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Research Paper

On linear combinations between Zagreb indices/coindices of a line graph

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Abstract. Let $G = (V, E)$, $V = \{v_1, v_2, \ldots, v_n\}$, be a simple graph of order n and size m. Denote by $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$, $d_i = d(v_i)$, and $\Delta_e = d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m) = \delta_e$, sequences of vertex and edge degrees, respectively. The first reformulated Zagreb index (coindex) is defined as $EM_1(G) = \sum_{i=1}^{m} d(e_i)^2 = \sum_{e_i \sim e_j} (d(e_i) + d(e_j))$ $\left(\overline{EM}_1(G) = \sum_{e_i \nsim e_j} (d(e_i) + d(e_j))\right)$. We consider relationship between reformulated Zagreb indices/coindices and determine their bounds in terms of some basic graph parameters.

Keywords: topological indices; zagreb indices; line graph
Mathematics Subject Classification (2010): 05C09.

1 Introduction

Let $G = (V, E)$, where $V = \{v_1, v_2, \ldots, v_n\}$ and $E = \{e_1, e_2, \ldots, e_m\}$ be a simple graph with n vertices and m edges. Denote by $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$, $d_i = d(v_i)$, and $\Delta_e = d(e_1) \geq d(e_2) \geq \cdots \geq d(e_m) = \delta_e$, sequences of vertex and edge degrees, respectively. If vertices v_i and v_j (edges e_i and e_j) are adjacent, we denote it as $i \sim j$ ($e_i \sim e_j$), otherwise we write $i \nsim j$ (i.e. $e_i \nsim e_j$).

A line graph, $L(G)$, of a graph G is the graph derived from G such that the edges in G are replaced by vertices in $L(G)$. Two vertices in $L(G)$ are connected whenever the correspond-

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ing edges in G are adjacent. The number of vertices in $L(G)$ is equal to the number of edges in G, i.e. $n_L = m$, and number of edges (see, for example, [10, 24]) is

$$m_L = \frac{1}{2}\sum_{i\sim j}(d_i + d_j - 2).$$

In graph theory, a graph invariant is property of the graph that is preserved by isomorphisms. The graph invariants that assume only numerical values are usually referred to as topological indices in chemical graph theory. Topological indices are important tools used to relate molecular structure with physicochemical characteristics of chemical compounds, especially those relevant for their pharmacological, medical, toxicological, and similar properties.

The first Zagreb index, $M_1(G)$, is defined as the sum of the squares of the degrees of the vertices [11]

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

and the second Zagreb index as the sum of the product of the degrees of adjacent vertices [12]

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

In [22] it was proven that the first Zagreb index satisfies the identity

$$M_1(G) = \sum_{i\sim j}(d_i + d_j). \tag{1}$$

It can be easily verified that the number of edges in a graph $L(G)$ holds in

$$m_L = \frac{1}{2}M_1(G) - m. \tag{2}$$

More on the mathematical properties and chemical applications of the Zagreb indices can be found in [1, 4, 5, 13, 14] and in the references cited therein.

The Zagreb indices can be reformulated in terms of the edges degree instead of the vertices degree. The first and the second reformulated Zagreb indices, $EM_1(G)$ and $EM_2(G)$, are defined as [18]:

$$EM_1(G) = \sum_{i=1}^{m} d(e_i)^2 = \sum_{e_i\sim e_j}(d(e_i) + d(e_j)) \quad \text{and} \quad EM_2(G) = \sum_{e_i\sim e_j} d(e_i)d(e_j).$$

The original and reformulated Zagreb indices are related as follows:

$$EM_1(G) = M_1(L(G)) \quad \text{and} \quad EM_2(G) = M_2(L(G)).$$

Therefore, one can compute the reformulated Zagreb indices of a graph G as the Zagreb indices of the corresponding line graph $L(G)$. More on these indices can be found in [8, 15, 19, 25].

