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Some Mathematical Properties of the Geometric–Arithmetic Index/Coindex of Graphs

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Abstract. Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, be a simple connected graph of order n, size m with vertex degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, $d_i = d(v_i)$. The geometric–arithmetic topological index of G is defined as $GA(G) = \sum_{i\sim j} \frac{2\sqrt{d_i d_j}}{d_i+d_j}$, whereas the geometric–arithmetic coindex as $\overline{GA}(G) = \sum_{i\nsim j} \frac{2\sqrt{d_i d_j}}{d_i+d_j}$. New lower bounds for $GA(G)$ and $\overline{GA}(G)$ in terms of some graph parameters and other invariants are obtained.

1. Introduction

In this paper we are concerned with simple graphs, that is graphs without directed, weighted or multiple edges, and without self loops. Let $G = (V, E)$ be a such graph, where $V = \{v_1, v_2, \ldots, v_n\}$ is its vertex set and $E = \{e_1, e_2, \ldots, e_m\}$ is its edge set. The degree of vertex v_i, denoted by $d(v_i)$ (or d_i if it is clear from the context) is the number of first neighbors of v_i. Denote by $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$ the set of vertex degrees of G, and by $\Delta_{e_1} = d(e_1) + 2$ and $\delta_{e_1} = d(e_m) + 2$. The complement of G, sometimes called the edge-complement, is the graph $\overline{G} = (V, \overline{E})$, with the same vertex set but whose edge set consists of the edges not present in G. Since the graph sum $G + \overline{G}$ on a n-node graph G is the complete graph K_n, the number of edges in $\overline{G}$ is $\overline{m} = \frac{n(n-1)}{2} - m$. If vertices v_i and v_j are adjacent in G, we write $i \sim j$, otherwise we write $i \nsim j$. As usual, $L(G)$ denotes a line graph.

The numeric quantity associated with a graph which characterize the topology of graph and is invariant under graph automorphism is called graph invariant or topological index. Very often in chemistry the aim is the construction of chemical compounds with certain properties, which not only depend on the chemical formula but also strongly on the molecular structure. That's where various topological indices come into consideration. A large number of topological indices have been derived depending on vertex degrees. Most degree based topological indices are viewed as the contributions of pairs of adjacent vertices. But equally important are degree based topological indices that consider the non-adjacent pairs of vertices for computing some topological properties of graphs which are named as coindices.

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The first and second Zagreb indices are vertex–degree–based graph invariants introduced in [22] and [23], respectively, and defined as

$$M_1(G) = \sum_{i=1}^{n} d_i^2 \quad \text{and} \quad M_2(G) = \sum_{i \sim j} d_i d_j .$$

Both $M_1(G)$ and $M_2(G)$ were recognized to be a measure of the extent of branching of the carbon–atom skeleton of the underlying molecule. Bearing in mind that for the edge e connecting the vertices i and j,

$$d(e) = d_i + d_j - 2,$$

the index $M_1(G)$ can also be considered as an edge–degree–based topological index [27]

$$M_1(G) = \sum_{i=1}^{m} (d(e_i) + 2).$$

In [13] (see also [12]) it was observed that the first Zagreb index can be also represented as

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

and inspired by the above identity a concept of coindices was introduced. In this case the sum runs over the edges of the complement of G. Thus, the first and the second Zagreb coindices are defined as [13]

$$\overline{M}_1(G) = \sum_{i \nsim j} (d_i + d_j) \quad \text{and} \quad \overline{M}_2(G) = \sum_{i \nsim j} d_i d_j .$$

In [22], another quantity, the sum of cubes of vertex degrees

$$F(G) = \sum_{i=1}^{n} d_i^3$$

was encountered as well. This quantity is also a measure of branching and it was found that its predictive ability is quite similar to that of $M_1(G)$. However, for the unknown reasons, it did not attracted any attention until 2015 when it was reinvented in [17] and named the forgotten topological index. By analogy to the first Zagreb index, the following equalities hold

$$F(G) = \sum_{i \sim j} (d_i^2 + d_j^2) \quad \text{and} \quad F(G) + 2M_2(G) = \sum_{i \sim j} (d_i + d_j)^2 = \sum_{i=1}^{m} (d(e_i) + 2)^2 .$$

The forgotten topological coindex, or F-coindex, $\overline{F}(G)$, was encountered in [18] (see also [11]) as

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

The F-coindex has almost the same predictive ability for a chemically relevant property of a non-trivial class of molecules as a linear combination of $M_1(G)$ and $F(G)$ (see [43]).

Generalization of the second Zagreb index, reported in [6], known as general Randić index, $R_\alpha(G)$, is defined as

$$R_\alpha(G) = \sum_{i \sim j} (d_i d_j)^\alpha ,$$

where α is a real number. Some well known special cases are $R(G) = R_{-1/2}(G)$ (the branching index that is nowadays known as Randić index or connectivity index [33]), $R(G) = R_{-1}(G)$ (general Randić index $R_{-1}(G)$

which is referred to as modified second Zagreb index in [31]), $RR(G) = R_{1/2}(G)$ (reciprocal Randić index [24]), and so on.

