BOUNDS FOR THE GEOMETRIC-ARITHMETIC INDEX OF A GRAPH

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Abstract. The first geometric-arithmetic index $GA_1(G)$, which was introduced by D. Vukičević and B. Furtula recently, is a graph-based molecular structure descriptor. The aim of this paper is to obtain new inequalities involving the geometric-arithmetic index GA_1 and other well known topological indices. In particular, we relate the geometric-arithmetic index of a graph G with its first Zagreb index $M_1(G)$, its second Zagreb index $M_2(G)$, its modified Zagreb index $Z_{-1}(G)$ and its Randić index $R(G)$.

1. INTRODUCTION

The study of topological indices is a subject of increasing interest, both in pure and applied mathematics. Topological indices are interesting since they capture some of the properties of a molecule (or a graph) in a single number(see, e.g., [17, 22]). Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener [19] in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes. Probably, the Randić index $R(G)$ is the best know topological index (see, e.g., [5, 9, 10, 14, 15] and the references cited therein). The Randić index $R(G)$ is defined in [14] as

$$R = R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

During many years, scientists were trying to improve the predictive power of the Randić index. This led to the introduction of a large number of new topological

descriptors resembling the original Randić index. The first geometric-arithmetic index $GA_1(G)$, defined in [18] as

$$GA_1 = GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)},$$

where uv denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u, is one of the successors of the Randić index. Although GA_1 was introduced just five years ago, there are many papers dealing with this index. There are other geometric-arithmetic indices, like $Z_{p,q}$ ($Z_{0,1} = GA_1$), but the results in [2] show empirically that the GA_1 index gathers the same information on observed molecules as other $Z_{p,q}$ indices.

Topological indices based on end-vertex degrees of edges have been used over thirty years. Among them, several indices are recognized to be useful tools in chemical researches. The graph based molecular descriptors called Zagreb indices were introduced by Gutman and Trinajstić. Since then, several results concerning Zagreb indices have been communicated in the chemical and mathematical literature (see [1, 4, 6, 13, 21] and the references cited therein). The variable Zagreb index is defined in [11] as

$$Z_\alpha = Z_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha,$$

and was used in the structure-boiling point modeling of benzenoid hydrocarbons. The obtained model is practically identical to the model based on the variable vertex-connectivity index and this is due to close relationship between the formulas for the two indices.

The reason for introducing a new index is to gain prediction of some property of molecules somewhat better than obtained by already presented indices. Therefore, a test study of predictive power of a new index must be done. As a standard for testing new topological descriptors, the properties of octanes are commonly used. We can find 16 physico-chemical properties of octanes at www.moleculardescriptors.eu. The GA_1 index gives better correlation coefficients than Randić index for these properties, but the differences between them are not significant. However, the predicting ability of the GA_1 index compared with Randić index is reasonably better (see [2, Table 1]).

We begin by stating some notation and terminology. Let $G = (V, E) = (V(G), E(G))$ denotes a (non-oriented) finite simple connected graph of order $n = |V(G)|$ and size $m = |E(G)|$ with $E(G) \neq \varnothing$. We denote two adjacent vertices u and v by $u \sim v$. For a vertex $u \in V$ we denote $N(v) = \{u \in V : u \sim v\}$. The degree of a vertex $v \in V$ will be denoted by $d_v = |N(v)|$. We denote by δ and Δ the minimum and maximum degree of the graph, respectively. We use the classical notation uv for the edge of a graph joining the vertices u and v. Note that the connectivity of G is not an important restriction, since if G has connected components $G_1, \ldots, G_r$, then $GA_1(G) = GA_1(G_1) + \cdots + GA_1(G_r)$.

2. RESULTS

We start with the following basic results. In [18] (see also [2]) the following inequalities appear :

$$GA_1(G) \geq \frac{2(n-1)^{3/2}}{n}.$$

$$GA_1(G) \geq \frac{2m}{n}.$$

In [2] we find the bounds

$$\frac{2m\sqrt{\Delta\delta}}{\Delta+\delta} \leq GA_1(G) \leq m.$$

In [16] the authors obtain a lower bound of $GA_1(G)$, depending just on n and m, for every graph G.

$$GA_1(G) \geq \frac{2m\sqrt{n-1}}{n}.$$

Moreover, [16] provides a lower bound of $GA_1(G)$ for every graph G with $\delta \geq k$, for any fixed $k \geq 2$.

