

New Inequalities Involving the Geometric–Arithmetic Index

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Abstract

Let $G = (V, E)$ be a simple connected graph and d_i be the degree of its i th vertex. In a recent paper [J. Math. Chem. 46 (2009) 1369-1376] the *first geometric-arithmetic index* of a graph G was defined as

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

This graph invariant is useful for chemical proposes. The main use of GA_1 is for designing so-called quantitative structure-activity relations and quantitative structure-property relations. In this paper we obtain new inequalities involving the geometric-arithmetic index GA_1 and characterize the graphs which make the inequalities tight. In particular, we improve some known results, generalize other, and we relate GA_1 to other well-known topological indices.

1 Introduction

A graph invariant is a property of graphs that is preserved by isomorphisms. Around the middle of the last century theoretical chemists discovered that some interesting re-

relationships between various properties of organic substances and the molecular structure can be deduced by examining some invariants of the underlining molecular graph. Those graph invariants that are useful for chemical purposes were named *topological indices* or *molecular structure descriptors*. The Wiener index, introduced by Harry Wiener in 1947, is the oldest topological index related to molecular branching. Wiener defined this topological index as the sum of all shortest-path distances of a graph, and he showed that it is closely correlated with the boiling points of alkane molecules [33]. Based on its success, many other topological indices have been developed subsequently to Wiener's work.

Topological indices based on vertex degrees have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best known such descriptor is the Randić connectivity index [24]. There are more than thousand papers and a couple of books dealing with this molecular descriptor (see, e.g., [13, 16, 17, 27, 28] and the references therein). 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 , defined in [32] as

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

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 in 2009, there are many papers dealing with this index (see, e.g., [5–9, 20, 25, 26, 29, 32] and the references therein). There are other geometric-arithmetic indices, like $Z_{p,q}$ [6], where $Z_{0,1} = GA_1$, but the results in [6, p.598] show that GA_1 gathers the same information on observed molecule as $Z_{p,q}$.

As described in [6], the reason for introducing a new index is to gain prediction of target property (properties) 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.molecular-descriptors.eu. The GA_1 index gives better correlation coefficients than the 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 [6, Table 1]). Although only about 1000 benzenoid hydrocarbons are known, the number of possible benzenoid hydrocarbons is huge. For instance, the number of pos-

sible benzenoid hydrocarbons with 35 benzene rings is $5.85 \cdot 10^{21}$ [31]. Therefore, the modeling of their physico-chemical properties is very important in order to predict properties of currently unknown species. The graphic in [6, Fig.7] (from [6, Table 2], [30]) shows that there exists a good linear correlation between GA_1 and the heat of formation of benzenoid hydrocarbons (the correlation coefficient is equal to 0.972). Furthermore, the improvement in prediction with GA_1 index comparing to Randić index in the case of standard enthalpy of vaporization is more than 9%. That is why one can think that GA_1 index should be considered for designing so-called quantitative structure-activity relations and quantitative structure-property relations, where “structure” means molecular structure, “property” some physical or chemical property and “activity” some biologic, pharmacologic or similar property.

Some inequalities involving the geometric-arithmetic index and other topological indices were obtained in [5–8, 20, 25, 26, 29, 32]. The aim of this paper is to obtain new inequalities involving the geometric-arithmetic index GA_1 and characterize the graphs which make the inequalities tight. In particular, we improve some known results, generalize other, and we relate GA_1 to other well-known topological indices.

2 New equalities involving GA_1

Throughout this paper, $G = (V, E) = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) connected graph with $E \neq \emptyset$. Note that the connectivity of G is not an important restriction, since if G has connected components G_1, \dots, G_r , then

$$GA_1(G) = GA_1(G_1) + \dots + GA_1(G_r).$$

Furthermore, every molecular graph is connected.

From now on, the order (the cardinality of $V(G)$), size (the cardinality of $E(G)$), and maximum and minimum degree of G will be denoted by n, m, Δ, δ , respectively.

We will denote by M_1 and M_2 the first and second Zagreb indices, respectively, defined as

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

These topological indices have attracted growing interest, see e.g., [3, 4, 10, 14, 18] (in particular, they are included in a number of programs used for the routine computation of topological indices).

The following inequality was given in [20] (see also [6, p.610]) and [25, Theorem 3.7],

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

Since $M_1(G) \geq \delta^2 n$, Theorem 2.1 below improves (1).

Theorem 2.1. *For any graph G ,*

$$GA_1(G) \leq \frac{\sqrt{nM_1(G)}}{2},$$

and the equality holds if and only if G is a regular graph.