Multiplicative versions of the first and the second Zagreb indices, $\Pi_1(G)$ and $\Pi_2(G)$, were first considered in [37]. These indices are defined as:

$$\Pi_1(G) = \prod_{i=1}^{n} d_i^2 \quad \text{and} \quad \Pi_2(G) = \prod_{i\sim j} d_i d_j .$$

Multiplicative variants of the first and the second Zagreb coindices were introduced in [45]

$$\overline{\Pi}_1(G) = \prod_{i\nsim j} (d_i + d_j) \quad \text{and} \quad \overline{\Pi}_2(G) = \prod_{i\nsim j} d_i d_j .$$

In [15] the multiplicative–sum first Zagreb index, $\Pi_1^*(G)$, was introduced as

$$\Pi_1^*(G) = \prod_{i\sim j} (d_i + d_j).$$

The inverse degree and harmonic indices are defined as

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

These indices first attracted attention through numerous conjectures generated by the computer programme Graffiti [16].

A family of 148 discrete Adriatic indices was introduced and analyzed in [41] (see also [42]). The so-called inverse sum indeg index, was singled out in [42] as being a significantly accurate predictor of total surface area of octane isomers. It is defined as

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

The geometric–arithmetic index, $GA(G)$ index for short, proposed in [44], is defined to be

$$GA(G) = \sum_{i\sim j} \frac{2\sqrt{d_i d_j}}{d_i + d_j} .$$

In [44] it was noted that the predictive power of GA index is somewhat better than the predictive power of the Randić connectivity index [33] for physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and acentric factor.

The corresponding GA-coindex could be defined as

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

A number of papers have been reported in the literature dealing with bounds for $GA(G)$, see for example [1–3, 5, 8–10, 30, 35, 36, 40, 44, 46]. In this paper we are concerned with lower bounds for $GA(G)$ and $\overline{GA}(G)$ depending on some of the graph parameters and invariants introduced above.

2. Preliminaries

In this section we recall some analytical inequalities for real number sequences that will be used subsequently.

Let $a = (a_i)$, $i = 1, 2, \dots, m$, be positive real number sequence. In [47] (see also [26]) was proved that

$$\left(\sum_{i=1}^{m} \sqrt{a_i} \right)^2 \geq \sum_{i=1}^{m} a_i + m(m-1) \left(\prod_{i=1}^{m} a_i \right)^{\frac{1}{m}} . \tag{1}$$

Let $x = (x_i)$ and $a = (a_i)$, $i = 1, 2, \dots, m$, be two positive real number sequences. Then for any $r \geq 0$ holds [32]

$$\sum_{i=1}^{m} \frac{x_i^{r+1}}{a_i^r} \geq \frac{\left(\sum_{i=1}^{m} x_i \right)^{r+1}}{\left(\sum_{i=1}^{m} a_i \right)^{r}} . \tag{2}$$

For two real number sequences, $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \dots, m$, Cauchy's inequality holds (see e.g. [28])

$$\left(\sum_{i=1}^{m} a_i b_i \right)^2 \leq \left(\sum_{i=1}^{m} a_i^2 \right) \left(\sum_{i=1}^{m} b_i^2 \right) . \tag{3}$$

Let $a_1 \geq a_2 \geq \cdots \geq a_m$ be positive real number sequence. Then (see [7])

$$\sum_{i=1}^{m} a_i \geq m \left(\prod_{i=1}^{m} a_i \right)^{\frac{1}{m}} + \left(\sqrt{a_1} - \sqrt{a_m} \right)^2 . \tag{4}$$

Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \dots, m$, be two real number sequences with the properties $p_1 + p_2 + \cdots + p_m = 1$ and $0 < r \leq a_i \leq R < +\infty$. In [34] the following inequality was proved

$$\sum_{i=1}^{m} p_i a_i + rR \sum_{i=1}^{m} \frac{p_i}{a_i} \leq r + R . \tag{5}$$

3. New lower bounds for *GA* index

In the following theorem we determine lower bound for GA in terms of parameter m and invariants $H(G)$, $R_{-1}(G)$, $\Pi_1^*(G)$ and $\Pi_2(G)$.

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

$$GA(G) \geq \sqrt{ \frac{H(G)^2}{R_{-1}(G)} + 4m(m-1) \frac{(\Pi_2(G))^{\frac{1}{m}}}{\left(\Pi_1^*(G) \right)^{\frac{2}{m}}} } . \tag{6}$$

Equality holds if and only if for any two pairs of adjacent vertices, $i \sim j$ and $u \sim v$, i.e. for any two edges ij and uv in graph G holds

$$\frac{d_i}{d_j} + \frac{d_j}{d_i} = \frac{d_u}{d_v} + \frac{d_v}{d_u} .$$

Proof. For $a_i := \frac{d_id_j}{(d_i+d_j)^2}$, where summation is performed over all edges in graph G, the inequality (1) becomes

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

i.e.

$$\left(\frac{1}{2}GA(G)\right)^2 \geq \sum_{i\sim j}\frac{d_id_j}{(d_i+d_j)^2}+m(m-1)\frac{(\Pi_2(G))^{\frac{1}{m}}}{\left(\Pi_1^*(G)\right)^{\frac{2}{m}}}. \tag{7}$$