(1) If $n \leq 10$, then $GA_1(G) \geq \frac{nk}{2}$.

(2) If $n \geq 11$, then $GA_1(G) \geq \min\left\{ \frac{nk}{2}, \frac{(k+1)\sqrt{k}(n-1)^{3/2}}{n-1+k} \right\}$.

We will denote by $M_1(G)$ and $M_2(G)$ the first and the second Zagreb indices of the graph G, respectively, defined in [7] as

$$M_1(G) = \sum_{u \in V(G)} d_u^2, \qquad M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

These indices have attracted growing interest, see e.g., [20] and [7].

In [3] (see also [2]) we find the bound:

$$GA_1(G) \leq \frac{\sqrt{mM_2(G)}}{\delta}.$$

A similar lower bound is obtained in [16]:

$$GA_1(G) \geq \frac{2}{\Delta+\delta} \sqrt{\frac{\delta m M_2(G)}{\Delta}}.$$

Theorem 1 below improves these lower bounds. In order to prove it, we need the following lemmas (see [16] and [8]).

Lemma 1. *Let g be the function $g(x,y) = \frac{2\sqrt{xy}}{x+y}$ with $0 < a \leq x, y \leq b$. Then*

$$\frac{2\sqrt{ab}}{a+b} \leq g(x,y) \leq 1.$$

The equality in the lower bound is attained if and only if either $x = a$ and $y = b$, or $x = b$ and $y = a$, and the equality in the upper bound is attained if and only if $x = y$. Besides, $g(x, y) = g(x', y')$ if and only if x/y is equal to either x'/y' or y'/x'.

Proof. Let f be the function $f(t) = \frac{2t}{1+t^2}$ on the interval $[0, \infty)$. Then f strictly increases in $[0, 1]$, strictly decreases in $[1, \infty)$, $f(t) = 1$ if and only if $t = 1$ and $f(t) = f(t_0)$ if and only if either $t = t_0$ or $t = t_0^{-1}$. The statements follow from $f'(t) = \frac{2(1-t^2)}{(1+t^2)^2}$. Now, taking $g(x, y) = f(t)$ with $t = \sqrt{\frac{x}{y}}$, and $\sqrt{\frac{a}{b}} \le t \le \sqrt{\frac{b}{a}}$, the result follows. $\square$

The following result provides a converse of Cauchy-Schwarz inequality.

Lemma 2. *If $0 < n_1 \le a_j \le N_1$ and $0 < n_2 \le b_j \le N_2$ for $1 \le j \le k$, then*

$$\Big(\sum_{j=1}^{k} a_j^2\Big)^{1/2} \Big(\sum_{j=1}^{k} b_j^2\Big)^{1/2} \le \frac{1}{2}\Big(\sqrt{\frac{N_1 N_2}{n_1 n_2}} + \sqrt{\frac{n_1 n_2}{N_1 N_2}}\Big)\Big(\sum_{j=1}^{k} a_j b_j\Big).$$

Theorem 1. *We have for any graph G*

$$\frac{2\sqrt{2\sqrt{\Delta\delta}(\Delta+\delta)m M_2(G)}}{\Delta(\sqrt{\Delta}+\sqrt{\delta})^2} \le GA_1(G) \le \frac{M_2(G)}{\delta^2},$$

and the equality in each inequality is attained if and only if G is a regular graph.

Proof. By Lemma 1, taking $a = \delta$ and $b = \Delta$, we have

$$\frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \le \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} \le 1.$$

Lemma 2 gives

$$GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} \ge \frac{\Big(\sum_{uv \in E(G)} \frac{4 d_u d_v}{(d_u + d_v)^2}\Big)^{1/2} \Big(\sum_{uv \in E(G)} 1\Big)^{1/2}}{\frac{1}{2}\Big(\sqrt{\frac{\Delta+\delta}{2\sqrt{\Delta\delta}}} + \sqrt{\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}}\Big)}$$

$$\ge \frac{2\sqrt{2\sqrt{\Delta\delta}(\Delta+\delta)m}}{(\sqrt{\Delta}+\sqrt{\delta})^2}\Big(\sum_{uv \in E(G)} \frac{1}{\Delta^2} d_u d_v\Big)^{1/2}$$

$$= \frac{2\sqrt{2\sqrt{\Delta\delta}(\Delta+\delta)m M_2(G)}}{\Delta(\sqrt{\Delta}+\sqrt{\delta})^2}.$$