Proof. First of all, note that for every function $f : [\delta, \Delta] \rightarrow \mathbb{R}$, we have

$$\sum_{uv \in E(G)} (f(d_u) + f(d_v)) = \sum_{u \in V(G)} d_u f(d_u).$$

Since $\frac{4}{d_u + d_v} \leq \frac{1}{d_u} + \frac{1}{d_v}$, by taking $f(d_u) = \frac{1}{d_u}$ we deduce

$$\sum_{uv \in E(G)} \frac{1}{d_u + d_v} \leq \frac{1}{4} \sum_{uv \in E(G)} \left(\frac{1}{d_u} + \frac{1}{d_v} \right) = \frac{n}{4}.$$

Cauchy-Schwarz inequality gives

$$\begin{aligned} GA_1(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \leq \sum_{uv \in E(G)} \sqrt{d_u + d_v} \frac{1}{\sqrt{d_u + d_v}} \\ &\leq \left(\sum_{uv \in E(G)} (d_u + d_v) \right)^{1/2} \left(\sum_{uv \in E(G)} \frac{1}{d_u + d_v} \right)^{1/2} \\ &\leq \left(\sum_{u \in V(G)} d_u d_u \right)^{1/2} \left(\frac{n}{4} \right)^{1/2} = \frac{\sqrt{nM_1(G)}}{2}. \end{aligned}$$

Notice that all the equalities above hold if and only if the graph is regular. ■

The following elementary lemma will be an important tool to derive some results.

Lemma 2.2. *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, $g(x, y) = g(x', y')$ for some $x', y' > 0$ if and only if x/y is equal to either x'/y' or y'/x' . Finally, if $0 \leq x' < x \leq y$, then $g(x', y) < g(x, y)$.

Theorem 2.3. For any graph G ,

$$\frac{\sqrt{(\Delta + \delta)^2 M_2(G) + 4\Delta^3 \delta m(m-1)}}{\Delta(\Delta + \delta)} \leq GA_1(G) \leq \frac{\sqrt{M_2(G) + \delta^2 m(m-1)}}{\delta},$$

and each equality holds if and only if G is regular.

Proof. By Lemma 2.2, for any edge $uv \in E(G)$ we have

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} \geq \frac{2\sqrt{\Delta\delta}}{\Delta + \delta}. \tag{2}$$

Notice also that

$$\frac{1}{\Delta^2} \leq \frac{4}{(d_u + d_v)^2} \leq \frac{1}{\delta^2} \tag{3}$$

Inequalities (2) and (3) lead to

$$\begin{aligned} (GA_1(G))^2 &= \left(\sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right)^2 \\ &= \sum_{uv \in E(G)} \frac{4d_u d_v}{(d_u + d_v)^2} + 2 \sum_{\substack{uv, xy \in E(G), \\ uv \neq xy}} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \frac{2\sqrt{d_x d_y}}{d_x + d_y} \\ &\geq \frac{1}{\Delta^2} \sum_{uv \in E(G)} d_u d_v + \sum_{\substack{uv, xy \in E(G), \\ uv \neq xy}} \frac{8\Delta\delta}{(\Delta + \delta)^2} \\ &= \frac{M_2(G)}{\Delta^2} + \frac{4\Delta\delta}{(\Delta + \delta)^2} m(m-1) \\ &= \frac{(\Delta + \delta)^2 M_2(G) + 4\Delta^3 \delta m(m-1)}{\Delta^2(\Delta + \delta)^2}. \end{aligned}$$

In a similar way, we obtain

$$\begin{aligned} (GA_1(G))^2 &= \sum_{uv \in E(G)} \frac{4d_u d_v}{(d_u + d_v)^2} + 2 \sum_{\substack{uv, xy \in E(G), \\ uv \neq xy}} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \frac{2\sqrt{d_x d_y}}{d_x + d_y} \\ &\leq \frac{1}{\delta^2} \sum_{uv \in E(G)} d_u d_v + 2 \sum_{\substack{uv, xy \in E(G), \\ uv \neq xy}} 1 = \frac{M_2(G)}{\delta^2} + m(m-1) \\ &= \frac{M_2(G) + \delta^2 m(m-1)}{\delta^2}. \end{aligned}$$

To conclude the proof we can observe that equality (2) holds for $uv \in E(G)$ if and only if $d_u = \Delta$ and $d_v = \delta$ or $d_u = \delta$ and $d_v = \Delta$. Furthermore, the equalities in (3) hold for every $uv \in E(G)$ if and only if G is regular. ■

We recall that the Randić index is defined as

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

The following result provides a bound on GA_1 involving the Randić index.

