results from the literature for linear combinations of the topological indices $M_1(G)$ and $M_2(G)$.

In [5], the following inequality for connected graphs was proven

$$M_2(G) - M_1(G) \geq 11m - 12n,$$

and in [7] it was shown that

$$M_1(G) + 2M_2(G) \leq 4m^2.$$

Inspired by these results, in [25], the following inequalities were established:

$$\delta M_1(G) - M_2(G) \leq m\delta^2, \tag{3}$$

$$\Delta M_1(G) - M_2(G) \leq m\Delta^2, \tag{4}$$

and

$$\Delta M_1(G) - M_2(G) \geq m\Delta\delta. \tag{5}$$

The inequalities presented in this section are the inspiration for current work.

3. Main Results

3.1. Inequalities between $\boldsymbol{ISI(G)}$ and $\boldsymbol{H(G)}$, and their coindices

First, we prove a result involving the inverse sum indeg index and the harmonic index when the size and minimum degree or maximum degree of the considered graph are known.

Theorem 3.1. *Let G be a connected graph of size m and minimum degree δ. Then*

$$ISI(G) + \frac{\delta^2}{2}H(G) \geq m\delta \tag{6}$$

with equality if and only if each edge of G is incident to at least one vertex of degree δ. However, if G is a connected graph of size m and maximum degree Δ, then

$$ISI(G) + \frac{\Delta^2}{2}H(G) \geq m\Delta, \tag{7}$$

where the equality in (7) holds if and only if each edge of G is incident to at least one vertex of degree Δ.

Proof. Let $(d_1, d_2, \cdots, d_n)$ be the sequence of vertex degrees of G satisfying $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. For any i and j with $1 \leq i \leq n$ and $1 \leq j \leq n$, it holds that

$$(d_i - \delta)(d_j - \delta) \geq 0 \quad \text{and} \quad (\Delta - d_i)(\Delta - d_j) \geq 0,$$

that is

$$d_i d_j + \delta^2 \geq \delta(d_i + d_j) \quad \text{and} \quad d_i d_j + \Delta^2 \geq \Delta(d_i + d_j). \tag{8}$$

After multiplying the inequalities in (8) by $\frac{1}{d_i+d_j}$ we obtain

$$\frac{d_i d_j}{d_i + d_j} + \frac{\delta^2}{d_i + d_j} \geq \delta \quad \text{and} \quad \frac{d_i d_j}{d_i + d_j} + \frac{\Delta^2}{d_i + d_j} \geq \Delta. \tag{9}$$

The summation of (9) over all pairs of adjacent vertices v_i and v_j of G, yields

$$\sum_{i\sim j} \frac{d_i d_j}{d_i + d_j} + \frac{\delta^2}{2} \sum_{i\sim j} \frac{2}{d_i + d_j} \geq \delta \sum_{i\sim j} 1, \quad \sum_{i\sim j} \frac{d_i d_j}{d_i + d_j} + \frac{\Delta^2}{2} \sum_{i\sim j} \frac{2}{d_i + d_j} \geq \Delta \sum_{i\sim j} 1,$$

from which we arrive at (6) and (7).

Equality in the first inequality in (8), and consequently in (6), holds if and only if each edge e_i of G is incident to at least one vertex v_i of degree δ.

Equality in the second inequality in (8), therefore in (7), holds if and only if each edge e_i of G is incident to at least one vertex v_i of degree Δ. □

Remark 3.2. *Certainly, equalities in (6) and (7) hold for all regular connected graphs. However, it seems to be interesting to note that the equalities in (6) and (7) hold also for many well–known classes of non-regular connected graphs. Figure 1 illustrates some graphs for which the equality in (6) is attained, while Figure 2 depicts some graphs for which the equality in (7) holds.*

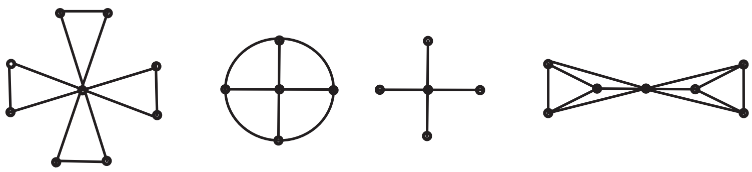

Figure 1: Examples of graphs satisfying the equality in (6)