Therefore,

$$\frac{2\sqrt{2\sqrt{\Delta\delta}(\Delta+\delta)m M_2(G)}}{\Delta(\sqrt{\Delta}+\sqrt{\delta})^2} \le GA_1(G).$$

On the other hand,

$$GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} = \sum_{uv \in E(G)} \frac{d_u d_v}{\frac{1}{2}(d_u + d_v)\sqrt{d_u d_v}} \le \sum_{uv \in E(G)} \frac{d_u d_v}{\delta\dot{\delta}}.$$

Thus, we have

$$GA_1(G) \le \frac{M_2(G)}{\delta^2}.$$

If the graph is regular, then $M_2(G) = \delta^2 m$, the lower and upper bound are the same, and they are equal to $GA_1(G) = m$. If the equality holds in the lower bound, then $4(d_u + d_v)^{-2} = \Delta^{-2}$ for every $uv \in E(G)$; hence, $d_u = \Delta$ for every $u \in V(G)$ and the graph is regular. If the equality is attained in the upper bound, then $\frac{1}{2}(d_u + d_v) = \delta$ for every $uv \in E(G)$ and we conclude $d_u = \delta$ for every $u \in V(G)$. $\square$

Theorem 1 improves the previous lower bound, as the following result shows.

Remark 1. For any $0 < \delta \le \Delta$ we have

$$\frac{\sqrt{2\sqrt{\Delta\delta}(\Delta + \delta)}}{\Delta(\sqrt{\Delta} + \sqrt{\delta})^2} \ge \frac{1}{\Delta + \delta}\sqrt{\frac{\delta}{\Delta}}.$$

Proof. First of all, note that the polynomial $p(x) = 2x^6 - x^5 + 2x^4 - 6x^3 + 2x^2 - x + 2$ verifies $p(x) \ge 0$ if $x \ge 1$, since $p(x) = (x-1)^2(2x^4 + 3x^3 + 6x^2 + 3x + 2)$. Hence,

$$2x^6 + 2x^4 + 2x^2 + 2 \ge x(x^4 + 6x^2 + 1), \quad if \ x \ge 1,$$

$$2\left(\frac{\Delta}{\delta}\right)^3 + 2\left(\frac{\Delta}{\delta}\right)^2 + 2\frac{\Delta}{\delta} + 2 \ge \sqrt{\frac{\Delta}{\delta}}\left(\left(\frac{\Delta}{\delta}\right)^2 + 6\frac{\Delta}{\delta} + 1\right),$$

$$2\Delta^3 + 2\Delta^2\delta + 2\Delta\delta^2 + 2\delta^3 \ge \Delta^2\sqrt{\Delta\delta} + 6\Delta\delta\sqrt{\Delta\delta} + \delta^2\sqrt{\Delta\delta},$$

$$2(\Delta + \delta)^3 \ge \sqrt{\Delta\delta}(\sqrt{\Delta} + \sqrt{\delta})^4,$$

and this implies the inequality. $\square$

In [2] appears the inequality

$$GA_1(G) \le \frac{1}{2} M_1(G).$$

In [16] appears the following result

$$GA_1(G) \le \frac{1}{2\delta} M_1(G).$$

Our next result improves both inequalities and also gives a lower bound of GA_1 involving the first Zagreb index.

Theorem 2. *We have for any graph G*

$$\frac{2\delta M_1(G)}{(\Delta+\delta)^2} \leq GA_1(G) \leq \sqrt{\frac{mM_1(G)}{2\delta}}\,.$$

Furthermore, the equality in each inequality is attained if and only if G is regular.