For $r=1$, $x_i := \frac{1}{d_i+d_j}$, $a_i := \frac{1}{d_id_j}$, where summation goes over all edges in G, the inequality (2) becomes

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

that is

$$\sum_{i\sim j}\frac{d_id_j}{(d_i+d_j)^2} \geq \frac{H(G)^2}{4R_{-1}(G)}. \tag{8}$$

According to (7) and (8) we obtain

$$\left(\frac{1}{2}GA(G)\right)^2 \geq \frac{H(G)^2}{4R_{-1}(G)}+m(m-1)\frac{(\Pi_2(G))^{\frac{1}{m}}}{\left(\Pi_1^*(G)\right)^{\frac{2}{m}}},$$

wherefrom we get (6).

Equality in (1) holds if and only if $a_1=a_2=\cdots=a_m$, therefore equality in (7) holds if and only if for any two pairs of adjacent vertices, $i\sim j$ and $u\sim v$, holds $\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_u}{d_v}+\frac{d_v}{d_u}$. Equality in (2) holds if and only if $\frac{x_1}{a_1}=\frac{x_2}{a_2}=\cdots=\frac{x_m}{a_m}$, therefore equality in (8) holds if and only if for any two pairs of adjacent vertices, $i\sim j$ and $u\sim v$, holds $\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_u}{d_v}+\frac{d_v}{d_u}$. Since the inequality (6) is obtained according to (7) and (8), equality in (6) is attained if and only if for any two pairs of adjacent vertices, $i\sim j$ and $u\sim v$, i.e. for any two edges ij and uv in graph G holds $\frac{d_i}{d_j}+\frac{d_j}{d_i}=\frac{d_u}{d_v}+\frac{d_v}{d_u}$. $\square$

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

$$GA(G) \geq 2\sqrt{\frac{RR(G)^2}{F(G)+2M_2(G)}+m(m-1)\frac{(\Pi_2(G))^{\frac{1}{m}}}{\left(\Pi_1^*(G)\right)^{\frac{2}{m}}}}. \tag{9}$$

Equality holds if G is a regular or semiregular bipartite graph.

Proof. For $r=1$, $x_i := \sqrt{d_id_j}$, $a_i := (d_i+d_j)^2$, where summation goes over all edges in G, the inequality (2) becomes

$$\sum_{i\sim j}\frac{d_id_j}{(d_i+d_j)^2}=\sum_{i\sim j}\frac{(\sqrt{d_id_j})^2}{(d_i+d_j)^2} \geq \frac{\left(\sum\limits_{i\sim j}\sqrt{d_id_j}\right)^2}{\sum\limits_{i\sim j}(d_i+d_j)^2},$$

i.e.

$$\sum_{i\sim j} \frac{d_i d_j}{(d_i+d_j)^2} \geq \frac{RR(G)^2}{F(G)+2M_2(G)}.$$

From the above and (7) we obtain (9). □

Corollary 3.3. *Let G be a simple connected graph with $m \geq 2$ edges. Then*

$$GA(G) \geq 2\sqrt{\frac{m^4}{(F(G)+2M_2(G))R(G)^2} + m(m-1)\frac{(\Pi_2(G))^{\frac{1}{m}}}{\left(\Pi_1^*(G)\right)^{\frac{2}{m}}}}.$$

Equality holds if G is a regular or semiregular bipartite graph.

Proof. According to the arithmetic–harmonic mean inequality for real numbers (see, for example, [28]), it holds

$$RR(G)R(G) \geq m^2.$$

From the above and (9) we get what is stated. □

In the next theorem we give lower bound for $GA(G)$ in terms of maximal and minimal edge degrees and indices $RR(G)$, $R(G)$ and $H(G)$.

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

$$GA(G) \geq \frac{2}{\Delta_{e_1}+\delta_{e_1}}\left(RR(G) + \frac{\Delta_{e_1}\delta_{e_1}H(G)^2}{4R(G)}\right). \tag{10}$$

Equality holds if and only if $L(G)$ is regular or semiregular bipartite graph.

Proof. For $p_i := \frac{2\sqrt{d_i d_j}}{(d_i+d_j)GA}$, $a_i := d_i + d_j$, $r = \delta_{e_1}$, $R = \Delta_{e_1}$, where summation is performed over all edges of G, the inequality (5) transforms into

$$2\sum_{i\sim j}^{m} \sqrt{d_i d_j} + 2\Delta_{e_1}\delta_{e_1}\sum_{i\sim j}\frac{\sqrt{d_i d_j}}{(d_i+d_j)^2} \leq (\Delta_{e_1}+\delta_{e_1})GA(G),$$

that is

$$(\Delta_{e_1}+\delta_{e_1})GA(G) \geq 2\left(RR(G) + \Delta_{e_1}\delta_{e_1}\sum_{i\sim j}\frac{\sqrt{d_i d_j}}{(d_i+d_j)^2}\right). \tag{11}$$

For $r = 1$, $x_i := \frac{1}{d_i+d_j}$ and $a_i := \frac{1}{\sqrt{d_i d_j}}$, where summation goes over all edges of G, the inequality (2) becomes

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

that is

$$\sum_{i\sim j}\frac{\sqrt{d_i d_j}}{(d_i+d_j)^2} \geq \frac{H(G)^2}{4R(G)}. \tag{12}$$

Based on (11) and (12) we get

$$(\Delta_{e_1}+\delta_{e_1})GA(G)\geq 2\left(RR(G)+\Delta_{e_1}\delta_{e_1}\frac{H(G)^2}{4R(G)}\right),$$

wherefrom (10) is obtained.