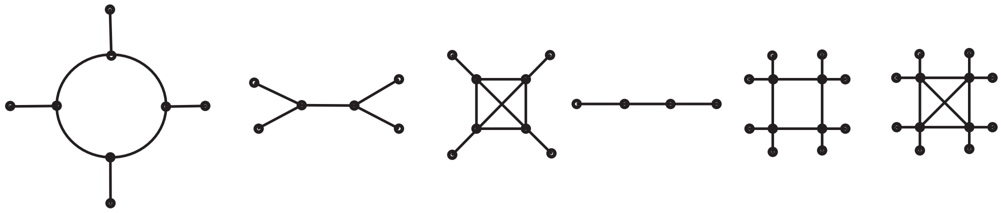

Figure 2: Examples of graphs satisfying the equality in (7)

Next, we present some corollaries of Theorem 3.1.

Corollary 3.3. *Let G be a connected graph with size m and minimum degree 1. Then*

$$ISI(G) + \frac{1}{2}H(G) \geq m.$$

Equality holds if and only if G is the star graph.

Corollary 3.4. *Let G be a connected graph with size m, minimum degree δ and maximum degree Δ. Then*

$$2ISI(G) + \frac{(\Delta^2 + \delta^2)H(G)}{2} \geq m(\Delta + \delta).$$

Equality holds if and only if G is either a regular graph or a complete bipartite graph.

Corollary 3.5. *Let G be a connected graph with n vertices and m edges such that the maximum degree of G is $n-1$. Then*

$$ISI(G) + \frac{(n-1)^2}{2}H(G) \geq m(n-1).$$

Equality holds if and only if each edge of G is incident to at least one vertex of degree $n-1$.

Corollary 3.6. *Let G be a connected graph of order n, size m and minimum degree δ such that $G \ncong K_n$. Then*

$$\overline{ISI}(G) + \frac{\delta^2}{2}\overline{H}(G) \geq \frac{\delta}{2}(n(n-1) - 2m) \tag{10}$$

with equality if and only if each edge of $\overline{G}$ is incident to at least one vertex of degree δ. Also, if G is a connected graph of order n, size m and maximum degree Δ such that $G \ncong K_n$, then

$$\overline{ISI}(G) + \frac{\Delta^2}{2}\overline{H}(G) \geq \frac{\Delta}{2}(n(n-1) - 2m). \tag{11}$$

Equality in (11) *holds if and only if each edge of $\overline{G}$ is incident to at least one vertex of degree Δ.*

Proof. As before, let $(d_1, d_2, \cdots, d_n)$ be the sequence of vertex degrees of G satisfying $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. After summation of (9) over all pairs of non-adjacent vertices v_i and v_j in G we obtain

$$\sum_{i \nsim j} \frac{d_i d_j}{d_i + d_j} + \frac{\delta^2}{2} \sum_{i \nsim j} \frac{2}{d_i + d_j} \geq \delta \sum_{i \nsim j} 1, \quad \sum_{i \nsim j} \frac{d_i d_j}{d_i + d_j} + \frac{\Delta^2}{2} \sum_{i \nsim j} \frac{2}{d_i + d_j} \geq \Delta \sum_{i \nsim j} 1,$$

from which (10) and (11) are obtained. Also, the equalities characterizations follow directly. □

Remark 3.7. *After summation of* (8) *over all pairs of adjacent vertices v_i and v_j in G we obtain* (3) *and* (4).

Corollary 3.8. *Let G be a connected graph of order n, size m and minimum degree δ. Then*

$$\delta\overline{M}_1(G) - \overline{M}_2(G) \le \frac{\delta^2}{2}(n(n-1) - 2m)$$

with equality if and only if each edge of $\overline{G}$ *is incident to at least one vertex of degree δ. Also, if G is a connected graph of order n, size m and maximum degree Δ, then*

$$\Delta\overline{M}_1(G) - \overline{M}_2(G) \le \frac{\Delta^2}{2}(n(n-1) - 2m),$$

where the equality holds if and only if each edge of $\overline{G}$ *is incident to at least one vertex of degree Δ.*

Proof. The desired results follow after applying the summation on (8) over all pairs of non-adjacent vertices v_i and v_j of G. □

Next, we establish an inequality involving the inverse sum indeg index and the harmonic index when the size, minimum degree and maximum degree of the considered graph are known.