Theorem 2.4. *The following statements hold for any graph G .*

- $GA_1(G) \geq 2m - \Delta R(G)$.
- $GA_1(G) \geq 2m - \frac{M_1(G)}{2\delta}$.

Furthermore, the equalities hold if and only if G is a regular graph.

Proof. It is well-known that for all $a, b > 0$,

$$\frac{a}{b} + \frac{b}{a} \geq 2,$$

and the equality holds if and only if $a = b$. Applying this inequality, we obtain

$$\sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}} \geq 2m.$$

Hence,

$$\sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + \sum_{uv \in E(G)} \frac{\Delta}{\sqrt{d_u d_v}} \geq 2m$$

and

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

which implies that $GA_1(G) + \Delta R(G) \geq 2m$ and $GA_1(G) + \frac{M_1(G)}{2\delta} \geq 2m$.

To conclude the proof we only need to observe that the above equalities hold if and only if $2\sqrt{d_u d_v} = d_u + d_v = 2\Delta$ and $2\delta = 2\sqrt{d_u d_v} = d_u + d_v$ for every $uv \in E(G)$. ■

In order to compare the above bounds we consider the following examples. If $G \cong K_{r,s}$ is a complete bipartite graph, where $r < s$, then $\Delta R_1(G) = s\sqrt{rs} < \frac{s(r+s)}{2} = \frac{M_1(G)}{2\delta}$. Now, if $G \cong K_1 + C_n$ is a wheel graph obtained as the join of K_1 and the cycle graph of order $n \geq 4$, then $\Delta R_1(G) = n \left(\frac{n}{3} + \frac{n}{\sqrt{3n}} \right) > \frac{n^2+9n}{6} = \frac{M_1(G)}{2\delta}$.

In 1998 Bollobás and Erdős [2] generalized the Randić index by replacing $1/2$ by any real number. Thus, for $\alpha \in \mathbb{R} \setminus \{0\}$, the *general Randić index* is defined as

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

The general Randić index, also called *variable Zagreb index* in 2004 by Milicević and Nikolić [19], has been extensively studied [16]. Note that $R_{-1/2}$ is the usual Randić index, R_1 is the second Zagreb index M_2 , R_{-1} is the modified Zagreb index [23], etc. In Randić's original paper [24], in addition to the particular case $\alpha = -1/2$, also the index with $\alpha = -1$ was briefly considered.

Next, we will prove some bounds on GA_1 involving the general Randić index. To this end, we need the following additional tool.

Lemma 2.5. [29, Lemma 3] *Let h be the function $h(x, y) = \frac{2xy}{x+y}$ with $\delta \leq x, y \leq \Delta$. Then*

$$\delta \leq h(x, y) \leq \Delta .$$

Furthermore, the lower (respectively, upper) bound is attained if and only if $x = y = \delta$ (respectively, $x = y = \Delta$).

As we will show in Theorems 2.6 and 2.8, bounds on R_α immediately impose bounds on GA_1 .

Theorem 2.6. *Let G be a graph and $\alpha \in \mathbb{R} \setminus \{0\}$. Then the following statements hold.*

(a) *If $\alpha \leq -1/2$, then $\delta^{-2\alpha} R_\alpha(G) \leq GA_1(G) \leq \Delta^{-2\alpha} R_\alpha(G)$.*

(b) *$\alpha \geq -1/2$, then $\delta \Delta^{-2\alpha-1} R_\alpha(G) \leq GA_1(G) \leq \Delta \delta^{-2\alpha-1} R_\alpha(G)$.*

Furthermore, each equality holds if and only if G is a regular graph.

Proof. Lemma 2.5 gives

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

If $\alpha \geq -1/2$, then

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

If $\alpha \leq -1/2$, then

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

We obtain the results by summing up these inequalities for $uv \in E(G)$.

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $GA_1(G)$. If the equality holds in the lower bound, then Lemma 2.5 gives $d_u = d_v = \delta$ 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 upper bound, then Lemma 2.5 gives $d_u = d_v = \Delta$ for every $uv \in E(G)$ and we conclude $d_u = \Delta$ for every $u \in V(G)$. ■

We would emphasize the following direct consequence of Theorem 2.6. The upper bound was previously stated in [25] and the lower bound in [29].

