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On the Geometric–Arithmetic Index

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Abstract

The concept of geometric-arithmetic index was introduced in the chemical graph theory recently, but it has shown to be useful. The aim of this paper is to obtain new inequalities involving the geometric-arithmetic index GA_1 and characterize graphs extremal with respect to them. In particular, we improve some known inequalities and we relate GA_1 to other well known topological indices.

1 Introduction

A single number, representing a chemical structure in graph-theoretical terms via the molecular graph, is called a topological descriptor and if it in addition correlates with a molecular property it is called topological index; it is used to understand physicochemical properties of chemical compounds. Topological indices are interesting since they capture some of the properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener [30] in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes.

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches.

Probably, the best know such descriptor is the Randić connectivity index (R) [25]. There are more than thousand papers and a couple of books dealing with this index (see, e.g., [13], [17], [18] 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 [28] as

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

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 [7, p.598] show empirically that the GA_1 index gathers the same information on observed molecules as other $Z_{p,q}$ 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 [7, Table 1]).

Although only about 1000 benzenoid hydrocarbons are known, the number of possible benzenoid hydrocarbons is huge. For instance, the number of possible benzenoid hydrocarbons with 35 benzene rings is 5851000265625801806530 [24]. Therefore, the modeling of their physico-chemical properties is very important in order to predict properties of currently unknown species.

The graphic in [7, Fig.7] (from [7, Table 2], [27]) 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%. Hence, one can think that GA_1 index should be considered in the QSPR/QSAR researches.

The aim of this paper is to obtain new inequalities involving the geometric-arithmetic index GA_1 and characterize graphs extremal with respect to them. In particular, we improve some known inequalities in Theorems 2.4, 3.7 and 3.10, and we relate GA_1 to other well known topological indices in Section 3.

Throughout this paper, $G = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) connected graph with $E(G) \neq \emptyset$. Note that the connectivity of G is not an important restriction, since if G has connected components $G_1, \dots, G_r$, then $GA_1(G) = GA_1(G_1) + \cdots + GA_1(G_r)$; furthermore, every molecular graph is connected.

2 Bounds for Geometric-Arithmetic Index

We start with the following elementary result which allows to compute GA_1 for many graphs. 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.

Proposition 2.1. *Let G be any graph. Then the following statements hold:*

- *G is a regular graph if and only if $GA_1(G) = m$.*
- *If G is a (Δ, δ)-biregular graph, then*

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

- *If C_n is the cycle graph with n vertices, then $GA_1(C_n) = n$.*
- *If K_n is the complete graph with n vertices, then $GA_1(K_n) = \binom{n}{2}$.*
- *If Q_n is the n-cube graph with 2^n vertices, then $GA_1(Q_n) = n2^{n-1}$.*
- *If K_{n_1,n_2} is the complete bipartite graph with n_1, n_2 vertices, then*

$$GA_1(K_{n_1,n_2}) = \frac{2(n_1 n_2)^{3/2}}{n_1 + n_2}.$$

- *If S_n is the star graph with n vertices, then*

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

- *If W_n is the wheel graph with n vertices, then*

$$GA_1(W_n) = n - 1 + \frac{6\sqrt{3}}{n+2}\,(n-1)^{3/2}.$$

- *If P_n is the path graph with n vertices, then*

$$GA_1(P_2) = 1, \qquad GA_1(P_n) = n - 3 + \frac{4\sqrt{2}}{3}\,, \quad \text{if } n \geq 3.$$

- *The double star graph S_{n_1,n_2} is the graph consisting of the union of two star graphs S_{n_1+1} and S_{n_2+1} together with an edge joining their centers. We have*

$$GA_1(S_{n_1,n_2}) = \frac{2n_1\sqrt{n_1+1}}{n_1+2} + \frac{2n_2\sqrt{n_2+1}}{n_2+2} + \frac{2\sqrt{(n_1+1)(n_2+1)}}{n_1+n_2+2}\,.$$

- *If $K_{n_1,\dots,n_k}$ is the complete multipartite graph with $n = n_1 + \cdots + n_k$ vertices, then*

$$GA_1(K_{n_1,\dots,n_k}) = \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} \frac{2n_in_j\sqrt{(n-n_i)(n-n_j)}}{2n-n_i-n_j}\,.$$

We will need the following result.