Proof. By Lemma 1, taking $a = \delta$ and $b = \Delta$, we have

$$\frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \leq \frac{2\sqrt{d_u d_v}}{d_u+d_v} \leq 1\,.$$

Hence,

$$1 \leq \frac{(d_u+d_v)^2}{4d_u d_v} \leq \frac{(\Delta+\delta)^2}{4\Delta\delta}\,, \qquad \frac{d_u+d_v}{2\sqrt{d_u d_v}} \leq \frac{(\Delta+\delta)^2}{4\Delta\delta}\frac{2\sqrt{d_u d_v}}{d_u+d_v}\,.$$

Note that

$$M_1(G) = \sum_{v \in V(G)} d_v^2 = \sum_{uv \in E(G)} (d_u+d_v)\,.$$

Thus, we have

$$\frac{M_1(G)}{2\Delta} = \sum_{uv \in E(G)} \frac{d_u+d_v}{2\Delta} \leq \sum_{uv \in E(G)} \frac{d_u+d_v}{2\sqrt{d_u d_v}} \leq \frac{(\Delta+\delta)^2}{4\Delta\delta} GA_1(G)\,.$$

Therefore,

$$\frac{2\delta M_1(G)}{(\Delta+\delta)^2} \leq GA_1(G)\,.$$

Cauchy-Schwarz inequality and $\frac{1}{d_u+d_v} \leq \frac{1}{2\delta}$ give

$$GA_1(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \leq \sum_{uv \in E(G)} \frac{\sqrt{d_u+d_v}}{\sqrt{d_u+d_v}}$$

$$\leq \Big(\sum_{uv \in E(G)} (d_u+d_v) \Big)^{1/2} \Big(\sum_{uv \in E(G)} \frac{1}{d_u+d_v} \Big)^{1/2} \leq \sqrt{\frac{mM_1(G)}{2\delta}}\,.$$

If the graph is regular, then $M_1(G) = n\delta^2 = 2m\delta$, the lower and upper bound are the same, and they are equal to $GA_1(G) = m$. If the equality holds in the lower bound, then $\sqrt{d_u d_v} = \Delta$ for every $uv \in E(G)$; hence, $d_u = \Delta$ for every $u \in V(G)$ and G is regular. If the equality is attained in the upper bound, then $d_u + d_v = 2\delta$ for every $uv \in E(G)$ and we conclude $d_u = \delta$ for every $u \in V(G)$. $\qquad\square$

Note that Theorem 2 improves the upper bound $\frac{1}{2\delta} M_1(G)$: since $2\delta m \leq M_1(G)$, we have

$$\sqrt{\frac{mM_1(G)}{2\delta}} \leq \frac{1}{2\delta} M_1(G)\,.$$

Recall that the variable Zagreb index is defined as $Z_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$. Note that $Z_{-1/2}$ is the usual Randić index $R(G)$, Z_1 is the second Zagreb index M_2, Z_{-1} is the modified Zagreb index [12], etc.

Next, we obtain new inequalities relating the geometric-arithmetic index with the modified Zagreb index. We will need also the following lemmas.

Lemma 3. *We have for any graph G and every $uv \in E(G)$*

$$\delta \leq \frac{2d_u d_v}{d_u + d_v} \leq \Delta,$$

and the lower (or upper) bound is attained for every $uv \in E(G)$ if and only if G is a regular graph.

Proof. We know that

$$d_u(d_v - \delta) + d_v(d_u - \delta) \geq 0, \qquad d_u d_v + d_v d_u \geq d_u \delta + d_v \delta.$$

Therefore,

$$\delta \leq \frac{2d_u d_v}{d_u + d_v}.$$

On the other hand, using the fact that the geometric mean is at most the arithmetic mean, we obtain

$$\frac{2d_u d_v}{d_u + d_v} \leq \frac{(d_u + d_v)^2}{2(d_u + d_v)} = \frac{d_u + d_v}{2} \leq \Delta.$$

If G is a regular graph, then it is clear that both inequalities are attained for every $uv \in E(G)$. Assume that the lower bound is attained for every $uv \in E(G)$. Then $d_v - \delta = d_u - \delta = 0$ for every $uv \in E(G)$, and $d_v = \delta$ for every $v \in V(G)$. Hence, G is a regular graph. If the upper bound is attained for every $uv \in E(G)$, then $4d_u d_v = (d_u + d_v)^2$ for every $uv \in E(G)$, $d_u = d_v$ for every $uv \in E(G)$, and we conclude that G is regular since it is connected. $\qquad\square$

In order to prove our next result we need the following particular case of Jensen's inequality.

Lemma 4. *If f is a convex function in $\mathbb{R}_+$ and $x_1, \ldots, x_m > 0$, then*

$$f\left(\frac{x_1 + \cdots + x_m}{m}\right) \leq \frac{1}{m}\left(f(x_1) + \cdots + f(x_m)\right).$$

Theorem 3. *We have for any graph G*

$$\sqrt{\frac{m^3}{\Delta^2 Z_{-1}(G)}} \leq GA_1(G) \leq \Delta^2 Z_{-1}(G).$$

Furthermore, the equality in each inequality is attained if and only if G is regular.