Equality in (11) holds if and only if for any edge in G holds $d_i+d_j=\Delta_{e_1}$ or $d_i+d_j=\delta_{e_1}$. Therefore equality in (10) holds if and only if $L(G)$ is regular or semiregular bipartite graph. □

Corollary 3.5. *Let G be a simple connected graph with $m\geq 2$ edges. Then*

$$GA(G)\geq \frac{2}{\Delta_{e_1}+\delta_{e_1}}\left(RR(G)+m\Delta_{e_1}\delta_{e_1}\frac{(\Pi_2(G))^{\frac{1}{2m}}}{\left(\Pi_1^*(G)\right)^{\frac{2}{m}}}\right).$$

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

Corollary 3.6. *Let G be a simple connected graph with $m\geq 2$ edges. Then*

$$GA(G)\geq \frac{1}{2(\Delta_{e_1}+\delta_{e_1})R(G)}\left(4m^2+\Delta_{e_1}\delta_{e_1}H(G)^2\right)\geq \frac{2mH(G)\sqrt{\Delta_{e_1}\delta_{e_1}}}{(\Delta_{e_1}+\delta_{e_1})R(G)}.$$

Equalities hold if and only if G is a regular or semiregular bipartite graph.

In the next theorem we establish lower bound for $GA(G)$ in terms of parameter m and invariants $M_2(G)$, $F(G)$ and $R_{-1}(G)$.

Theorem 3.7. *Let G be a simple connected graph with m edges. Then*

$$GA(G)\geq \frac{2m^2}{\sqrt{(F(G)+2M_2(G))R_{-1}(G)}}. \tag{13}$$

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

Proof. According to the arithmetic–harmonic mean inequality for real numbers (see, for example, [28]), we have that

$$\left(\sum_{i\sim j}\frac{d_i+d_j}{\sqrt{d_id_j}}\right)\left(\sum_{i\sim j}\frac{\sqrt{d_id_j}}{d_i+d_j}\right)\geq m^2. \tag{14}$$

Applying the Cauchy's inequality we get

$$\sum_{i\sim j}\frac{d_i+d_j}{\sqrt{d_id_j}}\leq\left(\sum_{i\sim j}(d_i+d_j)^2\right)^{1/2}\left(\sum_{i\sim j}\frac{1}{d_id_j}\right)^{1/2},$$

i.e.

$$\sum_{i\sim j}\frac{d_i+d_j}{\sqrt{d_id_j}}\leq \sqrt{(F(G)+2M_2(G))R_{-1}(G)}. \tag{15}$$

The inequality (13) follows from (14) and (15). □

Remark 3.8. *Since*

$$\sum_{i\sim j}\frac{d_i+d_j}{\sqrt{d_id_j}}=\sum_{i\sim j}\left(\sqrt{\frac{d_i}{d_j}}+\sqrt{\frac{d_j}{d_i}}\right)\le m\left(\sqrt{\frac{\Delta}{\delta}}+\sqrt{\frac{\delta}{\Delta}}\right)=\frac{m(\Delta+\delta)}{\sqrt{\Delta\delta}},$$

according to (14) *follows*

$$GA(G)\ge\frac{2m\sqrt{\Delta\delta}}{\Delta+\delta}.$$

This inequality was proven in [8].

In the following theorem we establish a lower bound for $GA(G)$ in terms of m, $\Pi_1^*(G)$ and $\Pi_2(G)$.

Theorem 3.9. *Let G be a simple connected graph with m edges. Then*

$$GA(G)\ge\frac{2m\left(\Pi_2(G)\right)^{\frac{1}{2m}}}{\left(\Pi_1^*(G)\right)^{\frac{1}{m}}}. \tag{16}$$

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

Proof. According to the arithmetic–geometric mean inequality (see e.g. [28]), we have

$$\begin{aligned}GA(G)&=\sum_{i\sim j}\frac{2\sqrt{d_id_j}}{d_i+d_j}\ge m\left(\prod_{i\sim j}\frac{2\sqrt{d_id_j}}{d_i+d_j}\right)^{\frac{1}{m}}\\&=2m\left(\frac{\prod_{i\sim j}\sqrt{d_id_j}}{\prod_{i\sim j}(d_i+d_j)}\right)^{\frac{1}{m}}=\frac{2m\left(\Pi_2(G)\right)^{\frac{1}{2m}}}{\left(\Pi_1^*(G)\right)^{\frac{1}{m}}},\end{aligned}$$

which completes the proof. □

Corollary 3.10. *Let G be a simple connected graph with $m\ge 2$ edges. Then*

$$GA(G)\ge\frac{2m^2\left(\Pi_2(G)\right)^{\frac{1}{2m}}}{M_1(G)-\left(\sqrt{\Delta_{e_1}}-\sqrt{\delta_{e_1}}\right)^2}. \tag{17}$$