Lemma 2.2. *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 $t = t_0^{-1}$.*

Proof. The statements follow from

$$f'(t) = \frac{2(1-t^2)}{(1+t^2)^2}\,.$$

■

Corollary 2.3. *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. It suffices to apply Lemma 2.2, since $g(x,y) = f(t)$ with $t = \sqrt{\frac{x}{y}}$, and $\sqrt{\frac{a}{b}} \leq t \leq \sqrt{\frac{b}{a}}$. ■

In [21] and [28] (see also [7, p.609-610]) appear the following inequalities:

$$GA_1(G) \geq \frac{2(n-1)^{3/2}}{n}, \qquad GA_1(G) \geq \frac{2m}{n}. \tag{2.1}$$

Our next result provides a lower bound of $GA_1(G)$ depending just on n and m, improving both inequalities in (2.1).

Theorem 2.4. *We have for any graph G*

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

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

Proof. Recall that $1 \leq d_u \leq n-1$ for every $u \in V(G)$. By Corollary 2.3, taking $a = 1$ and $b = n-1$, we have

$$GA_1(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \geq \sum_{uv \in E(G)} \frac{2\sqrt{(n-1)\cdot 1}}{n-1+1} = \frac{2m\sqrt{n-1}}{n}.$$

By Corollary 2.3, the equality holds for G if and only if every edge joins a vertex of degree 1 with a vertex of degree $n-1$, and this holds if and only if G is a star graph. ∎

In [6] (see also [7, p.609-610]) we find the bounds

$$\frac{2m\sqrt{\Delta\delta}}{\Delta+\delta} \leq GA_1(G) \leq m. \tag{2.2}$$

In the papers [29] and [31] the authors obtain lower bounds of sum-connectivity and harmonic indices, respectively, depending just on n, for every graph with $\delta \geq 2$. The following inequality provides a lower bound of $GA_1(G)$ for every graph G with $\delta \geq k$, for any fixed $k \geq 2$. This result improves the first inequality in (2.1).

Theorem 2.5. *Consider any graph G with $\delta \geq k \geq 2$.*

(1) *If $n \leq 10$, then*

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

(2) *If $n \geq 11$, then*

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

Proof. We have

$$2m = \sum_{v\in V(G)} d_v \geq (n-1)\delta + \Delta\,.$$

We obtain from this inequality and (2.2)

$$GA_1(G) \geq \frac{2m\sqrt{\Delta\delta}}{\Delta+\delta} \geq \big((n-1)\delta+\Delta\big)\frac{\sqrt{\Delta\delta}}{\Delta+\delta} = \sqrt{\delta}\,U(\Delta),$$

where we consider the function

$$U(t) = \big((n-1)\delta + t\big)\frac{\sqrt{t}}{t+\delta} = \frac{t^{3/2}+(n-1)\delta t^{1/2}}{t+\delta}$$

for $t \in [\delta, n-1]$. Since

$$U'(t) = \frac{t^2+(4-n)\delta t+(n-1)\delta^2}{2\sqrt{t}\,(t+\delta)^2}\,,$$

we have $U'(t) = 0$ if and only if

$$t = t_{\pm} = \frac{\delta}{2}\left(n-4 \pm \sqrt{(n-2)(n-10)}\,\right).$$

Hence, if $n \leq 10$ then $U'(t) \geq 0$ for every t, and we conclude $U(t) \geq U(\delta)$ for every $t \in [\delta, n-1]$. Therefore,

$$GA_1(G) \geq \sqrt{\delta}\,U(\Delta) \geq \sqrt{\delta}\,U(\delta) = \frac{n\delta}{2} \geq \frac{nk}{2}\,.$$