Theorem 3.9. *Let G be a connected graph of size m, minimum degree δ and maximum degree Δ. Then*

$$2ISI(G) + \Delta\delta H(G) \le m(\Delta + \delta). \tag{12}$$

Equality holds if and only if G is a regular graph.

Proof. Let $(d_1, d_2, \cdots, d_n)$ be the sequence of vertex degrees of G satisfying $\Delta = d_1 \ge d_2 \ge \cdots \ge d_n = \delta$. For any i and j with $1 \le i \le n$ and $1 \le j \le n$, we have

$$(\Delta - d_i)(d_j - \delta) \ge 0 \quad \text{and} \quad (d_i - \delta)(\Delta - d_j) \ge 0,$$

i.e.

$$d_id_j + \Delta\delta \le \delta d_i + \Delta d_j \quad \text{and} \quad d_id_j + \Delta\delta \le \Delta d_i + \delta d_j. \tag{13}$$

By summing up the inequalities in (13), we get

$$2d_id_j + 2\Delta\delta \le (\Delta + \delta)(d_i + d_j). \tag{14}$$

After multiplying the both sides of (14) with $\frac{1}{d_i+d_j}$ we get

$$2\frac{d_id_j}{d_i + d_j} + \frac{2\Delta\delta}{d_i + d_j} \le \Delta + \delta. \tag{15}$$

Finally, after summation of (15) over all pairs of adjacent vertices v_i and v_j in G we obtain (12).

It remains to prove the equality characterization. Suppose that v_i and v_j are two adjacent vertices in G. Then equality in (14) holds if and only if either $d_i = \delta$ or $d_j = \Delta$, and $d_i = \Delta$ or $d_j = \delta$. This implies that equality in (14) holds if and only if $d_i = d_j = \Delta = \delta$, which means that equality in (12) holds if and only if G is a regular graph. □

Next, we give several corollaries of Theorem 3.9

Corollary 3.10. *Let G be a connected graph of size m, minimum degree δ and maximum degree Δ. Then*

$$ISI(G) + \frac{\Delta\delta}{2}H(G) \le \Delta m.$$

Equality holds if and only if G is a regular graph.

Proof. Based on (13) we have

$$d_i d_j + \Delta\delta \leq \Delta(d_i + d_j). \tag{16}$$

If we divide this inequality with $d_i + d_j$ we get

$$\frac{d_i d_j}{d_i + d_j} + \frac{\Delta\delta}{d_i + d_j} \leq \Delta.$$

Now, after applying the summation on the above inequality over all pairs of adjacent vertices v_i and v_j of G, we obtain the desired result. □

Corollary 3.11. *Let G be a connected graph of size m, minimum degree δ and maximum degree Δ. Then*

$$2ISI(G) + \frac{2m^2\Delta\delta}{M_1(G)} \leq m(\Delta + \delta). \tag{17}$$

Equality holds if and only if G is a regular graph.

Proof. In [12] it was proven that

$$H(G)M_1(G) \geq 2m^2.$$

From the above and inequality (12) we obtain (17). □

Corollary 3.12. *Let G be a connected graph of order at least 2, size m, minimum degree δ and maximum degree Δ. Then*

$$2ISI(G) + \frac{2m^2\Delta\delta}{2m(\Delta + \delta) - n\Delta\delta} \leq m(\Delta + \delta).$$

Equality holds if and only if G is a regular graph.

Proof. In [8] it was proven that

$$M_1(G) \leq 2m(\Delta + \delta) - n\Delta\delta.$$

From the above and inequality (17) we obtain the desired result. □

Corollary 3.13. *Let G be a connected graph of order n, size m, minimum degree δ and maximum degree Δ such that $G \ncong K_n$. Then*

$$2\overline{ISI}(G) + \Delta\delta\overline{H}(G) \leq \frac{1}{2}(\Delta + \delta)(n(n-1) - 2m).$$

Equality holds if and only if each edge e_i of $\overline{G}$ is incident to two vertices v_i and v_j in G of degrees δ, or e_i is incident to two vertices v_i and v_j in G of degrees Δ.