Corollary 2.7. *For any graph G ,*

$$\delta R(G) \leq GA_1(G) \leq \Delta R(G),$$

and each equality holds if and only if G is regular.

Theorem 2.8. *Let G be a graph and $\alpha \in \mathbb{R} \setminus \{0\}$. Then the following statements hold.*

(a) *If $\alpha \leq 1/2$, then $\delta^{-2\alpha+1}\Delta^{-1}R_\alpha(G) \leq GA_1(G) \leq \Delta^{-2\alpha+1}\delta^{-1}R_\alpha(G)$.*

(b) *$\alpha \geq 1/2$, then $\Delta^{-2\alpha}R_\alpha(G) \leq GA_1(G) \leq \delta^{-2\alpha}R_\alpha(G)$.*

Furthermore, each equality holds if and only if G is a regular graph.

Proof. Notice that

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

Now, if $\alpha \leq 1/2$, then $\delta^{-2\alpha+1} \leq (d_u d_v)^{-\alpha+1/2} \leq \Delta^{-2\alpha+1}$, which implies that

$$\delta^{-2\alpha+1}\Delta^{-1}R_\alpha(G) \leq GA_1(G) \leq \Delta^{-2\alpha+1}\delta^{-1}R_\alpha(G).$$

Analogously, if $\alpha \geq 1/2$, then $\Delta^{-2\alpha+1} \leq (d_u d_v)^{-\alpha+1/2} \leq \delta^{-2\alpha+1}$, which implies that

$$\Delta^{-2\alpha}R_\alpha(G) \leq GA_1(G) \leq \delta^{-2\alpha}R_\alpha(G).$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $GA_1(G)$. If a bound is attained, then we have either $d_u d_v = \delta$ or $d_u d_v = \Delta$ for every $uv \in E(G)$, so that G is a regular graph. ■

It is readily seen that if $\alpha < 0$, then Theorem 2.6 gives better results than Theorem 2.8 and, if $\alpha > 0$, then Theorem 2.8 gives better results than Theorem 2.6.

The well-known Pólya-Szegő inequality can be stated as follows.

Lemma 2.9. [15, p.62] *If $0 < n_1 \leq a_j \leq N_1$ and $0 < n_2 \leq b_j \leq N_2$ for $1 \leq j \leq k$, then*

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

Theorems 2.10, 2.11 and 2.12 will show the usefulness of Pólya-Szegő inequality to deduce lower bounds on GA_1 .

Theorem 2.10. *For any graph G ,*

$$\frac{2\Delta\delta^2}{\Delta^2 + \delta^2} \sqrt{mR_{-1}(G)} \leq GA_1(G) \leq \Delta\sqrt{mR_{-1}(G)},$$

and each equality holds if and only if G is a regular graph.

Proof. First of all, Lemma 2.5 gives

$$\delta \leq \frac{2d_u d_v}{d_u + d_v} \leq \Delta. \tag{4}$$

We also have

$$\frac{1}{\Delta} \leq \frac{1}{\sqrt{d_u d_v}} \leq \frac{1}{\delta}. \tag{5}$$

These inequalities and Pólya-Szegő inequality give

$$\begin{aligned} GA_1(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \geq \frac{\left(\sum_{uv \in E(G)} \frac{1}{d_u d_v}\right)^{1/2} \left(\sum_{uv \in E(G)} \frac{(2d_u d_v)^2}{(d_u + d_v)^2}\right)^{1/2}}{\frac{1}{2} \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right)} \\ &\geq \frac{2\Delta\delta}{\Delta^2 + \delta^2} \sqrt{R_{-1}(G)} \left(\sum_{uv \in E(G)} \delta^2\right)^{1/2} = \frac{2\Delta\delta^2}{\Delta^2 + \delta^2} \sqrt{mR_{-1}(G)}. \end{aligned}$$

The upper bound is a direct consequence of Theorem 2.1, as

$$GA_1(G) \leq \frac{\sqrt{nM_1(G)}}{2} \leq \frac{\sqrt{2nm\Delta}}{2} \leq \Delta\sqrt{mR_{-1}(G)}. \tag{6}$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $GA_1(G)$. If the equality holds in the lower bound, then the left hand side equality holds in (4), so that Lemma 2.5 gives $d_u = d_v = \delta$ for every $uv \in E(G)$; hence, $d_u = \delta$ for every $u \in V(G)$ and the graph is regular. Analogously, if the equality holds in the upper bound, then the equalities hold in (6), so that $M_1(G) = 2m\Delta$, which implies that G is a regular graph. ■

Theorem 2.11. *For any graph G ,*

$$\frac{4\Delta^2\delta^2\sqrt{2\delta M_1(G)R_{-1}(G)}}{(\Delta^2 + \delta^2)(\delta + \Delta)^2} \leq GA_1(G) \leq \frac{\sqrt{2\Delta M_1(G)R_{-1}(G)}}{2},$$

and each equality holds if and only if G is a regular graph.