The concept of coindices was introduced in [9] (see also [2]). In this case the sum runs over the edges of the complement of G. In a view of (1), the corresponding first Zagreb coindex of G is defined as

$$\overline{M}_1(G) = \sum_{i \nsim j} (d_i + d_j),$$

and the second Zagreb coindex as

$$\overline{M}_2(G) = \sum_{i \nsim j} d_i d_j .$$

Analogously, reformulated first and second Zagreb coindices, $\overline{EM}_1(G)$ and $\overline{EM}_2(G)$, are defined as

$$\overline{EM}_1(G) = \sum_{e_i \nsim e_j} (d(e_i) + d(e_j)) = \sum_{i=1}^{m} (m - 1 - d(e_i)) d(e_i), \tag{3}$$

and

$$\overline{EM}_2(G) = \sum_{e_i \nsim e_j} d(e_i) d(e_j) . \tag{4}$$

In the present paper we consider linear combinations between reformulated Zagreb indices/coindices and determine their bounds in terms of some basic graph parameters.

2 Preliminaries

In this section we recall some results reported in the literature for $EM_1(G)$ and $EM_2(G)$ that are of interest for our work.

In [15] the following relations between reformulated Zagreb indices and the first Zagreb index was proven.

Lemma 2.1. [15] *Let G be a simple graph with n vertices and m edges. Then*

$$EM_1(G) - EM_2(G) \le \frac{1}{2} M_1(G) - m, \tag{5}$$

with equality if and only if G is a union of isolated vertices and paths P_2 and P_3.

Lemma 2.2. [15] *Let G be a simple graph with n vertices and m edges. Then*

$$EM_2(G) \ge \frac{(M_1(G) - 2m)^3}{2m^2}, \tag{6}$$

with equality if and only if $L(G)$ is regular.

Let us note that the inequality (6) was independently proven in [8], but with wrong equality conditions. Also, in the same paper the following result was established.

Lemma 2.3. [8] *Let G be a simple graph with n vertices and m edges. Then*

$$EM_1(G) \geq \frac{(M_1(G)-2m)^2}{m}, \tag{7}$$

with equality if and only if G is regular.

Let us note that the equality condition in (7) is not correct. Namely, one can easily see that equality (7) holds if and only if $L(G)$ is regular graph. The inequality (7) was also proven later in [23].

For the number of edges of a line graph $L(G)$, we have the following result.

Lemma 2.4. *Let G be a simple graph with m edges. Then*

$$\frac{1}{2}m\delta_e \leq m_L \leq \frac{1}{2}m\Delta_e, \tag{8}$$

with equality if and only if $L(G)$ is regular.

Proof. For any edge e_i, $i=1,2,\ldots,m$, in a graph G we have

$$\delta_e \leq d(e_i) \leq \Delta_e, \tag{9}$$

i.e. for any two adjacent vertices v_i and v_j in G

$$\delta_e \leq d_i + d_j - 2 \leq \Delta_e.$$

After summing up the above inequality over all adjacent vertices v_i and v_j in G, we get

$$\delta_e \sum_{i\sim j} 1 \leq \sum_{i\sim j}(d_i+d_j) - 2\sum_{i\sim j} 1 \leq \Delta_e \sum_{i\sim j} 1,$$

that is

$$m\delta_e \leq M_1(G) - 2m \leq m\Delta_e.$$

From the above and (2) we arrive at (8).

Equality (9) holds if and only if $d(e_i) = \Delta_e = \delta_e$ for every $i=1,2,\ldots,m$. Therefore, equality (8) holds if and only if $L(G)$ is regular. □

3 Main results

In the next theorem we determine a relationship between the first and second reformulated Zagreb indices.