Proof. The desired result is obtained after applying summation on (15) over all pairs of non-adjacent vertices v_i and v_j in G. □

Remark 3.14. *After applying the summation on* (16) *over all pairs of adjacent vertices v_i and v_j in G we obtain* (5).

Corollary 3.15. *Let G be a connected graph of order n, size m, minimum degree δ and maximum degree Δ. Then*

$$\Delta\overline{M}_1(G) - \overline{M}_2(G) \geq \frac{\Delta\delta}{2}(n(n-1) - 2m).$$

Equality holds if and only if G is a regular graph.

Corollary 3.16. *Let G be a connected graph of order n, size m, minimum degree δ and maximum degree Δ. Then*

$$(\Delta + \delta)\overline{M}_1(G) - 2\overline{M}_2(G) \geq \Delta\delta(n(n-1) - 2m).$$

Equality holds if and only if each edge e_i of $\overline{G}$ is incident to two vertices v_i and v_j in G of degrees δ, or e_i is incident to two vertices v_i and v_j in G of degrees Δ.

3.2. Inequalities between $\boldsymbol{M_1(G)}$ and $\boldsymbol{SDD(G)}$, and their coindices

The next result reveals a connection between the first Zagreb index and symmetric division deg index when the order, size, and minimum degree or maximum degree of the considered graph are known.

Theorem 3.17. *Let G be a connected graph of order n, size m and minimum degree δ. Then*

$$M_1(G) - \delta SDD(G) \geq \delta(2m - n\delta) \tag{18}$$

with equality if and only if each edge of G is incident to at least one vertex of degree δ. Also, if G is a connected graph of order n, size m and maximum degree Δ, then

$$\Delta SDD(G) - M_1(G) \leq \Delta(n\Delta - 2m), \tag{19}$$

where the equality in (19) *holds if and only if each edge of G is incident to at least one vertex of degree Δ.*

Proof. Let $(d_1, d_2, \cdots, d_n)$ be the sequence of vertex degrees of G satisfying $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. After multiplying (8) with $\frac{1}{d_i} + \frac{1}{d_j}$ we get

$$\begin{aligned} d_i + d_j + \delta^2\left(\frac{1}{d_i} + \frac{1}{d_j}\right) &\geq \delta\frac{(d_i + d_j)^2}{d_id_j}, \\ d_i + d_j + \Delta^2\left(\frac{1}{d_i} + \frac{1}{d_j}\right) &\geq \Delta\frac{(d_i + d_j)^2}{d_id_j}, \end{aligned} \tag{20}$$

i.e.

$$d_i + d_j + \delta^2\left(\frac{1}{d_i} + \frac{1}{d_j}\right) \geq \delta\left(\frac{d_i^2 + d_j^2}{d_id_j} + 2\right),$$

$$d_i + d_j + \Delta^2\left(\frac{1}{d_i} + \frac{1}{d_j}\right) \geq \Delta\left(\frac{d_i^2 + d_j^2}{d_id_j} + 2\right).$$

After applying the summation on the above inequalities over all pairs of adjacent vertices v_i and v_j of G, we obtain

$$\sum_{i\sim j}(d_i + d_j) + \delta^2\sum_{i\sim j}\left(\frac{1}{d_i} + \frac{1}{d_j}\right) \geq \delta\left(\sum_{i\sim j}\frac{d_i^2 + d_j^2}{d_id_j} + 2m\right),$$

$$\sum_{i\sim j}(d_i + d_j) + \Delta^2\sum_{i\sim j}\left(\frac{1}{d_i} + \frac{1}{d_j}\right) \geq \Delta\left(\sum_{i\sim j}\frac{d_i^2 + d_j^2}{d_id_j} + 2m\right).$$

Since

$$\sum_{i\sim j}\left(\frac{1}{d_i} + \frac{1}{d_j}\right) = \sum_{i=1}^{n} d_i\frac{1}{d_i} = n,$$

from the above we arrive at (18) and (19).