Assume now that $n \geq 11$, then $t_-, t_+ \in \mathbb{R}$ and $t_- < t_+$. Since $\sqrt{(n-2)(n-10)} < n-6$, we have

$$\delta = \frac{\delta}{2}\big(n-4-(n-6)\big) < \frac{\delta}{2}\left(n-4-\sqrt{(n-2)(n-10)}\,\right) = t_-.$$

Furthermore, since $n \geq 11$ and $\delta \geq 2$, $\sqrt{(n-2)(n-10)} \geq 3$ and

$$n-1 \leq \frac{\delta}{2}\big(n-4+3\big) \leq \frac{\delta}{2}\left(n-4+\sqrt{(n-2)(n-10)}\,\right) = t_+.$$

We have two possibilities:

(i) If $t_- < n-1$, then $\delta < t_- < n-1 \leq t_+$, U increases on $[\delta, t_-]$ and decreases on $[t_-, n-1]$, and $U(t) \geq \min\big\{U(\delta), U(n-1)\big\}$ for every $t \in [\delta, n-1]$.

(ii) If $n-1 \leq t_-$, then $\delta \leq n-1 \leq t_-$, U increases on $[\delta, n-1]$, and $U(t) \geq U(\delta) = \min\big\{U(\delta), U(n-1)\big\}$ for every $t \in [\delta, n-1]$.

Hence, in both cases

$$GA_1(G) \geq \sqrt{\delta}\, U(\Delta) \geq \sqrt{\delta}\, \min\big\{U(\delta), U(n-1)\big\} = \min\left\{ \frac{n\delta}{2}\,, \frac{(\delta+1)\sqrt{\delta}\,(n-1)^{3/2}}{n-1+\delta} \right\}$$

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

■

Remark 2.6. *One can check that if $k = 2$, then*

$$\min\left\{ n, \frac{3\sqrt{2}\,(n-1)^{3/2}}{n+1} \right\} = \begin{cases} n, & \text{if } n = 11, \\ \frac{3\sqrt{2}\,(n-1)^{3/2}}{n+1}, & \text{if } n \geq 12, \end{cases}$$

and that if $k = 3$, then

$$\min\left\{ \frac{3n}{2}\,, \frac{4\sqrt{3}\,(n-1)^{3/2}}{n+2} \right\} = \begin{cases} \frac{3n}{2}, & \text{if } n = 11, 12, \\ \frac{4\sqrt{3}\,(n-1)^{3/2}}{n+2}, & \text{if } n \geq 13. \end{cases}$$

The study of Gromov hyperbolic graphs is a subject of increasing interest, both in pure and applied mathematics (see, e.g., [1], [2], [3], [4], [20] and the references cited therein). We say that a graph is *t-hyperbolic* ($t \geq 0$) if any side of every geodesic triangle is contained in the t-neighborhood of the union of the other two sides. We define the *hyperbolicity constant* $\delta(G)$ of a graph G as the infimum of the constants $t \geq 0$ such that G is t-hyperbolic. We consider that every edge has length 1.

The following inequality relates the geometric-arithmetic index with the hyperbolicity constant $\delta(G)$.

Theorem 2.7. *We have for any graph G that is not a tree*

$$GA_1(G) \geq \frac{2(4\delta(G)-1)^{3/2}}{4\delta(G)}.$$

Proof. It is well known that if G is not a tree then $\delta(G) > 0$. We have that $\delta(G)$ is always an integer multiple of $\frac{1}{4}$ by [1, Theorem 2.6] and that $\delta(G) \notin \{\frac{1}{4}, \frac{1}{2}\}$ by [20, Theorem 11], since G has not loops or multiple edges. Hence, $\delta(G) \geq \frac{3}{4}$.