Theorem 3.1. *Let G be a simple graph with $m \geq 2$ edges. Then*

$$\delta_e EM_1(G) - EM_2(G) \leq \delta_e^2 m_L, \tag{10}$$

and

$$\Delta_e EM_1(G) - EM_2(G) \leq \Delta_e^2 m_L. \tag{11}$$

Equality (10) *holds if and only if for every pair of adjacent edges e_i and e_j in G, holds that at least one is of degree δ_e, whereas in* (11) *if and only if at least one in the pair is of degree Δ_e.*

Proof. For every i and j, $1 \leq i,j \leq m$,

$$(d(e_i)-\delta_e)(d(e_j)-\delta_e) \geq 0 \qquad \text{and} \qquad (\Delta_e - d(e_i))(\Delta_e - d(e_j)) \geq 0\,,$$

that is

$$\begin{aligned} d(e_i)d(e_j) + \delta_e^2 &\geq \delta_e(d(e_i)+d(e_j))\,, \\ d(e_i)d(e_j) + \Delta_e^2 &\geq \Delta_e(d(e_i)+d(e_j))\,. \end{aligned} \tag{12}$$

After summation of the above inequalities over all pairs of adjacent edges e_i and e_j in G, we obtain

$$\sum_{e_i \sim e_j} d(e_i)d(e_j) + \delta_e^2 \sum_{e_i \sim e_j} 1 \geq \delta_e \sum_{e_i \sim e_j} (d(e_i)+d(e_j))\,,$$

and

$$\sum_{e_i \sim e_j} d(e_i)d(e_j) + \Delta_e^2 \sum_{e_i \sim e_j} 1 \geq \Delta_e \sum_{e_i \sim e_j} (d(e_i)+d(e_j))\,,$$

that is

$$\begin{aligned} &EM_2(G) + \delta_e^2 m_L \geq \delta_e EM_1(G) \quad \text{and} \\ &EM_2(G) + \Delta_e^2 m_L \geq \Delta_e EM_1(G)\,, \end{aligned} \tag{13}$$

from which we obtain the inequalities (10) and (11). inequality (10) holds if and only if every pair of adjacent edges e_i and e_j in G, has at least one edge of degree δ_e. Similarly, inequality (11) holds if and only if every pair of adjacent edges e_i and e_j in G, has at least one edge of degree Δ_e. □

Remark 1. The inequalities (10) and (11) are incomparable. Thus, for example, for a graph with vertex degree sequence $(d_1, d_2, \dots, d_n) = \left(\frac{n}{2}, \frac{n}{2}, 1, \dots, 1\right)$, for even n, the inequality (10) is stronger than (11). On the other hand, for the graph with vertex degree sequence $(d_1, d_2, \dots, d_n) = (n-1, 2, \dots, 2)$, where n is odd, the inequality (11) is stronger than (10).

Corollary 3.2. *Let G be a connected graph with $m \geq 2$ edges. Then we have*

$$\delta_e EM_1(G) - EM_2(G) \leq \frac{m\Delta_e\delta_e^2}{2}\,,$$

and

$$\Delta_e EM_1(G) - EM_2(G) \leq \frac{m\Delta_e^3}{2}\,.$$

Equalities hold if and only if $L(G)$ is a regular graph.

Proof. Since

$$m\delta_e \leq 2m_L \leq m\Delta_e\,, \tag{14}$$

from the right hand part of inequality (14) and inequalities (10) and (11) we obtain the required result. □

Remark 2. Since

$$d(e_i) \geq \delta_e \geq 1,$$

from the first inequality (12) we have

$$d(e_i)d(e_j) + 1 \geq d(e_i) + d(e_j).$$

After summation of the above inequality over all pairs of adjacent edges e_i and e_j in G, we obtain the inequality (5). Therefore inequality (10) is stronger than (5).

In the next theorem we determine a relationship between EM_1 and $\overline{EM}_1(G)$.

Theorem 3.3. *Let G be a connected graph with $m \geq 2$ edges. Then we have*

$$m(m-1)\delta_e \leq EM_1(G) + \overline{EM}_1(G) \leq m(m-1)\Delta_e. \tag{15}$$

Equality holds if and only if $L(G)$ is regular.

Proof. Since

$$\overline{EM}_1(G) = \sum_{e_i \nsim e_j} (d(e_i) + d(e_j)) = \sum_{i=1}^{m} (m-1-d(e_i))d(e_i) =$$

$$= (m-1)\sum_{i=1}^{m} d(e_i) - \sum_{i=1}^{m} d(e_i)^2 = 2m_L(m-1) - EM_1(G),$$

we have that the following identity is valid

$$EM_1(G) + \overline{EM}_1(G) = 2m_L(m-1). \tag{16}$$

From the above and equality (14) we arrive at wquality (15).