Proof. Using Lemma 3, we have

$$\delta \le \frac{2d_u d_v}{d_u + d_v} \le \Delta,$$

$$\frac{\delta}{d_u d_v} \le \frac{2}{d_u + d_v} \le \frac{\Delta}{d_u d_v}.$$

Moreover,

$$\sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \le \Delta \sum_{uv \in E(G)} \frac{2}{d_u + d_v} \le \Delta \sum_{uv \in E(G)} \frac{\Delta}{d_u d_v} = \Delta^2 Z_{-1}(G).$$

Since $f(x) = 1/x^2$ is a convex function in $\mathbb{R}_+$, Lemma 4 gives

$$\frac{m^2}{\left(\sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right)^2} \le \frac{1}{m} \sum_{uv \in E(G)} \frac{(d_u + d_v)^2}{4 d_u d_v} \le \frac{\Delta^2}{m} \sum_{uv \in E(G)} \frac{1}{d_u d_v},$$

$$\frac{m^2}{(GA_1(G))^2} \le \frac{\Delta^2}{m} Z_{-1}(G).$$

If the graph is regular, then $Z_{-1}(G) = m\Delta^{-2}$, the lower and upper bound are the same, and they are equal to $GA_1(G) = m$. If the equality holds in the upper bound, then $\sqrt{d_u d_v} = \Delta$ for every $uv \in E(G)$; hence, $d_u = \Delta$ for every $u \in V(G)$ and the graph is regular. If the equality is attained in the lower bound, then $(d_u + d_v)^2 = 4\Delta^2$ for every $uv \in E(G)$ and we conclude $d_u = \Delta$ for every $u \in V(G)$.   □

The following result gives a lower and upper bounds for GA_1 involving the Zagreb indices $M_2(G)$ and $Z_{-1}(G)$.

Theorem 4. *We have for any graph G*

$$\frac{2\delta^2 \sqrt{M_2(G)Z_{-1}(G)}}{\Delta^2 + \delta^2} \le GA_1(G) \le \sqrt{M_2(G)Z_{-1}(G)},$$

and the equality in each inequality is attained if and only if G is a regular graph.

Proof. Lemma 3 gives

$$\delta \le \frac{2d_u d_v}{d_u + d_v} \le \Delta.$$

It is easy to see that

$$\frac{1}{\Delta} \le \frac{1}{\sqrt{d_u d_v}} \le \frac{1}{\delta}.$$

Thus Lemma 2 gives

$$GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} = \sum_{uv \in E(G)} \frac{2 d_u d_v}{d_u + d_v} \frac{1}{\sqrt{d_u d_v}}$$

$$\geq \frac{\left(\sum_{uv \in E(G)} \frac{4(d_u d_v)^2}{(d_u + d_v)^2} \right)^{1/2} \left(\sum_{uv \in E(G)} \frac{1}{d_u d_v} \right)^{1/2}}{\frac{1}{2} \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta} \right)}$$

$$\geq \frac{2\Delta\delta \sqrt{Z_{-1}(G)}}{\Delta^2 + \delta^2} \left(\sum_{uv \in E(G)} \frac{4(d_u d_v)^2}{(d_u + d_v)^2} \right)^{1/2}$$

$$\geq \frac{2\Delta\delta \sqrt{Z_{-1}(G)}}{\Delta^2 + \delta^2} \frac{2\delta}{2\Delta} \left(\sum_{uv \in E(G)} d_u d_v \right)^{1/2}$$

$$= \frac{2\delta^2 \sqrt{M_2(G) Z_{-1}(G)}}{\Delta^2 + \delta^2} .$$

Since

$$4 d_u d_v \leq (d_u + d_v)^2,$$

Cauchy-Schwarz inequality gives

$$GA_1(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \leq \left(\sum_{uv \in E(G)} d_u d_v \right)^{1/2} \left(\sum_{uv \in E(G)} \frac{4}{(d_u + d_v)^2} \right)^{1/2}$$

$$\leq \left(\sum_{uv \in E(G)} d_u d_v \right)^{1/2} \left(\sum_{uv \in E(G)} \frac{1}{d_u d_v} \right)^{1/2} = \sqrt{M_2(G) Z_{-1}(G)} .$$

