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Bounds on the Arithmetic-Geometric Index

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Abstract: The concept of arithmetic-geometric index was recently introduced in chemical graph theory, but it has proven to be useful from both a theoretical and practical point of view. The aim of this paper is to obtain new bounds of the arithmetic-geometric index and characterize the extremal graphs with respect to them. Several bounds are based on other indices, such as the second variable Zagreb index or the general atom-bond connectivity index), and some of them involve some parameters, such as the number of edges, the maximum degree, or the minimum degree of the graph. In most bounds, the graphs for which equality is attained are regular or biregular, or star graphs.

Keywords: arithmetic-geometric index; variable Zagreb index; general atom-bond connectivity index; symmetric division deg index; vertex-degree-based topological index

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1. Introduction

In chemical graph theory, a topological descriptor is a function that associates each molecular graph with a real value. If it correlates well with some chemical property, then it is called a topological index. Since Winer's work (see [1]), numerous topological indices have been defined and discussed, the growing interest in their study is because there are several applications in theoretical chemistry, especially in QSPR/QSAR research (see [2–4]).

In particular, vertex-degree-based topological indices belong to one of the largest and most studied classes of topological descriptors. The Randić index [5] and the Zagreb indices [6] are probably the best known such descriptors.

In [7–9], the *first and second variable Zagreb indices* are defined, for each $\alpha \in \mathbb{R}$, as

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

where d_u denotes the degree of $u \in V(G)$.

Note that, for $\alpha = 2$, $\alpha = -1$ and $\alpha = 3$, the index M_1^α is the first Zagreb index M_1, the inverse index ID, and the forgotten index F, respectively; also, for $\alpha = 1$, $\alpha = -1/2$ and $\alpha = -1$, the index M_2^α is the second Zagreb index M_2, the Randić index R and the modified Zagreb index.

The *geometric-arithmetic index* GA is defined in [10] as

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

There are many papers studying the mathematical and computational properties of the GA index (see [10–17]).

In 2015, the *arithmetic-geometric index* [18] was defined as

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

The AG index of path graphs with pendant vertices attached was discussed in the papers [18,19]. Additionally, the arithmetic-geometric index of graphene, which is the most conductive and effective material for electromagnetic interference shielding, was computed in [20]. The paper [21] studied the spectrum and energy of arithmetic-geometric matrix, in which the sum of all elements is equal to $2AG$. Other bounds of the arithmetic-geometric energy appeared in [22,23]. The paper [24] studies extremal AG-graphs for various classes of simple graphs, and it includes inequalities that involve $AG + GA$, $AG - GA$, $AG \cdot GA$, and AG/GA. In [25–28], there are more bounds on the AG index and a discussion on the effect of deleting an edge from a graph on the arithmetic-geometric index.

Along the paper, we denote, by G, a simple graph without isolated vertices.

An important subject in the study of topological indices is to bind them in terms of some parameters. Reference [29] proves that many upper bounds of GA are not useful, and it shows the importance of obtaining upper bounds of GA less than the number of edges m. In a similar way, it is important to find lower bounds of AG that are greater than m. With this aim, in this paper we obtain several new lower bounds of AG, which are greater than m, and we characterize the extremal graphs.

2. Bounds Involving Other Indices

A graph is said *biregular* if it is bipartite and the degree of any vertex in one side of the bipartition is the maximum degree Δ and the degree of any vertex in the other side is the minimum degree δ.

One can check that the following result holds.

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

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

The equality in the upper bound is attained if and only if either $x = a$ and $y = b$, or $x = b$ and $y = a$, and the equality in the lower bound is attained if and only if $x = y$.

The following inequalities follow from Lemma 1:

$$m \le AG(G) \le \frac{\Delta + \delta}{2\sqrt{\Delta\delta}}\, m. \tag{1}$$

The lower bound in (1) also follows from the inequalities $GA(G) \cdot AG(G) \ge m^2$ and $GA(G) \le m$, see [11,12]. The upper bound in (1) appears in [27].

The following result improves the lower bound in (1), see Remark 1.

Theorem 1. *If G is a graph with m edges, maximum degree Δ, and minimum degree δ, then*

$$m + \frac{M_1(G) - 2M_2^{1/2}(G)}{2\Delta} \le AG(G) \le m + \frac{M_1(G) - 2M_2^{1/2}(G)}{2\delta}.$$

The equality in each bound is attained if and only if G is a regular graph.