Equality in (15), and consequently in (14), holds if and only if $L(G)$ is regular. □

Theorem 3.4. *Let G be a connected graph with $m \geq 2$ edges. Then we have*

(17) Equality on the left hand side holds if and only if G is regular or $d_2 = \cdots = d_{n-1} = \frac{\Delta+\delta}{2}$. Equality on the right hand side holds if and only if $d_i \in \{\Delta, \delta\}$, for all i, $1 \leq i \leq n$.

Proof. The equality (16) can be considered as

$$EM_1(G) + \overline{EM}_1(G) = (m-1)(M_1(G) - 2m). \tag{18}$$

In [20] (see also [5, 17]) it was proven that

$$M_1(G) \geq \frac{4m^2}{n} + \frac{1}{2}(\Delta - \delta)^2,$$

with equality holding if and only if G is either regular or $d_2 = \cdots = d_{n-1} = \frac{\Delta+\delta}{2}$. From the above and identity (18) we obtain the left hand side of inequality (3.4).

In [6] it was proven that

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

with equality holding if and only if $d_i \in \{\Delta, \delta\}$, for all i, $1 \leq i \leq n$. So the proof is completed. □

Since $(\Delta-\delta)^2 \geq 0$, we obtain the following result.

Corollary 3.5. *Let G be a connected graph with $n \geq 3$ vertices and m edges. Then we have*

$$EM_1(G) + \overline{EM}_1(G) \geq \frac{2m(m-1)(2m-n)}{n}.$$

Equality holds if and only if G is regular.

In the next theorem we establish relationship between $\overline{EM}_1(G)$ and the first Zagreb index, $M_1(G)$.

Theorem 3.6. *Let G be a connected graph with $m \geq 2$ edges. Then we have*

$$\overline{EM}_1(G) \geq (m-1-\Delta_e-\delta_e)(M_1(G)-2m) + m\Delta_e\delta_e. \tag{19}$$

Equality holds if $d(e_i) \in \{\Delta_e, \delta_e\}$, for all i, $1 \leq i \leq m$.

Proof. For every i, $i = 1,2,\ldots,m$, the following inequality is valid

$$(d(e_i)-\delta_e)(\Delta_e - d(e_i)) \geq 0, \tag{20}$$

that is

$$d(e_i)^2 + \Delta_e\delta_e \leq (\Delta_e+\delta_e)d(e_i).$$

After summation of the above inequality over i, $i = 1,2,\ldots,m$, we obtain

$$\sum_{i=1}^{m} d(e_i)^2 + \Delta_e\delta_e\sum_{i=1}^{m} 1 \leq (\Delta_e+\delta_e)\sum_{i=1}^{m} d(e_i),$$

that is

$$EM_1(G) \leq (\Delta_e+\delta_e)(M_1(G)-2m) - m\Delta_e\delta_e.$$

From the above inequality and identity (18) we arrive at (19).

Equality in (20), and therefore in (19), holds if and only if $d(e_i) \in \{\Delta_e, \delta_e\}$, for all i, $i = 1,2,\ldots,m$.

□

Denote by $\overline{m}_L$ the number of nonadjacent edges in $L(G)$. Then the following identity is valid

$$\overline{m}_L = \frac{m(m-1)}{2} - m_L = \frac{1}{2}(m(m+1) - M_1(G)).$$

The proof of the next theorem is analogous to that of Theorem 3.1, hence omitted. The following theorem reveals a relationship between reformulated Zagreb coindices.

Theorem 3.7. *Let G be a connected graph with $m \geq 2$ edges. Then we have*

$$\delta_e\overline{EM}_1(G) - \overline{EM}_2(G) \leq \delta_e^2\overline{m}_L.$$

and

$$\Delta_e\overline{EM}_1(G) - \overline{EM}_2(G) \leq \Delta_e^2\overline{m}_L,$$

Equality in the first inequality holds if and only if for every pair of nonadjacent edges e_i and e_j in G, holds that at least one is of degree δ_e, whereas in the second one if and only if at least one edge in each pair of nonadjacent edges is of degree Δ_e.