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

Proof. For $a_i := d_i+d_j$, $a_1=\Delta_{e_1}$ and $a_m=\delta_{e_1}$, where summation goes over all edges in G, the inequality (4) transforms into

$$\sum_{i\sim j}(d_i+d_j)\ge m\left(\prod_{i\sim j}(d_i+d_j)\right)^{\frac{1}{m}}+\left(\sqrt{\Delta_{e_1}}-\sqrt{\delta_{e_1}}\right)^2,$$

i.e.

$$M_1(G)\ge m\left(\Pi_1^*(G)\right)^{\frac{1}{m}}+\left(\sqrt{\Delta_{e_1}}-\sqrt{\delta_{e_1}}\right)^2.$$

From this and inequality (16) we arrive at (17). □

Remark 3.11. *Since* $\left(\sqrt{\Delta_{e_1}}-\sqrt{\delta_{e_1}}\right)^2\ge 0$, *according to* (17) *follows*

$$GA(G)\ge\frac{2m^2\left(\Pi_2(G)\right)^{\frac{1}{2m}}}{M_1(G)}. \tag{18}$$

Also, since $M_1(G) \leq m\Delta_{e_1} \leq 2m\Delta$, *the following is valid*

$$GA(G) \geq \frac{2m\,(\Pi_2(G))^{\frac{1}{2m}}}{\Delta_{e_1}} \geq \frac{m\,(\Pi_2(G))^{\frac{1}{2m}}}{\Delta}.$$

The second inequality was proven in [35].

Since $(\Pi_2(G))^{\frac{1}{2m}} \geq \delta$, *according to* (18) *we get*

$$GA(G) \geq \frac{2m^2\delta}{M_1(G)}.$$

This inequality was proven in [35].

4. New lower bounds for *GA* coindex

In the next theorem we establish lower bound for $\overline{GA}(G)$ in terms of n, m and $ID(G)$.

Theorem 4.1. *Let* $G \ncong K_n$ *be a simple connected graph with* $n \geq 3$ *vertices and* m *edges. Then*

$$\overline{GA}(G) \geq \frac{n^2(n(n-1)-2m)^3}{8m^2((n-1)ID(G)-n)^2}. \tag{19}$$

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

Proof. Based on the geometric–harmonic mean inequality, GM–HM inequality, see for example [28], we have that

$$\sqrt{d_id_j} \geq \frac{2}{\frac{1}{d_i}+\frac{1}{d_j}},$$

i.e.

$$2\sqrt{d_id_j} \geq \frac{4d_id_j}{d_i+d_j}. \tag{20}$$

After multiplying the above inequality with $\frac{1}{d_i+d_j}$ and summing over all nonadjacent vertices in G, we obtain

$$\overline{GA}(G) = \sum_{i\nsim j} \frac{2\sqrt{d_id_j}}{d_i+d_j} \geq \sum_{i\nsim j} \frac{4d_id_j}{(d_i+d_j)^2}. \tag{21}$$

For $r = 1$, $x_i := \frac{d_id_j}{d_i+d_j}$, $a_i := d_id_j$, with summation performed over all nonadjacent vertices in G, the inequality (2) becomes

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

that is

$$\sum_{i\nsim j} \frac{d_id_j}{(d_i+d_j)^2} \geq \frac{\left(\sum\limits_{i\nsim j} \frac{d_id_j}{d_i+d_j}\right)^2}{\overline{M}_2(G)}. \tag{22}$$

From the arithmetic–harmonic mean inequality, we have that

$$\sum_{i\nsim j}\frac{d_i+d_j}{d_id_j}\sum_{i\nsim j}\frac{d_id_j}{d_i+d_j}\ge \overline{m}^2. \tag{23}$$

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

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

from (23) we obtain

$$\sum_{i\nsim j}\frac{d_id_j}{d_i+d_j}\ge\frac{(n(n-1)-2m)^2}{4((n-1)ID(G)-n)}. \tag{24}$$

In [4] the following identity was proven

$$\overline{M}_2(G)=\frac{1}{2}(4m^2-M_1(G)-2M_2(G)), \tag{25}$$

and in [14] and [25]

$$M_1(G)\ge\frac{4m^2}{n}\quad\text{and}\quad M_2(G)\ge\frac{4m^3}{n^2}.$$

From the above and (25) we get

$$\overline{M}_2(G)\le\frac{2m^2}{n^2}(n(n-1)-2m). \tag{26}$$

From the above and (22) and (24) we have that

$$\sum_{i\nsim j}\frac{d_id_j}{(d_i+d_j)^2}\ge\frac{n^2(n(n-1)-2m)^3}{32m^2((n-1)ID(G)-n)^2}. \tag{27}$$

Now, (19) follows from to (21) and (27).