Equalities in (20) hold under the same conditions as in (8) and (9). Therefore equalities in (18) and (19) hold under the same conditions as in (6) and (7). □

Corollary 3.18. *Let G be a connected graph of order n, size m, minimum degree δ and maximum degree Δ. Then*

$$\delta SDD(G) \leq 2m\Delta - n\delta(\Delta - \delta)$$

and

$$\Delta SDD(G) \leq 2m\delta + n\Delta(\Delta - \delta).$$

Equality in the first inequality holds if and only if G is a bidegreed graph in which every edge of G is incident to at least one vertex of degree δ. Also, equality in the second inequality holds if and only if G is a bidegreed graph in which every edge of G is incident to at least one vertex of degree Δ.

Corollary 3.19. *Let G be a connected graph of order n, size m and minimum degree δ such that $G \ncong K_n$. Then*

$$\overline{M}_1(G) + \delta^2(n-1)ID(G) - \delta\overline{SDD}(G) \geq \delta(n(n-1) - 2m + n\delta) \tag{21}$$

with equality in if and only if each edge of $\overline{G}$ is incident to at least one vertex of degree δ. Also, if G is a connected graph of order n, size m and maximum degree Δ such that $G \ncong K_n$, then

$$\overline{M}_1(G) + \Delta^2(n-1)ID(G) - \Delta\overline{SDD}(G) \geq \Delta(n(n-1) - 2m + n\Delta), \tag{22}$$

where equality in (22) *holds if and only if each edge of $\overline{G}$ is incident to at least one vertex of degree Δ.*

Proof. Let $(d_1, d_2, \cdots, d_n)$ be the sequence of vertex degrees of G satisfying $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. After applying the summation on (20) over all pairs of non-adjacent vertices v_i and v_j of G, we obtain

$$\sum_{i \nsim j}(d_i + d_j) + \delta^2 \sum_{i \nsim j}\left(\frac{1}{d_i} + \frac{1}{d_j}\right) \geq \delta \sum_{i \nsim j}\left(\frac{d_i^2 + d_j^2}{d_i d_j} + 2\right),$$

$$\sum_{i \nsim j}(d_i + d_j) + \Delta^2 \sum_{i \nsim j}\left(\frac{1}{d_i} + \frac{1}{d_j}\right) \geq \Delta \sum_{i \nsim j}\left(\frac{d_i^2 + d_j^2}{d_i d_j} + 2\right).$$

Since

$$\sum_{i \nsim j}\left(\frac{1}{d_i} + \frac{1}{d_j}\right) = \sum_{i=1}^{n}(n-1-d_i)\frac{1}{d_i} = (n-1)ID(G) - n,$$

the above inequalities become

$$\overline{M}_1(G) + \delta^2((n-1)ID(G) - n) \geq \delta(\overline{SDD}(G) + n(n-1) - 2m)$$

and

$$\overline{M}_1(G) + \Delta^2((n-1)ID(G) - n) \geq \Delta(\overline{SDD}(G) + n(n-1) - 2m),$$

from which we get (21) and (22).

Equalities in (21) and (22) hold under the same conditions as in (10) and (11). □

Theorem 3.20. *Let G be a connected graph of order n, size m, minimum degree δ and maximum degree Δ. Then*

$$2M_1(G) - (\Delta + \delta)SDD(G) \leq 2m(\Delta + \delta) - 2n\Delta\delta \tag{23}$$

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

Proof. After multiplying (14) with $\frac{1}{d_i} + \frac{1}{d_j}$ we get

$$2(d_i + d_j) + 2\Delta\delta\left(\frac{1}{d_i} + \frac{1}{d_j}\right) \leq (\Delta + \delta)\left(\frac{d_i^2 + d_j^2}{d_i d_j} + 2\right), \tag{24}$$

where $(d_1, d_2, \cdots, d_n)$ is the sequence of vertex degrees of G satisfying $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. After applying the summation on (24) over all pairs of adjacent vertices v_i and v_j of G, we obtain

$$2\sum_{i \sim j}(d_i + d_j) + 2\Delta\delta \sum_{i \sim j}\left(\frac{1}{d_i} + \frac{1}{d_j}\right) \leq (\Delta + \delta)\left(\sum_{i \sim j}\frac{d_i^2 + d_j^2}{d_i d_j} + 2m\right),$$

from which we get (23).

