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A note on the first Zagreb index and coindex of graphs

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Abstract: Let $G=(V,E)$, $V=\{v_1,v_2,\dots,v_n\}$, be a simple graph with n vertices, m edges and a sequence of vertex degrees $\Delta=d_1\geq d_2\geq\cdots\geq d_n=\delta$, $d_i=d(v_i)$. If vertices v_i and v_j are adjacent in G, it is denoted as $i\sim j$, otherwise, we write $i\nsim j$. The first Zagreb index is vertex-degree-based graph invariant defined as $M_1(G)=\sum_{i=1}^n d_i^2$, whereas the first Zagreb coindex is defined as $\overline{M}_1(G)=\sum_{i\nsim j}(d_i+d_j)$. A couple of new upper and lower bounds for $M_1(G)$, as well as a new upper bound for $\overline{M}_1(G)$, are obtained.

Keywords: Topological indices, first Zagreb index, first Zagreb coindex

AMS Subject classification: 05C50

1. Introduction

Let $G=(V,E)$, $V=\{v_1,v_2,\dots,v_n\}$, be a simple graph with n vertices, m edges and a sequence of vertex degrees $\Delta=d_1\geq d_2\geq\cdots\geq d_n=\delta>0$, $d_i=d(v_i)$. The complement of 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 of G are adjacent, we write $i\sim j$. On the other hand, if v_i and v_j are adjacent in $\overline{G}$, we write $i\nsim j$.

A topological index of a graph is a numerical quantity which is invariant under automorphisms of the graph. Topological indices are important and useful tools in mathematical chemistry, used for quantifying physical and chemical properties of molecules. A vertex-degree-based graph invariant, later named the first Zagreb index

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[3], $M_1(G)$, is defined as [14]

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

The first Zagreb index is the oldest and most extensively studied topological index and one of the most popular and most extensively studied graph-based molecular structure descriptors. Details of their theory and applications can be found in surveys [1, 4, 5, 12] and in the references quoted therein.
In [17] it was shown that $M_1(G)$ can be also represented as

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

Inspired by the above identity, in [10] a concept of coindices was introduced. In this case the sum runs over the edges of the complement of G. Thus, the first Zagreb coindex is defined as

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

The inverse degree index [11] is defined as

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

Considering the fact that obtaining the exact and easy to compute formula for various topological indices is not always possible, it is useful to know approximating expressions. In this paper we obtain some inequalities related to the first Zagreb index and coindex that establish new upper and lower bounds for these invariants in terms of some of the structural graph parameters (number of vertices, number of edges, maximal and minimal vertex degree) and $ID(G)$.

2. Preliminaries

In this section we recall some results for $M_1(G)$ and $\overline{M}_1(G)$, as well as one analytical inequality for real number sequences that will be used later in the paper.
In [9] the following inequality was proven

$$M_1(G) \le 2m(\Delta + \delta) - n\Delta\delta, \tag{1}$$

with equality if and only if $d_i \in \{\delta, \Delta\}$ for every i, $i = 1, 2, \ldots, n$.
Let us note that inequality (1) is the best possible upper bound for $M_1(G)$ determined in terms of parameters n, m, Δ and δ.

Let T be an arbitrary tree with $n \geq 2$ vertices. In [8] it was proven

$$M_1(T) \leq n(n-3) + 2(\Delta + 1). \tag{2}$$

In [18] the following upper bound for $M_1(T)$ was obtained. If $n \equiv p \pmod{\Delta - 1}$ then

$$M_1(T) \leq \begin{cases} (\Delta+2)n - 4\Delta + 4, & \text{if } p = 0 \\ (\Delta+2)n - 3\Delta, & \text{if } p = 1 \\ (\Delta+2)n - 2\Delta - 2, & \text{if } p = 2 \\ (\Delta+2)n - p\Delta + p(p-3), & \text{if } p \geq 3 \end{cases}. \tag{3}$$

Let $p = (p_i)$, $i = 1, 2, \ldots, n$, be a sequence of non-negative real numbers, and $a = (a_i)$, $i = 1, 2, \ldots, n$, a sequence of positive real numbers. Then for any real r, $r \leq 0$ or $r \geq 1$, the following holds [15, 16]

$$\left(\sum_{i=1}^{n} p_i\right)^{r-1} \sum_{i=1}^{n} p_i a_i^r \geq \left(\sum_{i=1}^{n} p_i a_i\right)^r. \tag{4}$$

When $0 \leq r \leq 1$, the opposite inequality is valid. Equality holds if and only if either $r = 0$, or $r = 1$, or $a_1 = a_2 = \cdots = a_n$, or $p_1 = p_2 = \cdots = p_t = 0$ and $a_{t+1} = \cdots = a_n$, for some t, $1 \leq t \leq n-1$.