Equality in (20) holds if and only if $d_i=d_j$ for every pair of nonadjacent vertices in G. Equality in (22) holds if and only if d_i+d_j is a constant for every pair of nonadjacent vertices. Equality in (23) is attained if and only if $\frac{1}{d_i}+\frac{1}{d_j}$ is a constant for every pair of nonadjacent vertices in G. Equality in (27) holds if and only if G is a regular graph, i.e. if and only if $d_i=d_j$ for every pair of adjacent vertices. Therefore, equality in (19) holds if and only if G, $G\ncong K_n$, is regular. □

Corollary 4.2. *Let G, $G\ncong K_n$, be a simple connected graph with n vertices and m edges. Then*

$$\overline{GA}(G)\ge\frac{4\overline{ISI}(G)^2}{\overline{M}_2(G)}. \tag{28}$$

Equality holds if and only if d_i+d_j is a constant for every pair of nonadjacent vertices in G.

Proof. The inequality (28) is obtained from (21) and (22). □

Before we give some other bounds for $\overline{GA}(G)$, we will prove some auxiliary results.

Lemma 4.3. *Let G be a simple connected graph with $n\ge 3$ vertices. If d_i+d_j is a constant for every pair of nonadjacent vertices v_i and v_j in G, then d_id_j is a constant for every pair of nonadjacent vertices v_i and v_j in G also, and vice versa.*

Proof. It is suffices to consider three vertices v_1, v_2 and v_3 in G. The following two cases may occur.

Case 1. Let vertices v_1, v_2 and v_3 be mutually nonadjacent. Then we have $d_1+d_2 = d_1+d_3$, $d_1+d_2 = d_2+d_3$ and $d_1 + d_3 = d_2 + d_3$, and therefore $d_1 = d_2 = d_3$. Now we have $d_1d_2 = d_1d_3 = d_2d_3$. Reverse is valid also. From the equalities $d_1d_2 = d_2d_3$, $d_1d_2 = d_1d_3$ and $d_1d_3 = d_2d_3$ we have that $d_1 = d_2 = d_3$, and consequently $d_1 + d_2 = d_1 + d_3 = d_2 + d_3$.

Case 2. Let vertices v_1 and v_2 be nonadjacent, vertices v_1 and v_3 be nonadjacent and vertices v_2 and v_3 be adjacent. From $d_1 + d_2 = d_1 + d_3$ we have that $d_2 = d_3$, and therefore $d_1d_2 = d_1d_3$. Likewise, from the equality $d_1d_2 = d_1d_3$ we have that $d_2 = d_3$, and consequently $d_1 + d_2 = d_1 + d_3$. □

By a similar procedure the following results are obtained.

Lemma 4.4. *Let G be a simple connected graph with $n \geq 3$ vertices. If $d_i + d_j$ is a constant for every pair of nonadjacent vertices v_i and v_j in G, then the same is valid for $\frac{1}{d_i} + \frac{1}{d_j}$ and vice versa.*

Lemma 4.5. *Let G be a simple connected graph with $n \geq 3$ vertices. If $d_i + d_j$ is a constant for every pair of nonadjacent vertices v_i and v_j in G, then the same is valid for $\frac{\sqrt{d_id_j}}{d_i+d_j}$.*

In the next lemma we determine a relationship between $\overline{\Pi}_1(G)$ and $\overline{\Pi}_2(G)$.

Lemma 4.6. *Let G, $G \ncong K_n$, be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$\overline{\Pi}_2(G) \geq \left(\frac{\overline{m}}{(n-1)ID(G)-n}\right)^{\overline{m}} \overline{\Pi}_1(G). \tag{29}$$

Equality holds if and only if $d_i + d_j$ is constant for every pair of nonadjacent vertices v_i and v_j in graph G.

Proof. Based on the arithmetic–geometric mean inequality, AM–GM inequality, we have that

$$(n-1)ID(G) - n = \sum_{i \nsim j} \frac{d_i + d_j}{d_id_j} \geq \overline{m}\left(\prod_{i \nsim j} \frac{d_i + d_j}{d_id_j}\right)^{\frac{1}{\overline{m}}} = \overline{m}\frac{\overline{\Pi}_1(G)^{\frac{1}{\overline{m}}}}{\overline{\Pi}_2(G)^{\frac{1}{\overline{m}}}}, \tag{30}$$

from which (29) is obtained.

Equality in (30) holds if and only if $\frac{1}{d_i} + \frac{1}{d_j}$ is a constant for every pair of nonadjacent vertices in G. From Lemma 4.4 we get that equality in (29) holds if and only if $d_i + d_j$ is a constant for every pair of nonadjacent vertices in G. □

In [45] the following inequality was proven

$$\overline{\Pi}_1(G) \geq 2^{\overline{m}}\overline{\Pi}_2(G)^{\frac{1}{2}},$$

which is opposite to (29).

In the following theorem we establish a lower bound for $\overline{GA}(G)$ in terms of $\overline{m}$, $\overline{M}_2(G)$, $\overline{ISI}(G)$, $\overline{\Pi}_1(G)$ and $\overline{\Pi}_2(G)$.