Equality in (23) is attained under the same condition as in (12). □

Corollary 3.21. *Let G be a connected graph of order n, size m and minimum degree δ such that $G \ncong K_n$. Then*

$$2\overline{M}_1(G) + 2\Delta\delta((n-1)ID(G) - n) - (\Delta + \delta)\overline{SDD}(G) \le (\Delta + \delta)(n(n-1) - 2m) - 2n\Delta\delta.$$

Equality holds if and only if both the end vertices of each edge of $\overline{G}$ have either degree δ or degree Δ.

3.3. Inequalities between $M_2(G)$, $M_2^*(G)$ and $SDD(G)$, and their coindices

In the next theorem, we establish a connection between topological indices $M_2(G)$, $M_2^*(G)$ and $SDD(G)$, when either the minimum degree or the maximum degree of the considered graph is given.

Theorem 3.22. *Let G be a connected graph with the minimum degree δ. Then*

$$M_2(G) - \delta^2 SDD(G) + \delta^4 M_2^*(G) \ge 0 \tag{25}$$

with equality if and only if each edge of G is incident to at least one vertex of degree δ. Also, if G is a connected graph with the maximum degree Δ, then

$$M_2(G) - \Delta^2 SDD(G) + \Delta^4 M_2^*(G) \ge 0. \tag{26}$$

Equality in (26) *holds if and only if each edge of G is incident to at least one vertex of degree Δ.*

Proof. Let $(d_1, d_2, \cdots, d_n)$ be the sequence of vertex degrees of G satisfying $\Delta = d_1 \ge d_2 \ge \cdots \ge d_n = \delta$. After squaring the inequality (8) we get

$$(d_i d_j)^2 + \delta^4 \ge \delta^2(d_i^2 + d_j^2) \quad \text{and} \quad (d_i d_j)^2 + \Delta^4 \ge \Delta^2(d_i^2 + d_j^2).$$

If we divide these inequalities with $d_i d_j$ we have that

$$d_i d_j + \frac{\delta^4}{d_i d_j} \ge \delta^2 \frac{d_i^2 + d_j^2}{d_i d_j} \quad \text{and} \quad d_i d_j + \frac{\Delta^4}{d_i d_j} \ge \Delta^2 \frac{d_i^2 + d_j^2}{d_i d_j}. \tag{27}$$

After applying the summation on (27) over all pairs of adjacent vertices v_i and v_j of G, we obtain

$$\sum_{i \sim j} d_i d_j + \delta^4 \sum_{i \sim j} \frac{1}{d_i d_j} \ge \delta^2 \sum_{i \sim j} \frac{d_i^2 + d_j^2}{d_i d_j}, \ \sum_{i \sim j} d_i d_j + \Delta^4 \sum_{i \sim j} \frac{1}{d_i d_j} \ge \Delta^2 \sum_{i \sim j} \frac{d_i^2 + d_j^2}{d_i d_j},$$

from which we arrive at (25) and (26).

Equalities in (25) and (26) hold under the same conditions as in (6) and (7), respectively. □

Corollary 3.23. *Let G be a connected graph with the minimum degree δ. Then*

$$\overline{M}_2(G) - \delta^2 \overline{SDD}(G) + \delta^4 \overline{M_2^*}(G) \ge 0. \tag{28}$$

Equality in (28) *holds if and only if each edge of $\overline{G}$ is incident to at least one vertex of degree δ. Also, if G is a connected graph with the maximum degree Δ, then*

$$\overline{M}_2(G) - \Delta^2 \overline{SDD}(G) + \Delta^4 \overline{M_2^*}(G) \ge 0. \tag{29}$$

Equality in (29) *holds if and only if each edge of $\overline{G}$ is incident to at least one vertex of degree Δ.*

Proof. The desired inequalities follow after applying the summation on (27) over all pairs of non-adjacent vertices v_i and v_j of G. □