Proof. We have

$$\frac{d_u + d_v}{2\sqrt{d_u d_v}} = 1 + \frac{\left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2}{2\sqrt{d_u d_v}},$$

$$AG(G) = m + \sum_{uv \in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2}{2\sqrt{d_u d_v}}.$$

Because

$$\begin{aligned}\sum_{uv \in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2}{2\sqrt{d_u d_v}} &\geq \frac{1}{2\Delta} \sum_{uv \in E(G)} \left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2 \\ &= \frac{1}{2\Delta}\Big(\sum_{uv \in E(G)} (d_u + d_v) - 2 \sum_{uv \in E(G)} \sqrt{d_u d_v} \Big) \\ &= \frac{M_1(G) - 2M_2^{1/2}(G)}{2\Delta},\end{aligned}$$

we conclude

$$AG(G) \geq m + \frac{M_1(G) - 2M_2^{1/2}(G)}{2\Delta}.$$

Because

$$\begin{aligned}\sum_{uv \in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2}{2\sqrt{d_u d_v}} &\leq \frac{1}{2\delta} \sum_{uv \in E(G)} \left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2 \\ &= \frac{1}{2\delta}\Big(\sum_{uv \in E(G)} (d_u + d_v) - 2 \sum_{uv \in E(G)} \sqrt{d_u d_v} \Big) \\ &= \frac{M_1(G) - 2M_2^{1/2}(G)}{2\delta},\end{aligned}$$

we conclude

$$AG(G) \leq m + \frac{M_1(G) - 2M_2^{1/2}(G)}{2\delta}.$$

If G is regular, then both bounds are the same, and they are equal to $AG(G)$.

If the equality in some bound is attained, then we have either $d_u d_v = \Delta^2$ for every $uv \in E(G)$ or $d_u d_v = \delta^2$ for every $uv \in E(G)$, so $d_u = \Delta$ for every $u \in V(G)$ or $d_u = \delta$ for every $u \in V(G)$, and G is a regular graph. □

Remark 1. *Because Cauchy–Schwarz inequality gives*

$$\begin{aligned}M_1(G) - 2M_2^{1/2}(G) &= \sum_{uv \in E(G)} \left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2 \\ &= \sum_{uv \in E(G)} \left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2 \frac{1}{m} \sum_{uv \in E(G)} 1^2 \\ &\geq \frac{1}{m}\Big(\sum_{uv \in E(G)} \left|\sqrt{d_u} - \sqrt{d_v}\,\right| \Big)^2,\end{aligned}$$

we have $M_1(G) - 2M_2^{1/2}(G) \geq 0$ and, so, Theorem 1 improves the lower bound in (1).

The *misbalance rodeg index* [30] is

$$MR(G) = \sum_{uv \in E(G)} \left|\sqrt{d_u} - \sqrt{d_v}\,\right|.$$

Theorem 1 and Remark 1 have the following consequence.

Corollary 1. *If G is a graph with m edges, maximum degree* Δ*, and minimum degree* δ*, then*

$$m+\frac{MR(G)^2}{2\Delta m}\leq AG(G),$$

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

The following fact is elementary.

Lemma 2. *Let us consider the function* $f(x,y)=(xy)^{\alpha}$ *with* $\delta\leq x,y\leq\Delta$*. Then*

$$f(x,y)\leq\delta^{2\alpha},\quad \text{if } \alpha\leq 0,$$
$$f(x,y)\leq\Delta^{2\alpha},\quad \text{if } \alpha\geq 0.$$

The following result provides bounds that relate the arithmetic-geometric and the second variable Zagreb indices.