Theorem 4.7. *Let G, $G \ncong K_n$, be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$\overline{GA}(G) \geq 2\sqrt{\frac{\overline{ISI}(G)^2}{\overline{M}_2(G)} + \overline{m}(\overline{m}-1)\frac{\overline{\Pi}_2(G)^{\frac{1}{\overline{m}}}}{\overline{\Pi}_1(G)^{\frac{2}{\overline{m}}}}}. \tag{31}$$

Equality holds if and only if $d_i + d_j$ is a constant for every pair of nonadjacent vertices in G.

Proof. For $m := \overline{m}$, $a_i := \frac{d_id_j}{(d_i+d_j)^2}$, with summation performed over all nonadjacent vertices in G, the inequality (1) becomes

$$\left(\sum_{i\nsim j}\frac{\sqrt{d_id_j}}{d_i+d_j}\right)^2 \geq \sum_{i\nsim j}\frac{d_id_j}{(d_i+d_j)^2}+\overline{m}(\overline{m}-1)\left(\prod_{i\nsim j}\frac{d_id_j}{(d_i+d_j)^2}\right)^{\frac{1}{\overline{m}}},$$

that is

$$\frac{1}{4}\overline{GA}(G)^2 \geq \sum_{i\nsim j}\frac{d_id_j}{(d_i+d_j)^2}+\overline{m}(\overline{m}-1)\frac{\overline{\Pi}_2(G)^{\frac{1}{\overline{m}}}}{\overline{\Pi}_1(G)^{\frac{2}{\overline{m}}}}. \tag{32}$$

From the above and (22) we arrive at (31).

Equality in (22) holds if and only if $d_i + d_j$ is a constant for every pair of nonadjacent vertices in G. Equality in (32) holds if and only if $\frac{\sqrt{d_id_j}}{d_i+d_j}$ is a constant for every pair of nonadjacent vertices in G. From Lemmas 4.3 and 4.5 we obtain that equality in (31) holds if and only if $d_i + d_j$ is a constant for every pair of nonadjacent vertices in G. □

Corollary 4.8. *Let G, $G \ncong K_n$, be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$\overline{GA}(G) \geq 2\sqrt{\frac{\overline{ISI}(G)^2}{\overline{M}_1(G)}+\frac{\overline{m}^2(\overline{m}-1)}{((n-1)ID(G)-n)\overline{\Pi}_1(G)^{\frac{1}{\overline{m}}}}}. \tag{33}$$

Equality holds if and only if $d_i + d_j$ is a constant for every pair of nonadjacent vertices in G.

Proof. The inequality (33) follows from (31) and (29). □

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References

[1] M. Aouchiche, I. El Hallaoui, P. Hansen, Geometric–arithmetic index and minimum degree of connected graphs, MATCH Commun. Math. Comput. Chem. 83 (1) (2020) 179–188.

[2] M. Aouchiche, P. Hansen, Comparing the geometric–arithmetic index and the spectral radius of graphs, MATCH Commun. Math. Comput. Chem. 84 (2) (2020) 473–482.

[3] M. Aouchiche, V. Ganesan, Adjusting geometric–arithmetic index to estimate boiling point, MATCH Commun. Math. Comput. Chem. 84 (2) (2020) 483–497.

[4] A. R. Ashrafi, T. Došlića, A. Hamzeh, The Zagreb coindices of graph operations, Discr. Appl. Math., **158** (2010), 1571–1578.

[5] S. Balachandran, H. Deng, S. Elumalai, T. Mansour, Extremal graphs on geometric–arithmetic index of tetracyclic chemical graphs, Int. J. Quantum Chem. 121 (2021) e26516.

[6] B. Bollobás, P. Erdős, Graphs of extremal weights, Ars Comb., **50** (1998), 225–233.

[7] V. Cirtoaje, The best lower bound depended on two fixed variables for Jensen's inequality with ordered variables, J. Ineq. Appl., **2010** (2010), Article ID 128258, 1–12.

[8] K. C. Das, On geometric–arithmetic index of graphs, MATCH Commun. Math. Comput. Chem., **64** (2010), 619–630.

[9] K. C. Das, I. Gutman, B. Furtula, On the first geometric–arithmetic index of graphs, Discr. Appl. Math., **159** (2011), 2030–2037.

[10] K. C. Das, I. Gutman, B. Furtula, Survey on geometric–arithmetic indices of graphs, MATCH Commun. Math. Comput. Chem., **65** (2011), 595–644.

[11] N. De, S. M. A. Nayeem, A. Pal, The F–coindex of some graph operations, SpringerPlus **5** (2016), #221.

[12] T. Došlić, B. Furtula, A. Graovac, I. Gutman, S. Moradi, Z. Yarahmadi, On vertex–degree–based molecular structure descriptors, MATCH Commun. Math. Comput. Chem., **66** (2011), 613–626.

[13] T. Došlić, Vertex–weighted Wiener polynomials for composite graphs, Ars Math. Contemp., **1** (2008), 66–80.

[14] C. S. Edwards, The largest vertex degree sum for a triangle in a graph, Bull. London Math. Soc., **9** (1977), 203–208.