Proof. The upper bound is a direct consequence of Theorem 2.1, as

$$GA_1(G) \leq \frac{\sqrt{nmM_1(G)}}{2} \leq \frac{\sqrt{2\Delta M_1(G)R_{-1}(G)}}{2}. \tag{7}$$

Let us prove the lower bound. Notice that

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} = \frac{4d_u d_v}{(d_u + d_v)^2} \frac{d_u + d_v}{2\sqrt{d_u d_v}}.$$

By Lemma 2.2, we have

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

Since

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

we have

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

Since $\delta \leq \frac{d_u + d_v}{2} \leq \Delta$, $\frac{1}{\Delta} \leq \frac{1}{\sqrt{d_u d_v}} \leq \frac{1}{\delta}$, the Pólya-Szegő inequality gives

$$\begin{aligned} \sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}} &\geq \frac{\left(\sum_{uv \in E(G)} \frac{(d_u + d_v)^2}{4} \right)^{1/2} \left(\sum_{uv \in E(G)} \frac{1}{d_u d_v} \right)^{1/2}}{\frac{1}{2} \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta} \right)} \\ &\geq \frac{\Delta\delta\sqrt{2\delta M_1(G)R_{-1}(G)}}{\Delta^2 + \delta^2}. \end{aligned}$$

Therefore,

$$GA_1(G) \geq \frac{4\delta\Delta}{(\delta + \Delta)^2} \frac{\Delta\delta\sqrt{2\delta M_1(G)R_{-1}(G)}}{\Delta^2 + \delta^2}.$$

If G is a regular graph, then the lower and upper bounds are the same, and they are equal to $GA_1(G)$. If we have the equality in the upper bound, then the equalities hold in (7), so that $R_{-1}(G) = \frac{n}{2\delta}$, which implies that G is a regular graph. Now, if we have the equality in the lower bound, then $d_u + d_v = 2\delta$ for every $uv \in E(G)$, and $d_u = \delta$ for every $u \in V(G)$. ■

Theorem 2.12. *For any graph G and $\alpha > 0$,*

$$k_\alpha \sqrt{R_\alpha(G)R_{-\alpha}(G)} \leq GA_1(G) \leq \sqrt{R_\alpha(G)R_{-\alpha}(G)},$$

with

$$k_\alpha := \begin{cases} \frac{2\Delta^{1/2}\delta^{3/2}}{\Delta^2 + \delta^2}, & \text{if } 0 < \alpha \leq 1, \\ \frac{2\Delta^{\alpha-1/2}\delta^{\alpha+1/2}}{\Delta^{2\alpha} + \delta^{2\alpha}}, & \text{if } \alpha \geq 1, \end{cases}$$

and each inequality holds only if G is a regular graph.

Proof. Cauchy-Schwarz inequality and Lemma 2.2 give

$$\begin{aligned} GA_1(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \leq \left(\sum_{uv \in E(G)} (d_u d_v)^{-\alpha} \right)^{1/2} \left(\sum_{uv \in E(G)} \frac{4d_u d_v (d_u d_v)^\alpha}{(d_u + d_v)^2} \right)^{1/2} \\ &\leq \left(\sum_{uv \in E(G)} (d_u d_v)^{-\alpha} \right)^{1/2} \left(\sum_{uv \in E(G)} (d_u d_v)^\alpha \right)^{1/2} = \sqrt{R_\alpha(G)R_{-\alpha}(G)}. \end{aligned}$$

Lemma 2.5 gives

$$\begin{aligned} \delta^\alpha &\leq \frac{2d_u d_v}{d_u + d_v} (d_u d_v)^{(\alpha-1)/2} \leq \Delta^\alpha, & \text{if } \alpha \geq 1, \\ \delta \Delta^{\alpha-1} &\leq \frac{2d_u d_v}{d_u + d_v} (d_u d_v)^{(\alpha-1)/2} \leq \Delta \delta^{\alpha-1}, & \text{if } 0 < \alpha \leq 1, \end{aligned}$$