The function $f(x) = \frac{2(x-1)^{3/2}}{x}$ is increasing in $[1, \infty)$, since

$$f'(x) = \frac{(x-1)^{1/2}}{x^2}\big(x+2\big) > 0$$

for every $x \in (1, \infty)$. We know by (2.1) that

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

Since $\delta(G) \le \frac{n}{4}$ by [20, Theorem 30], we have $n \ge 4\delta(G) \ge 3$ and

$$GA_1(G) \ge \frac{2(n-1)^{3/2}}{n} \ge \frac{2(4\delta(G)-1)^{3/2}}{4\delta(G)} .$$

■

One can think that perhaps it is possible to obtain an upper bound of $GA_1(G)$ in terms of $\delta(G)$, i.e., the inequality

$$GA_1(G) \le \Psi\big(\delta(G)\big),$$

for every graph G and some function Ψ. However, this is not possible, as the following example shows. For each integer $d \ge 3$ consider two copies A_d and B_d of the path graph with (ordered) vertices $a_1, \dots, a_d$ and $b_1, \dots, b_d$, respectively. Let G_d be the graph obtained from A_d and B_d by connecting with an edge the vertices a_i and b_i for every $i \in \{1, \dots, d\}$. One can check that $\delta(G) = \frac{3}{2}$ for every $d \ge 3$. However, $\lim_{d\to\infty} GA_1(G_d) = \infty$.

3 Relations between GA_1 and other well known topological indices

In order to obtain relations between GA_1 and other well known topological indices we need the following classical result, which provides a converse of Cauchy-Schwarz inequality (see [15, p.62]).

Lemma 3.1. *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*

$$\left(\sum_{j=1}^{k} a_j^2\right)^{1/2} \left(\sum_{j=1}^{k} b_j^2\right)^{1/2} \le \frac{1}{2}\left(\sqrt{\frac{N_1N_2}{n_1n_2}} + \sqrt{\frac{n_1n_2}{N_1N_2}}\right)\left(\sum_{j=1}^{k} a_jb_j\right).$$

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 [14] as

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

These indices have attracted growing interest, see e.g., [5], [14], [19] (in particular, they are included in a number of programs used for the routine computation of topological indices).

In [8] (see also [7, p.611]) we find the bound

$$GA_1(G) \le \frac{\sqrt{mM_2(G)}}{\delta} \,. \tag{3.3}$$

The following result gives a lower bound for GA_1 similar to (3.3).

Proposition 3.2. *We have for any graph G*

$$GA_1(G) \ge \frac{2\delta\sqrt{mM_2(G)}}{\Delta^2+\delta^2} \,,$$

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

Proof. Since

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

Lemma 3.1 gives

$$GA_1(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \ge \frac{\Big(\sum_{uv\in E(G)} d_u d_v\Big)^{1/2}\Big(\sum_{uv\in E(G)} \frac{4}{(d_u+d_v)^2}\Big)^{1/2}}{\frac{1}{2}\Big(\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\Big)}$$
$$\ge \frac{2\Delta\delta\big(M_2(G)\big)^{1/2}\Big(\sum_{uv\in E(G)} \frac{1}{\Delta^2}\Big)^{1/2}}{\Delta^2+\delta^2} \ge \frac{2\delta\sqrt{mM_2(G)}}{\Delta^2+\delta^2} \,.$$

If the graph is regular (i.e., $\delta = \Delta$), then the lower and upper bound are the same, and they are equal to $GA_1(G)$. If we have the equality, 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. ∎

We will use the following particular case of Jensen's inequality.

Lemma 3.3. *If f is a convex function in* $\mathbb{R}_+$ *and* $x_1,\dots,x_m > 0$, *then*

$$f\Big(\frac{x_1+\cdots+x_m}{m}\Big) \le \frac{1}{m}\big(f(x_1)+\cdots+f(x_m)\big).$$

As we have said, we will denote by $R(G)$ the Randić index of the graph G, defined in [25] as

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

We recall that probably R is the best know topological index (see, e.g., [13], [17], [18], [26] and the references cited therein). The following result provides lower and upper bounds of GA_1 involving the Randić index.