[15] M. Eliasi, A. Iranmanesh, I. Gutman, Multiplicative versions of first Zagreb index, MATCH Commun. Math. Comput. Chem., **68**(1) (2012), 217–230.

[16] S. Fajtlowicz, On conjectures on Graffiti-II, Congr. Numer., **60** (1987), 187–197.

[17] B. Furtula, I. Gutman, A forgotten topological index, J. Math. Chem., **53**(4) (2015), 1184–1190.
[18] B. Furtula, I. Gutman, Ž. Kovijanić Vukičević, G. Lekishvili, G. Popivoda, On an old/new degree–based topological index, Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.), **40** (2015), 19–31.
[19] I. Gutman, Multiplicative Zagreb indices of trees, Bull. Int. Math. Virt. Inst., **1** (2011), 13–19.
[20] I. Gutman, On the origin of two degree-based topological indices, Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.), **146** (2014), 39–52.
[21] I. Gutman, On coindices of graphs and their complements, Appl. Math. Comput., **305** (2017), 161–165.
[22] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. **17** (1972), 535–538.
[23] I. Gutman, B. Rušćić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, J. Chem. Phys. **62** (1975), 3399–3405.
[24] I. Gutman, B. Furtula, C. Elphick, Three new/old vertex–degree–based topological indices, MATCH Commun. Math. Comput. Chem., **72** (2014), 617–632.
[25] A. Ilić, D. Stevanović, On comparing Zagreb indices, MATCH Commun. Math. Comput. Chem., **62** (2009), 681–687.
[26] H. Kober, On the arithmetic and geometric means and on Hölder's inequality, Proc. Amer. Math. Soc., **9** (1958), 452–459.
[27] I. Ž. Milovanović, E. I. Milovanović, I. Gutman, B. Furtula, Some inequalities for the forgotten topological index, Int. J. Appl. Graph Theory, **1**(1) (2017), 1–15.
[28] D. S. Mitrinović, P. M. Vasić, Analytic inequalities, Springer Verlag, Berlin-Heidelberg-New York, 1970.
[29] D. S. Mitrinović, J. E. Pečarić, A. M. Fink, Classical and new inequalities in analysis, Kluwer Academic Publishers, Dorchrecht, 1993.
[30] M. Mogharrab, G. H. Fath-Tabar, Some bounds on GA_1 index of graphs, MATCH Commun. Math. Comput. Chem., **65** (2011), 33–38.
[31] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, Croat. Chem. Acta, **76** (2003), 113–124.
[32] J. Radon, Über die absolut additiven Mengenfunktionen, Wiener Sitzungsber., **122** (1913), 1295–1438.
[33] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc., **97** (1975), 6609–6615.
[34] B. C. Rennie, On a class of inequalities, J. Austral. Math. Soc., **3** (1963), 442–448.
[35] J. M. Rodriguez, J. M. Sigarreta, On the geometric–arithmetic index, MATCH Commun. Math. Comput. Chem., **74** (2015), 103–120.
[36] J. M. Rodriguez, J. A. Rodriguez-Velazquez, J. M. Sigarreta, New inequalities involving the geometric–arithmetic index, MATCH Commun. Math. Comput. Chem., **78** (2017), 361–374.
[37] R. Todeschini, V. Consonni, New local vertex invariants and molecular descriptors based on functions of the vertex degrees, MATCH Commun. Math. Comput. Chem., **64**(2) (2010), 359–372.
[38] R. Todeschini, V. Consonni, Handbook of molecular descriptors, Wiley VCH, Weinheim, 2000.
[39] R. Todeschini, V. Consonni, Molecular descriptors for chemoinformatics, Wiley VCH, Weinheim, 2009.
[40] S. Vujošević, G. Popivoda, Ž. K. Vukičević, B. Furtula, R.Škrekovski, Arithmetic–geometric index and its relations with geometric–arithmetic index, Appl. Math. Comput. 391 (2021) 125706.
[41] D. Vukičević, M. Gašparov, Bond additive modeling I. Adriatic indices, Croat. Chem. Acta, **83**(3) (2010), 243–260.
[42] B. Vukičević, Bond additive modeling 2. Mathematical properties of maximum radeg index, Croat. Chem. Acta, **83** (2010), 261–273.
[43] D. Vukičević, Q. Li, J. Sedlar, T. Došlić, Lanzhou index, MATCH Commun. Math. Comput. Chem., **80** (2018), 863–876.
[44] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end–vertex degrees of edges, J. Math. Chem., **46** (2009), 1369–1376.
[45] K. Xu, K. C. Das, K. Tang, On the multiplicative Zagreb coindex of graphs, Opuscula Math., **33**(1) (2013), 191–204.
[46] X. Zhao, Y. Shao, Y. Gao, The maximal geometric–arithmetic energy of trees, MATCH Commun. Math. Comput. Chem. 84 (2) (2020) 363–367.
[47] B. Zhou, I. Gutman, T. Aleksić, A note on Laplacian energy of graphs, MATCH Commun. Math. Comput. Chem., **60** (2008), 441–446.