If the graph is regular, then the lower and upper bound are the same, and they are equal to $GA_1(G)$. If the equality holds in the lower bound, then $d_u d_v = \delta^2$ for every $uv \in E(G)$; hence, $d_u = \delta$ for every $u \in V(G)$ and the graph is regular. If the equality is attained in the upper bound, then $4 d_u d_v = (d_u + d_v)^2$ for every $uv \in E(G)$, $d_u = d_v$ for every $uv \in E(G)$, and we conclude that G is regular since it is connected. $\square$

Next, we obtain inequalities relating the geometric-arithmetic index with the Zagreb indices $M_1(G)$, $M_2(G)$ and $Z_{-1}(G)$. Recall that a (Δ, δ)-biregular graph is a bipartite graph for which any vertex in one side of the given bipartition has degree Δ and any vertex in the other side of the bipartition has degree δ.

Theorem 5. *For any graph G,* $\frac{\Delta\delta \sqrt{(n M_1(G) + 4 M_2(G) - 4m^2) Z_{-1}(G)}}{\Delta^2 + \delta^2} \leq GA_1(G) \leq$ $\frac{\sqrt{(n M_1(G) + 4 M_2(G) - 4m^2) Z_{-1}(G)}}{2}$. *The equality in the lower bound is attained if and only if G is either regular or (Δ, δ)-biregular; the equality in the upper bound is attained if and only if G is regular.*

Proof. We have by Lemma 1

$$\frac{4\Delta\delta}{(\Delta+\delta)^2} \le \frac{4d_u d_v}{(d_u+d_v)^2} \le 1.$$

Hence,

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} \le \frac{d_u + d_v}{2\sqrt{d_u d_v}} \tag{2.1}$$

and

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} \ge \frac{4\Delta\delta}{(\Delta+\delta)^2} \frac{d_u + d_v}{2\sqrt{d_u d_v}}. \tag{2.2}$$

We have by (2.1)

$$GA_1(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \le \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}}.$$

Moreover,

$$\sum_{uv\in E(G)} (d_u + d_v)^2 = \sum_{uv\in E(G)} d_u^2 + 2\sum_{uv\in E(G)} d_u d_v + \sum_{uv\in E(G)} d_v^2$$

$$= \sum_{uv\in E(G)} (d_u^2 + d_v^2) + 2\sum_{uv\in E(G)} d_u d_v$$

$$= \sum_{uv\in E(G)} (d_u^2 + d_v^2) + 2M_2(G).$$

Since

$$\sum_{uv\in E(G)} (d_u^2 + d_v^2) = \sum_{v\in V(G)} d_v \cdot d_v^2 = \sum_{v\in V(G)} d_v^3,$$

we have

$$\sum_{uv\in E(G)} (d_u + d_v)^2 = \sum_{v\in V(G)} d_v^3 + 2M_2(G). \tag{2.3}$$

Using Cauchy-Schwarz inequality and the formula

$$\sum_{v\in V(G)} d_v^3 = nM_1(G) + 2M_2(G) - 4m^2 \tag{2.4}$$

(see, e.g., [21]), we obtain

$$\sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}} \leq \Big(\sum_{uv \in E(G)} \frac{(d_u + d_v)^2}{4} \Big)^{1/2} \Big(\sum_{uv \in E(G)} \frac{1}{d_u d_v} \Big)^{1/2}$$

$$= \frac{1}{2} \Big(\sum_{v \in V(G)} d_v^3 + 2M_2(G) \Big)^{1/2} \sqrt{Z_{-1}(G)}$$

$$= \frac{\sqrt{(nM_1(G) + 4M_2(G) - 4m^2)Z_{-1}(G)}}{2}.$$

Let us prove the lower bound. We have by (2.2)

$$GA_1(G) \geq \frac{4\delta\Delta}{(\delta + \Delta)^2} \sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}}.$$

Since

$$\delta \leq \frac{d_u + d_v}{2} \leq \Delta, \qquad \frac{1}{\Delta} \leq \frac{1}{\sqrt{d_u d_v}} \leq \frac{1}{\delta},$$