3. Main results

In the next theorem we establish bounds for $M_1(G)$ depending on parameters n, m, Δ and δ, and graph invariant $ID(G)$.

Theorem 1. *Let G be a simple (n, m)-graph, $n \geq 2$, without isolated vertices. Then*

$$M_1(G) \geq 2m(2\Delta + \delta) + \Delta^2 \delta ID(G) - n\Delta(\Delta + 2\delta) \tag{5}$$

and

$$M_1(G) \leq 2m(\Delta + 2\delta) + \Delta\delta^2 ID(G) - n\delta(2\Delta + \delta). \tag{6}$$

Equalities hold if and only if $\Delta = d_1 = \cdots = d_t \geq d_{t+1} = \cdots = d_n = \delta$, for some t, $1 \leq t \leq n-1$.

Proof. For every vertex v_i in graph G we have that

$$(\Delta - d_i)(d_i - \delta) \geq 0,$$

i.e.

$$d_i + \frac{\Delta\delta}{d_i} \leq \Delta + \delta. \tag{7}$$

After multiplying the above inequality by $\Delta - d_i$ and summing over i, $i = 1, 2, \ldots, n$, we get

$$\sum_{i=1}^{n}(\Delta - d_i)d_i + \Delta\delta \sum_{i=1}^{n} \frac{\Delta - d_i}{d_i} \leq (\Delta + \delta) \sum_{i=1}^{n}(\Delta - d_i), \tag{8}$$

that is

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

from which (5) is obtained.
Similarly, after multiplying (7) by $d_i - \delta$ and summing over i, $i = 1, 2, \ldots, n$, we obtain

$$\sum_{i=1}^{n} d_i(d_i - \delta) + \Delta\delta \sum_{i=1}^{n} \frac{d_i - \delta}{d_i} \leq (\Delta + \delta) \sum_{i=1}^{n}(d_i - \delta), \tag{9}$$

that is

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

from which (6) is obtained.
Equalities in (8) and (9) hold if and only if $d_i \in \{\delta, \Delta\}$ for every i, $i = 1, 2, \ldots, n$, and consequently equalities in (5) and (6) hold if and only if $\Delta = d_1 = \cdots = d_t \geq d_{t+1} = \cdots = d_n = \delta$, for some t, $1 \leq t \leq n - 1$. □

Remark 1. After summing up the inequality (7) over i, $i = 1, 2, \ldots, n$, we get

$$2m + \Delta\delta ID(G) \leq n(\Delta + \delta). \tag{10}$$

According to the above and (6), it follows

$$\begin{aligned} M_1(G) &\leq 2m(\Delta + 2\delta) + \Delta\delta^2 ID(G) - n\delta(2\Delta + \delta) \\ &\leq 2m(\Delta + 2\delta) + \delta(n(\Delta + \delta) - 2m) - n\delta(2\Delta + \delta) \\ &= 2m(\Delta + \delta) - n\delta\Delta, \end{aligned}$$

which means that the inequality (6) is stronger than (1).

In the following lemma we determine lower bound for $M_1(G)$ in terms of parameters n, m, Δ, δ and d_{n-1}.

Lemma 1. *Let G be a simple (n,m)-graph of size $n \geq 4$. Then*

$$M_1(G) \geq \Delta^2 + d_{n-1}^2 + \delta^2 + \frac{(2m - \Delta - d_{n-1} - \delta)^2}{n-3}. \tag{11}$$

Equality holds if and only if $\Delta = d_1 \geq d_2 = \cdots = d_{n-2} \geq d_{n-1} \geq d_n = \delta$.