Theorem 3.4. *We have for any graph G*

$$\frac{m^2}{\Delta R(G)} \leq GA_1(G) \leq \Delta R(G),$$

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

Proof. Since $f(x) = 1/x$ is a convex function in $\mathbb{R}_+$, Lemma 3.3 gives

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

If the equality holds, then $\frac{1}{2}(d_u + d_v) = \Delta$ for every $uv \in E(G)$ and we conclude $d_u = \Delta$ for every $u \in V(G)$.

In order to prove the upper bound note that

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

If the equality holds, then $\frac{1}{2}(d_u + d_v) = \Delta$ for every $uv \in E(G)$ and we conclude $d_u = \Delta$ for every $u \in V(G)$.

Reciprocally, if G is regular, then $R(G) = \frac{m}{\Delta}$. Hence, the lower and upper bound are the same, and they are equal to $m = GA_1(G)$. ■

Remark 3.5. *If we replace the function $f(x) = 1/x$ by the convex function $f(x) = x^2$ in the proof of Theorem 3.4, we obtain the known inequality* (3.3).

We will need also the following lemma.

Lemma 3.6. *We have for any graph G*

$$\sum_{uv\in E(G)} \frac{1}{d_u + d_v} \geq \frac{m^2}{M_1(G)}.$$

Furthermore, the equality is attained if only if G is regular or biregular.

Proof. Note that in the sum $\sum_{uv\in E(G)}(d_u + d_v)$ each term d_u appears exactly d_u times, since u is the endpoint of precisely d_u edges. Hence,

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

and Cauchy-Schwarz inequality gives

$$m^2 = \left(\sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \sqrt{d_u + d_v} \right)^2 \le \left(\sum_{uv \in E(G)} \frac{1}{d_u + d_v} \right) \left(\sum_{uv \in E(G)} (d_u + d_v) \right)$$
$$= M_1(G) \left(\sum_{uv \in E(G)} \frac{1}{d_u + d_v} \right).$$

Furthermore, by Cauchy-Schwarz inequality, the inequality is attained if only if there exists a constant μ such that, for every $uv \in E(G)$,

$$\frac{1}{\sqrt{d_u + d_v}} = \mu \sqrt{d_u + d_v}\,, \qquad d_u + d_v = \mu^{-1}. \tag{3.4}$$

If $uv, uw \in E(G)$, then

$$\mu^{-1} = d_u + d_v = d_u + d_w\,, \qquad d_w = d_v,$$

and we conclude that (3.4) is equivalent to the following: for each vertex $u \in V(G)$, every neighbor of u has the same degree. Since G is connected, this holds if and only if G is regular or biregular. ■

In [21] (see also [7, p.610]) appears the inequality

$$GA_1(G) \le \frac{1}{2} M_1(G). \tag{3.5}$$

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

Theorem 3.7. *We have for any graph G*

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

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

Proof. First of all we have

$$GA_1(G) \le m = \frac{1}{2} \sum_{u \in V(G)} d_u \le \frac{1}{2} \sum_{u \in V(G)} \frac{d_u^2}{\delta} = \frac{1}{2\delta} M_1(G).$$

If we have the equality, then $GA_1(G) = m$ and G is regular. If the graph is regular, then $M_1(G) = n\delta^2 = 2m\delta$, $GA_1(G) = m$ and the equality holds.

Lemma 3.6 gives

$$GA_1(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \geq 2\delta \sum_{uv\in E(G)} \frac{1}{d_u + d_v} \geq \frac{2\delta m^2}{M_1(G)} .$$

If the equality holds, 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 G is regular, then $M_1(G) = n\delta^2 = 2m\delta$, $GA_1(G) = m$ and the equality holds. ■

The following result gives a lower bound for GA_1 involving the Zagreb indices M_1 and M_2.