If $\alpha \geq 1$, then these inequalities, $\Delta^{-\alpha} \leq (d_u d_v)^{-\alpha/2} \leq \delta^{-\alpha}$ and Lemmas 2.9 and 2.5 give

$$\begin{aligned} GA_1(G) &= \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} \geq \frac{\left(\sum_{uv \in E(G)} (d_u d_v)^{-\alpha} \right)^{1/2} \left(\sum_{uv \in E(G)} \frac{4(d_u d_v)^2}{(d_u + d_v)^2} (d_u d_v)^{\alpha-1} \right)^{1/2}}{\frac{1}{2} \left(\frac{\Delta^\alpha}{\delta^\alpha} + \frac{\delta^\alpha}{\Delta^\alpha} \right)} \\ &= \frac{2\Delta^\alpha \delta^\alpha}{\Delta^{2\alpha} + \delta^{2\alpha}} \sqrt{R_{-\alpha}(G)} \left(\sum_{uv \in E(G)} \frac{2}{d_u + d_v} \frac{2d_u d_v}{d_u + d_v} (d_u d_v)^\alpha \right)^{1/2} \\ &\geq \frac{2\Delta^\alpha \delta^\alpha}{\Delta^{2\alpha} + \delta^{2\alpha}} \sqrt{R_{-\alpha}(G)} \left(\frac{\delta}{\Delta} \sum_{uv \in E(G)} (d_u d_v)^\alpha \right)^{1/2} \\ &= \frac{2\Delta^{\alpha-1/2} \delta^{\alpha+1/2}}{\Delta^{2\alpha} + \delta^{2\alpha}} \sqrt{R_\alpha(G)R_{-\alpha}(G)}. \end{aligned}$$

If $0 < \alpha \leq 1$, then similar computations (using the bounds for $0 < \alpha \leq 1$) give the lower bound.

If the graph is regular, then the two bounds are the same, and they are equal to $GA_1(G)$. If the lower bound is attained, then Lemma 2.5 gives $d_u = d_v = \delta$ for every $uv \in E(G)$ and we conclude $d_u = \delta$ for every $u \in V(G)$. If the upper bound is attained, then Lemma 2.5 gives $d_u = d_v = \Delta$ for every $uv \in E(G)$ and we conclude $d_u = \Delta$ for every $u \in V(G)$. ■

In [29, Theorem 4] appear the inequalities

$$\frac{2\delta^2}{\Delta^2 + \delta^2} \sqrt{M_2(G)R_{-1}(G)} \leq GA_1(G) \leq \sqrt{M_2(G)R_{-1}(G)}.$$

Theorem 2.12 generalizes these bounds. Furthermore, the following consequence of Theorem 2.12 (with $\alpha = 1$) improves the lower bound above.

Corollary 2.13. *We have for any graph G*

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

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

The modified Narumi-Katayama index

$$NK^* = NK^*(G) = \prod_{u \in V(G)} d_u^{d_u} = \prod_{uv \in E(G)} d_u d_v$$

was introduced in [11], inspired in the Narumi-Katayama index defined in [22] (see also [12], [21]). Next, we prove some inequalities relating the modified Narumi-Katayama index with others topological indices.

Theorem 2.14. *We have for any graph G and $\alpha \in \mathbb{R} \setminus \{0\}$*

$$R_\alpha(G) \geq m NK^*(G)^{\alpha/m},$$

and the equality holds if and only if $(d_u d_v)$ has the same value for every $uv \in E(G)$.

Proof. Using the fact that the geometric mean is at most the arithmetic mean, we obtain

$$\frac{1}{m} R_\alpha(G) = \frac{1}{m} \sum_{uv \in E(G)} (d_u d_v)^\alpha \geq \left(\prod_{uv \in E(G)} (d_u d_v)^\alpha \right)^{1/m} = NK^*(G)^{\alpha/m}.$$

The equality holds if and only if $(d_u d_v)$ has the same value for every $uv \in E(G)$. ■

Theorems 2.6 and 2.14 have the following consequence.

Corollary 2.15. *We have for any graph G and $\alpha \in \mathbb{R} \setminus \{0\}$*

$$GA_1(G) \geq \delta^{-2\alpha} m NK^*(G)^{\alpha/m}, \quad \text{if } \alpha \leq -1/2,$$

$$GA_1(G) \geq \delta \Delta^{-2\alpha-1} m NK^*(G)^{\alpha/m}, \quad \text{if } \alpha \geq -1/2,$$

and the equality holds if and only if G is regular.

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