Proof. For $r = 2$, the inequality (4) can be considered in the following form

$$\sum_{i=2}^{n-2} p_i \sum_{i=2}^{n-2} p_i a_i^2 \geq \left(\sum_{i=2}^{n-2} p_i a_i \right)^2 .$$

Now, for $p_i = 1$, $a_i = d_i$, $i = 2, \ldots, n-2$, the above inequality transforms into

$$\sum_{i=2}^{n-2} 1 \sum_{i=2}^{n-2} d_i^2 \geq \left(\sum_{i=2}^{n-2} d_i \right)^2 , \tag{12}$$

that is

$$(n-3)(M_1(G) - \Delta^2 - d_{n-1}^2 - \delta^2) \geq (2m - \Delta - d_{n-1} - \delta)^2,$$

from which we obtain (11).
Equality in (12) holds if and only if $d_2 = \cdots = d_{n-2}$, which implies that equality in (11) holds if and only if $\Delta = d_1 \geq d_2 = \cdots = d_{n-2} \geq d_{n-1} \geq d_n = \delta$. □

In the following corollary of Theorem 1 and Lemma 1 we obtain bounds for $M_1(T)$, where T is an arbitrary tree, in terms of parameters n and Δ.

Corollary 1. *Let T be an arbitrary tree with n vertices. If $n \geq 2$, then*

$$M_1(T) \leq 2(n-1) + (n-2)\Delta, \tag{13}$$

with equality holding if and only if T is a tree with the property $\Delta = d_1 = \cdots = d_t \geq d_{t+1} = \cdots = d_n = \delta = 1$, for some t, $1 \leq t \leq n-1$.
If $n \geq 4$, then

$$M_1(T) \geq \Delta^2 + 2 + \frac{(2n - 4 - \Delta)^2}{n-3}. \tag{14}$$

Equality is attained if and only if tree T is such that $\Delta = d_1 \geq d_2 = \cdots = d_{n-2} \geq d_{n-1} = d_n = \delta = 1$.

Proof. Let T be a tree with $n \geq 2$ vertices. Then $m = n-1$ and $\delta = 1$. Therefore according to (6) and (10) we get

$$M_1(T) \leq 2(n-1)(\Delta + 2) + \Delta ID(T) - n(2\Delta + 1)$$

and

$$\Delta ID(T) \leq n(\Delta+1) - 2(n-1),$$

wherefrom we arrive at (13).
Let T be a tree with $n \geq 4$ vertices. Since every tree has at least two vertices of degree 1, for $m = n-1$, $d_{n-1} = d_n = \delta = 1$, from (11) we obtain (14). □

Remark 2. Since

$$M_1(T) \leq 2(n-1) + (n-2)\Delta \leq n(n-3) + 2(\Delta+1),$$

the upper bound for $M_1(T)$ given by (13) is stronger than (2).

Remark 3. For the bounds given by (3) and (13) for $M_1(T)$ the following applies

- For $p = 0$ and $\Delta = 4$, or $p = 1$ and $\Delta = 3$, or $p \geq 3$ and $\Delta \geq p$, the inequality (3) is stronger than (13);
- For $p = 0$ and $\Delta = 3$, or $p = 1$ and $\Delta = 2$, or $p = 2$ regardless of Δ, or $p \geq 3$ and $\Delta = p-1$, the inequalities (3) and (13) coincide;
- For $p = 0$ and $\Delta = 2$, or $p = 1$ and $\delta = 2$, or $p \geq 3$ and $2 \leq \Delta \leq p-2$, the inequality (13) is stronger than (3).

Corollary 2. *Let T be an arbitrary tree with n vertices. If $n \geq 4$, then*

$$\overline{M}_1(T) \leq 2n(n-2) - \Delta^2 - \frac{(2n-4-\Delta)^2}{n-3}.$$

Equality is attained if and only if tree T is such that $\Delta = d_1 \geq d_2 = \cdots = d_{n-2} \geq d_{n-1} = d_n = \delta = 1$.
If $n \geq 2$, then

$$\overline{M}_1(T) \geq (n-2)(2n-2-\Delta).$$

Equality holds if and only if T is a tree with the property $\Delta = d_1 = \cdots = d_t \geq d_{t+1} = \cdots = d_n = \delta = 1$, for some t, $1 \leq t \leq n-1$.