Theorem 3.8. *We have for any graph G*

$$GA_1(G) \geq \frac{2\delta m}{\Delta^2 + \delta^2} \sqrt{\frac{2\Delta M_2(G)}{M_1(G)}} ,$$

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

Proof. Since

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

Lemmas 3.1 and 3.6 give

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

$$\geq \frac{2\Delta\delta\big(M_2(G)\big)^{1/2}\Big(\frac{2}{\Delta}\sum_{uv\in E(G)} \frac{1}{d_u+d_v}\Big)^{1/2}}{\Delta^2 + \delta^2} \geq \frac{2\delta m}{\Delta^2 + \delta^2}\sqrt{\frac{2\Delta M_2(G)}{M_1(G)}} .$$

If the equality holds, then $\frac{1}{2}(d_u + d_v) = \Delta$ for every $uv \in E(G)$; hence, $d_u = \Delta$ for every $u \in V(G)$. If G is regular, then $M_1(G) = n\Delta^2 = 2m\Delta$, $M_2(G) = m\Delta^2$, $GA_1(G) = m$ and we have the equality. ■

We deal now with two additional topological descriptors, called *harmonic* and *sum-connectivity* index, defined respectively as

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

These indices have attracted a great interest in the lasts years (see, e.g., [9], [10], [16], [29], [31], [32], [33] and [34]). Next, we relate them with the geometric-arithmetic index.

Proposition 3.9. *We have for any graph G*

$$\delta H(G) \le GA_1(G) \le \Delta H(G),$$

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

Proof. We have

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

for every $uv \in E(G)$. Hence, we obtain the inequalities by summing in $uv \in E(G)$.

The equality in the first (respectively, second) inequality is attained if and only if $\sqrt{d_u d_v} = \delta$ for every $uv \in E(G)$, i.e., $d_u = \delta$ (respectively, $d_u = \Delta$) for every $u \in V(G)$. Reciprocally, if G is regular, then both bounds have the same value, and they are equal to $GA_1(G)$. ■

Next, we obtain inequalities relating the geometric-arithmetic index with the second Zagreb index. Note that, since $n\delta \le 2m$ by the handshaking lemma, the upper bound improves the known inequality (3.3).

Theorem 3.10. *We have for any graph G*

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

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

Proof. Since

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

Lemma 3.1 gives

$$\begin{aligned} GA_1(G) = \sum_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u+d_v)} &\ge \frac{\left(\sum_{uv\in E(G)} \frac{4d_u d_v}{(d_u+d_v)^2}\right)^{1/2} \left(\sum_{uv\in E(G)} 1\right)^{1/2}}{\frac{1}{2}\left(\sqrt{\frac{\Delta}{\delta}}+\sqrt{\frac{\delta}{\Delta}}\right)} \\ &\ge \frac{2\sqrt{\Delta\delta m}}{\Delta+\delta}\left(\sum_{uv\in E(G)} \frac{1}{\Delta^2}\, d_u d_v\right)^{1/2} = \frac{2}{\Delta+\delta}\sqrt{\frac{\delta m M_2(G)}{\Delta}}\,. \end{aligned}$$

In order to prove the upper bound, fix any function h. Note that in the sum $\sum_{uv\in E(G)} \big(h(d_u)+h(d_v)\big)$ each term $h(d_u)$ appears exactly d_u times, since u is the endpoint of precisely d_u edges. Hence,

$$\sum_{uv\in E(G)} \big(h(d_u)+h(d_v)\big) = \sum_{u\in V(G)} d_u h(d_u), \qquad \sum_{uv\in E(G)} \left(\frac{1}{d_u}+\frac{1}{d_v}\right) = \sum_{u\in V(G)} d_u \frac{1}{d_u} = n.$$

Therefore, Lemma 3.3 with $f(x) = x^{-1}$ gives

$$\sum_{uv\in E(G)} \frac{2}{d_u + d_v} \le \sum_{uv\in E(G)} \frac{1}{2}\Big(\frac{1}{d_u} + \frac{1}{d_v}\Big) = \frac{n}{2}\,.$$

Cauchy-Schwarz inequality gives

$$\begin{aligned} GA_1(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} &\le \left(\sum_{uv\in E(G)} d_u d_v\right)^{1/2} \left(\sum_{uv\in E(G)} \frac{4}{(d_u+d_v)^2}\right)^{1/2} \\ &\le (M_2(G))^{1/2} \left(\frac{1}{\delta} \sum_{uv\in E(G)} \frac{2}{d_u + d_v}\right)^{1/2} \le \sqrt{\frac{nM_2(G)}{2\delta}}\,. \end{aligned}$$