References

[1] A. Ali, I. Gutman, E. Milovanović, I. Milovanović, *Sum of powers of the degrees of graphs: extremal results and bounds*, MATCH Commun. Math. Comput. Chem. 80 (2018) 5–84.
[2] A. Ali, I. Gutman, I. Redžepović, A. M. Albalahi, Z. Raza, A. E. Hamza, *Symmetric division deg index: extremal results and bounds*, MATCH Commun. Math. Comput. Chem., to appear.
[3] A. Ali, L. Zhong, I. Gutman, *Harmonic index and its generalizations: extremal results and bounds*, MATCH Commun. Math. Comput. Chem. 81 (2019) 249–311.
[4] B. Borovićanin, K. C. Das, B. Furtula, I. Gutman, *Bounds for the Zagreb indices*, MATCH Commun. Math. Comput. Chem. 78(1) (2017) 17–100.
[5] G. Caporossi, P. Hansen, D. Vukičević, *Comparing Zagreb indices of cyclic graphs*, MATCH Commun. Math. Comput. Chem. 63 (2010) 441–451.
[6] K. Ch. Das, M. Matejić, E. Milovanović, I. Milovanović, *Bounds for symmetric division deg index of graphs*, Filomat 33(3) (2019) 683–698.
[7] K. Ch. Das, I. Gutman, *Some properties of the second Zagreb index*, MATCH Commun. Math. Comput. Chem. 52 (2004) 103–112.
[8] K. C. Das, *Maximizing the sum of the squares of the degrees of a graph*, Discr. Math. 285 (2004) 57–66.
[9] J. Devillers, A. T. Balaban (Eds.), *Topological indices and related descriptors in QSAR and QSPR*, Gordon & Breach, New York, 1999.
[10] T. Došlić, *Vertex–weighted Wiener polynomials for composite graphs*, Ars Math. Contemp. 1 (2008) 66–80.
[11] S. Fajtlowicz, *On conjectures of graffiti II*, Congr. Numer. 60 (1987) 187–197.
[12] F. Falahati-Nezhad, M. Azari, T. Došlić, *Sharp bounds on the inverse sum indeg index*, Discrete Appl. Math. 217 (2017) 185–195.
[13] I. Gutman, N. Trinajstić, *Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. 17 (1972) 535–538.
[14] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, *Graph theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys. 62 (1975) 3399–3405.
[15] S. M. Hosamani, B. Basavanagoud, *New upper bounds for the first Zagreb index*, MATCH Commun. Math. Comput. Chem. 74 (2015) 97–101.
[16] A. Ilić, M. Ilić, B. Liu, *On the upper bounds for the first Zagreb index*, Kragujevac J. Math. 35 (2011) 173–182.
[17] J. Li, W. C. Shiu, A. Chang, *On the Laplacian Estrada index of a graph*, Appl. Anal. Discrete Math. 3 (2009) 147–156.
[18] M. Matejić, I. Milovanović, E. Milovanović, *On bounds for harmonic topological index*, Filomat 32(1) (2018) 311–317.
[19] M. M. Matejić, I. Ž. Milovanović, E. I. Milovanović, *Upper bounds for the inverse sum indeg index of graphs*, Discrete Appl. Math. 251 (2018) 258–267.
[20] E. Milovanović, I. Milovanović, M. Jamil, *Some properties of the Zagreb indices*, Filomat 32(7) (2018) 2667–2675.
[21] P. Milošević, I. Milovanović, E. Milovanović, M. Matejić, *Some inequalities for general zeroth–order Randić index*, Filomat 33(16) (2019) 5249–5258.
[22] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, *The Zagreb indices 30 years after*, Croat. Chem. Acta 76 (2003) 113–124.
[23] K. Pattabiraman, *A note on the symmetric division deg coindex of graphs*, Electron. J. Math. 2 (2021) 37–43.
[24] M. Randić, *On characterization of molecular branching*, J. Amer. Chem. Soc. 97 (1975) 6609–6615.
[25] T. Réti, *On the relationship between the first and second Zagreb indices*, MATCH Commun. Math. Comput. Chem. 68 (2012) 169–188.
[26] R. Todeschini, V. Consonni, *Handbook of molecular descriptors*, Wiley–VCH, Weinheim, 2000.
[27] D. Vukičević, M. Gašperov, *Bond additive modeling 1. Adriatic indices*, Croat. Chem. Acta 83 (2010) 243–260.