Proof. The following equality is valid [2, 7]

$$\overline{M}_1(G) + M_1(G) = 2m(n-1),$$

i.e.

$$\overline{M}_1(T) + M_1(T) = 2(n-1)^2.$$

The desired result follows from the above and (13) and (14). □

A vertex-degree-based topological index, known as the Narumi-Katayama index, is defined as [13]

$$NK(G) = \prod_{i=1}^{n} d_i \,.$$

In the next theorem we determine a relationship between $M_1(G)$ and $NK(G)$.

Theorem 2. *Let G be a simple connected graph with $n \geq 5$ vertices. Then*

$$M_1(G) \geq \Delta^2 + d_{n-1}^2 + \delta^2 + (n-3)\left(\frac{NK(G)}{\Delta\delta d_{n-1}}\right)^{2/(n-3)} + (d_2 - d_{n-2})^2 \,.$$

Equality holds if $\Delta = d_1 \geq d_2 = \cdots = d_{n-2} \geq d_{n-1} \geq d_n = \delta$, or $d_3 = \cdots = d_{n-3} = \frac{d_2+d_{n-2}}{2}$.

Proof. Let $a_1 \geq a_2 \geq \cdots \geq a_n \geq 0$ be positive real numbers. In [6] it was proven that

$$\sum_{i=1}^{n} a_i \geq n\left(\prod_{i=1}^{n} a_i\right)^{1/n} + (\sqrt{a_1} - \sqrt{a_n})^2 \,,$$

with equality if $a_2 = \cdots = a_{n-1} = \frac{a_2+a_n}{2}$. This inequality can be considered in the following form

$$\sum_{i=2}^{n-2} a_i \geq (n-3)\left(\prod_{i=2}^{n-2} a_i\right)^{1/(n-3)} + \left(\sqrt{a_2} - \sqrt{a_{n-2}}\right)^2 \,.$$

Now, for $a_i = d_i^2$, $i = 1, 2, \ldots, n-2$, the above inequality transforms into

$$\sum_{i=2}^{n-2} d_i^2 \geq (n-3)\left(\prod_{i=2}^{n-2} d_i^2\right)^{1/(n-3)} + \left(\sqrt{d_2^2} - \sqrt{d_{n-2}^2}\right)^2 \,,$$

that is

$$\sum_{i=1}^{n} d_i^2 \geq d_1^2 + d_{n-1}^2 + d_n^2 + (n-3)\left(\frac{\prod_{i=1}^{n} d_i}{d_1 d_{n-1} d_n}\right)^{2/(n-3)} + (d_2 - d_{n-2})^2 \,,$$

wherefrom we obtain the assertion of the theorem. $\square$

When G is a tree, $G \cong T$, with n vertices, we have the following corollary of Theorem 2.

Corollary 3. *Let T be a tree with $n \geq 5$ vertices. Then we have*

$$M_1(T) \geq \Delta^2 + 2 + (n-3)\left(\frac{NK(T)}{\Delta}\right)^{2/(n-3)} + (d_2 - d_{n-2})^2 .$$

Equality holds if $\Delta = d_1 \geq d_2 = \cdots = d_{n-2} \geq d_{n-1} = d_n = \delta = 1$, or $\Delta = d_1$, $d_3 = \cdots = d_{n-3} = \frac{d_2+d_{n-2}}{2}$, $d_{n-1} = d_n = \delta = 1$.

Theorem 3. *Let G be a simple connected graph with $n \geq 5$ vertices and m edges. Then*

$$M_1(G) \leq \Delta^2 + \delta^2 + d_{n-1}^2 + (2m - \Delta - \delta - d_{n-1})^2 - (n-3)(n-4)\left(\frac{NK(G)}{\Delta\delta d_{n-1}}\right)^{2/(n-3)} .$$

Equality holds if and only if $d_2 = d_3 = \cdots = d_{n-2}$.