Lemma 2, (2.3) and (2.4) give

$$\sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}} \geq \frac{\Big(\sum_{uv \in E(G)} \frac{(d_u + d_v)^2}{4} \Big)^{1/2} \Big(\sum_{uv \in E(G)} \frac{1}{d_u d_v} \Big)^{1/2}}{\frac{1}{2} \Big(\frac{\Delta}{\delta} + \frac{\delta}{\Delta} \Big)}$$

$$\geq \frac{\Delta\delta \sqrt{\Big(\sum_{v \in V(G)} d_v^3 + 2M_2(G) \Big)Z_{-1}(G)}}{\Delta^2 + \delta^2}$$

$$= \frac{\Delta\delta \sqrt{(nM_1(G) + 4M_2(G) - 4m^2)Z_{-1}(G)}}{\Delta^2 + \delta^2}.$$

If the graph is regular, then the lower and upper bound are the same, and they are equal to $GA_1(G)$.

If the equality in the lower bound is attained, then (2.2) holds for every $uv \in E(G)$; by Lemma 1 we have either $d_u = \Delta$ and $d_v = \delta$, or viceversa, for each $uv \in E(G)$. This happens if and only if G is a regular graph if $\Delta = \delta$ or a (Δ, δ)-biregular graph otherwise.

If the equality in the upper bound is attained, then (2.1) holds for every $uv \in E(G)$; by Lemma 1 we have $d_u = d_v$ for each $uv \in E(G)$, and G is a regular graph.   □

In [16] we find the bound

$$GA_1(G) \leq \Delta R(G), \tag{2.5}$$

where $R(G)$ is the Randić index. We recall that $R(G)$ is the best know topological index.

The following result provides lower and upper bounds of GA_1 involving the Randić index. Furthermore, it improves (2.5).

Theorem 6. *We have for any graph G*

$$\delta R(G) \leq GA_1(G) \leq \sqrt{\Delta m R(G)},$$

and the equality in each inequality holds if and only if G is regular.

Proof. Since $f(x) = x^2$ is a convex function in $\mathbb{R}_+$, Lemma 4 gives

$$\frac{1}{m^2} GA_1(G)^2 = \frac{1}{m^2} \left(\sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right)^2 \leq \frac{1}{m} \sum_{uv \in E(G)} \frac{4 d_u d_v}{(d_u + d_v)^2}.$$

Lemma 3 gives

$$\frac{2 d_u d_v}{d_u + d_v} \leq \Delta,$$

$$\frac{2 d_u d_v (2\sqrt{d_u d_v})}{(d_u + d_v)^2} \leq \frac{2 d_u d_v (d_u + d_v)}{(d_u + d_v)^2} = \frac{2 d_u d_v}{d_u + d_v} \leq \Delta,$$

$$\frac{4 d_u d_v}{(d_u + d_v)^2} \leq \frac{\Delta}{\sqrt{d_u d_v}},$$

$$\frac{1}{m^2} GA_1(G)^2 \leq \frac{1}{m} \sum_{uv \in E(G)} \frac{4 d_u d_v}{(d_u + d_v)^2} \leq \frac{\Delta}{m} \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

Hence,

$$GA_1(G) \leq \sqrt{\Delta m R(G)}.$$

In order to prove the lower bound, notice that Lemma 3 gives

$$\delta \leq \frac{2 d_u d_v}{d_u + d_v} = \frac{2\sqrt{d_u d_v}\sqrt{d_u d_v}}{d_u + d_v}.$$

Hence,

$$\sum_{uv \in E(G)} \frac{\delta}{\sqrt{d_u d_v}} \leq \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)},$$

$$\delta R(G) \leq GA_1(G).$$

If the graph is regular, then $R(G) = \frac{m}{\delta}$, the lower and upper bound are the same, and they are equal to $GA_1(G) = m$.

If the equality in the lower bound is attained, then

$$\delta = \frac{2 d_u d_v}{d_u + d_v}$$

for every $uv \in E(G)$. By Lemma 3, the graph G is regular.

If the equality in the upper bound is attained, then

$$\Delta = \frac{2d_u d_v}{d_u + d_v}$$

for every $uv \in E(G)$, and G is regular by Lemma 3.   □

Note that Theorem 6 improves the upper bound $GA_1(G) \leq \Delta R(G)$: since $\frac{m}{\Delta} \leq R(G)$, we have

$$\sqrt{\Delta m R(G)} \leq \Delta R(G).$$

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