In the next theorem we determine a relationship between the first and second reformulated Zagreb indices.

Theorem 3.8. *Let G be a connected graph with $m \geq 2$ edges. Then we have*

$$(\Delta_e + \delta_e)EM_1(G) - 2EM_2(G) \geq 2\Delta_e\delta_e m_L\,. \tag{21}$$

Equality holds if and only if $L(G)$ is regular.

Proof. For every i and j, $1 \leq i, j \leq m$, the following inequality is valid

$$(d(e_i) - \delta_e)(\Delta_e - d(e_j)) \geq 0\,,$$

that is

$$d(e_i)d(e_j) \leq \Delta_e d(e_i) + \delta_e d(e_j) - \delta_e\Delta_e\,. \tag{22}$$

Also, for every i and j, $1 \leq i, j \leq m$

$$(\Delta_e - d(e_i))(d(e_j) - \delta_e) \geq 0\,,$$

that is

$$d(e_i)d(e_j) \leq \delta_e d(e_i) + \Delta_e d(e_j) - \Delta_e\delta_e\,. \tag{23}$$

The sum of (22) and (23) yields

$$2d(e_i)d(e_j) \leq (\Delta_e + \delta_e)(d(e_i) + d(e_j)) - 2\Delta_e\delta_e\,.$$

After summation of the above inequality over all pairs of adjacent edges e_i and e_j in G, we obtain

$$2\sum_{e_i \sim e_j} d(e_i)d(e_j) \leq (\Delta_e + \delta_e)\sum_{e_i \sim e_j}(d(e_i) + d(e_j)) - \Delta_e\delta_e\sum_{e_i \sim e_j} 2\,,$$

that is

$$2EM_2(G) \leq (\Delta_e + \delta_e)EM_1(G) - 2\Delta_e\delta_e m_L.$$

In both (22) and (23) equality holds if and only if $\Delta_e = d(e_i) = d(e_j) = \delta_e$, which implies that equality (21) holds if and only if $L(G)$ is regular. □

Corollary 3.9. *Let G be a connected graph with $m \geq 2$ edges. Then we have*

$$EM_2(G) \leq \Delta_e(EM_1(G) - \delta_e m_L)\,.$$

Equality holds if and only if $L(G)$ is regular.

Proof. Since $\delta_e \leq \Delta_e$, from (22) we have

$$d(e_i)d(e_j) \leq \Delta_e(d(e_i) + d(e_j) - \delta_e)\,.$$

After summation of the above inequality over all pairs of adjacent edges e_i and e_j in G, we obtain the required result. □

Corollary 3.10. *Let G be a connected graph with $m \geq 2$ edges. Then we have*

$$EM_2(G) \leq \frac{(\Delta_e + \delta_e)^2 EM_1(G)^2}{8\Delta_e\delta_e(M_1(G) - 2m)}. \tag{24}$$

Equality holds if and only if $L(G)$ is regular.

Proof. According to inequality (21) we have that

$$(\Delta_e + \delta_e)EM_1(G) \geq 2EM_2(G) + 2\Delta_e\delta_e m_L = 2EM_2(G) + \delta_e\Delta_e(M_1(G) - 2m).$$

By the arithmetic–geometric mean inequality (see e.g. [21]) we have

$$(\Delta_e + \delta_e)EM_1(G) \geq 2\sqrt{2\Delta_e\delta_e EM_2(G)(M_1(G) - 2m)},$$

from which we arrive at (24).

□

Similarly as in the case of Theorem 3.8 the following result can be proven.

Theorem 3.11. *Let G be a connected graph with $m \geq 2$ edges. Then we have*

$$(\Delta_e + \delta_e)\overline{EM}_1(G) - 2\overline{EM}_2(G) \geq 2\Delta_e\delta_e\overline{m}_L.$$

Equality holds if and only if $L(G)$ is either a regular graph or $L(G) \cong P_3$.

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