Proof. The following identity is valid

$$\left(\sum_{i=2}^{n-2} d_i\right)^2 = \sum_{i=2}^{n-2} d_i^2 + 2\sum_{2\leq i<j\leq n-2} d_i d_j .$$

According to the arithmetic–geometric mean inequality, AM–GM inequality (see e.g. [16]), for real number sequences we have

$$\begin{aligned}
\left(\sum_{i=2}^{n-2} d_i\right)^2 &\geq \sum_{i=2}^{n-2} d_i^2 + (n-3)(n-4)\left(\prod_{2\leq i<j\leq n-2} d_i d_j\right)^{\frac{2}{(n-3)(n-4)}} \\
&= \sum_{i=2}^{n-2} d_i^2 + (n-3)(n-4)\left(\prod_{i=2}^{n-2} d_i^{n-4}\right)^{\frac{2}{(n-3)(n-4)}} \\
&= \sum_{i=2}^{n-2} d_i^2 + (n-3)(n-4)\left(\prod_{i=2}^{n-2} d_i\right)^{2/(n-3)}
\end{aligned}$$

From the above inequality we have that

$$\sum_{i=1}^{n} d_i^2 - \Delta^2 - \delta^2 - d_{n-1}^2 \leq \left(\sum_{i=1}^{n} d_i - \Delta - \delta - d_{n-1}\right)^2 - (n-3)(n-4)\left(\frac{\prod_{i=1}^{n} d_i}{\Delta\delta d_{n-1}}\right)^{2/(n-3)} ,$$

from which we obtain the required result. □

If G is a tree, $G \cong T$, with $n \geq 5$ vertices we have the following corollary of Theorem 3.

Corollary 4. *Let T be a tree with $n \geq 5$ vertices. Then we have that*

$$M_1(T) \leq \Delta^2 + 2 + (2n - \Delta - 4)^2 - (n-3)(n-4)\left(\frac{NK(T)}{\Delta}\right)^{2/(n-3)}.$$

Equality holds if and only if $\Delta = d_1$, $d_2 = d_3 = \cdots = d_{n-2}$, $d_{n-1} = d_n = \delta = 1$.

In the next theorem we establish an upper bound for $\overline{M}_1(G)$ and lower bound for $M_1(\overline{G})$ depending on parameters n, m, Δ and δ, and graph invariant $ID(G)$.

Theorem 4. *Let G be a simple (n,m)-graph, $n \geq 2$, without isolated vertices. Then*

$$\overline{M}_1(G) \leq (\Delta + \delta)(n(n-1) - 2m) - \Delta\delta((n-1)ID(G) - n) \tag{15}$$

and

$$M_1(\overline{G}) \geq \Delta\delta((n-1)ID(G) - n) - (\Delta + \delta - n + 1)(n(n-1) - 2m). \tag{16}$$

Equalities hold if and only if $\Delta = d_1 = \cdots = d_t \geq d_{t+1} = \cdots = d_n = \delta$, for some t, $1 \leq t \leq n-1$.

Proof. After multiplying (7) by $n - 1 - d_i$ and summing over i, $i = 1, 2, \ldots, n$, we get

$$\sum_{i=1}^{n} d_i(n-1-d_i) + \Delta\delta \sum_{i=1}^{n} \frac{n-1-d_i}{d_i} \leq (\Delta + \delta) \sum_{i=1}^{n} (n-1-d_i), \tag{17}$$

that is

$$\overline{M}_1(G) + \Delta\delta((n-1)ID(G) - n) \leq (\Delta + \delta)(n(n-1) - 2m),$$

from which (15) is obtained.
According to (7) we have that

$$d_i - n + 1 + \frac{\Delta\delta}{d_i} \leq \Delta + \delta - n + 1,$$

i.e.

$$(n-1-d_i) - \frac{\Delta\delta}{d_i} \geq n - 1 - \Delta - \delta.$$

Similarly, after multiplying the above inequality by $n - 1 - d_i$ and summing over i, $i = 1, 2, \ldots, n$, we obtain

$$\sum_{i=1}^{n} (n-1-d_i)^2 - \Delta\delta \sum_{i=1}^{n} \frac{n-1-d_i}{d_i} \geq (n-1-\Delta-\delta) \sum_{i=1}^{n} (n-1-d_i), \tag{18}$$

that is

$$M_1(\overline{G}) - \Delta\delta((n-1)ID(G) - n) \geq (n-1-\Delta-\delta)(n(n-1)-2m),$$

from which (16) is obtained.
Equalities in (17) and (18), and consequently in (15) and (16), hold if and only if $\Delta = d_1 = \cdots = d_t \geq d_{t+1} = \cdots = d_n = \delta$, for some t, $1 \leq t \leq n-1$. □

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