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 $4(d_u + d_v)^{-2} = \Delta^{-2}$ 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 $u \in V(G)$. ■

Theorem 3.11. *We have for any graph G*

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

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 3.3 gives

$$\begin{aligned} \frac{2\delta S(G)^2}{m^2} &= \left(\frac{\sqrt{2\delta}}{m} \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}\right)^2 \le \left(\frac{1}{m} \sum_{uv\in E(G)} \left(\frac{2\sqrt{d_u d_v}}{d_u + d_v}\right)^{1/2}\right)^2 \\ &\le \frac{1}{m} \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} = \frac{1}{m}\, GA_1(G). \end{aligned}$$

If the equality holds, then $\sqrt{d_u d_v} = \delta$ for every $uv \in E(G)$ and we conclude $d_u = \delta$ for every $u \in V(G)$.

In order to prove the upper bound note that

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

$$\begin{aligned} GA_1(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} &= \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{\sqrt{d_u + d_v}} \frac{1}{\sqrt{d_u + d_v}} \\ &\le \sum_{uv\in E(G)} \sqrt{2\Delta}\, \frac{1}{\sqrt{d_u + d_v}} = \sqrt{2\Delta}\, S(G). \end{aligned}$$

If the equality holds, then $d_u + d_v = 2\Delta$ for every $uv \in E(G)$ and we conclude $d_u = \Delta$ for every $u \in V(G)$.

Reciprocally, if G is regular, then $S(G) = \frac{m}{\sqrt{2\Delta}}$. Hence, the lower and upper bound are the same, and they are equal to $m = GA_1(G)$. ■

Theorem 3.12. *We have for any graph G*

$$GA_1(G) \geq \frac{2S(G)^2}{R(G)}\,,$$

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

Proof. Using the Cauchy-Schwarz inequality, we obtain

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

Hence, the equality is attained if and only if there exists a constant c such that for every $uv \in E(G)$

$$\sqrt{\frac{2\sqrt{d_u d_v}}{d_u+d_v}} = c\,\frac{1}{(d_u d_v)^{1/4}}\,, \qquad 2d_u d_v = c^2(d_u+d_v), \qquad \frac{2}{c^2} = \frac{1}{d_u} + \frac{1}{d_v}\,. \tag{3.6}$$

If $uv, uw \in E(G)$, then

$$\frac{2}{c^2} = \frac{1}{d_u} + \frac{1}{d_v} = \frac{1}{d_u} + \frac{1}{d_w}\,, \qquad d_w = d_v,$$

and we conclude that (3.6) is equivalent to the following: for each vertex $u \in V(G)$, every neighbor of u has the same degree. Since G is connected, this holds if and only if G is regular or biregular. ■

The *modified Narumi-Katayama index*

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

is introduced in [11], inspired in the Narumi-Katayama index defined in [23] (see also [12], [22]). Next, we prove an inequality relating the modified Narumi-Katayama index with the geometric-arithmetic index.

Theorem 3.13. *We have for any graph G*

$$GA_1(G) \geq \frac{m}{\Delta} NK^*(G)^{1/(2m)},$$

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

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

$$\begin{aligned}\frac{1}{m} GA_1(G) &= \frac{1}{m} \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \geq \left(\prod_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right)^{1/m} \\ &\geq \left(\frac{1}{\Delta^m} \prod_{uv \in E(G)} \sqrt{d_u d_v} \right)^{1/m} = \frac{1}{\Delta} NK^*(G)^{1/(2m)}.\end{aligned}$$

If the equality holds, then $\frac{1}{2}(d_u + d_v) = \Delta$ for every $uv \in E(G)$; hence, $d_u = \Delta$ for every $u \in V(G)$ and the graph is regular. If the graph is regular, then $NK^*(G) = \Delta^{2m}$ and the equality holds. ∎

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