Theorem 2. *If G is a graph with maximum degree* Δ *and minimum degree* δ*, and* $\alpha\in\mathbb{R}$*, then*

$$AG(G)\leq\Delta\delta^{2\alpha-1}M_2^{-\alpha}(G),\qquad \text{if } \alpha\leq 1/2,$$
$$AG(G)\leq\Delta^{2\alpha}M_2^{-\alpha}(G),\qquad \text{if } \alpha\geq 1/2,$$

and the equality in each bound is attained for some fixed α *if and only if G is regular.*

Proof. We have

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

If $\alpha\leq 1/2$, then Lemma 2 gives

$$AG(G)\leq\Delta\delta^{2\alpha-1}\sum_{uv\in E(G)}(d_ud_v)^{-\alpha}.$$

If $\alpha\geq 1/2$, then we have, by Lemma 2

$$AG(G)\leq\Delta^{2\alpha}\sum_{uv\in E(G)}(d_ud_v)^{-\alpha}.$$

If G is regular, then $AG(G)=m$, $M_2^{-\alpha}(G)=\delta^{-2\alpha}m=\Delta^{-2\alpha}m$ and $\Delta\delta^{2\alpha-1}=\Delta^{2\alpha}$, and the equality in each bound is attained.

If the equality is attained, then $d_u+d_v=2\Delta$ for every $uv\in E(G)$; thus, $d_u=\Delta$ for every $u\in V(G)$, and G is a regular graph. □

The *symmetric division deg index*

$$SDD(G)=\sum_{uv\in E(G)}\frac{d_u^2+d_v^2}{d_ud_v}=\sum_{uv\in E(G)}\left(\frac{d_u}{d_v}+\frac{d_v}{d_u}\right).$$

is another Adriatic index that appears in [30,31], see also [32].

We need the following inequality (see e.g., [14], Lemma 4) in the proof of Theorem 3 below.

Lemma 3. *Let* (X,μ) *be a measure space and* $f,g:X\to\mathbb{R}$ *measurable functions. If there exist positive constants* ω,Ω *with* $\omega|g|\leq|f|\leq\Omega|g|$ μ*-a.e., then*

$$\|f\|_2\|g\|_2\leq\frac{1}{2}\left(\sqrt{\frac{\Omega}{\omega}}+\sqrt{\frac{\omega}{\Omega}}\right)\|fg\|_1. \tag{2}$$

If these norms are finite, the equality in the bound is attained if and only if $\omega = \Omega$ and $|f| = \omega|g|$ μ-a.e. or $f = g = 0$ μ-a.e.

We have the following direct consequence.

Corollary 2. *If $a_j, b_j \geq 0$ and $\omega b_j \leq a_j \leq \Omega b_j$ for $1 \leq j \leq m$, then*

$$\Big(\sum_{j=1}^{m} a_j^2\Big)^{1/2}\Big(\sum_{j=1}^{m} b_j^2\Big)^{1/2} \leq \frac{1}{2}\left(\sqrt{\frac{\Omega}{\omega}} + \sqrt{\frac{\omega}{\Omega}}\right)\sum_{j=1}^{m} a_j b_j.$$

If $a_j > 0$ for some $1 \leq j \leq m$, then the equality holds if and only if $\omega = \Omega$ and $a_j = \omega b_j$ for every $1 \leq j \leq m$.

The following result provides an inequality relating the arithmetic-geometric and the symmetric division deg indices.

Theorem 3. *Let G be a graph with m edges, maximum degree Δ, and minimum degree δ. Subsequently,*

$$\frac{\sqrt{2\sqrt{\Delta\delta}\,(\Delta+\delta)}}{\big(\sqrt{\Delta}+\sqrt{\delta}\,\big)^2}\sqrt{m\big(SDD(G)+2m\big)} \leq AG(G) \leq \frac{1}{2}\sqrt{m\big(SDD(G)+2m\big)}\,.$$

The equality in the lower bound is attained if and only if G is a regular graph. The equality in the upper bound is attained if G is a regular or biregular graph.

Proof. Let us consider

$$a_j := \frac{d_u + d_v}{2\sqrt{d_u d_v}}, \qquad b_j := 1.$$

We have, by Corollary 1,

$$1 \leq \frac{a_j}{b_j} \leq \frac{\Delta+\delta}{2\sqrt{\Delta\delta}}\,.$$

Thus, Corollary 2 gives

$$\begin{aligned}\Big(\sum_{uv\in E(G)} 1\Big)\Big(\sum_{uv\in E(G)} \frac{(d_u+d_v)^2}{4d_u d_v}\Big) &\leq \frac{1}{4}\left(\sqrt{\frac{\Delta+\delta}{2\sqrt{\Delta\delta}}} + \sqrt{\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}}\right)^2\Big(\sum_{uv\in E(G)} \frac{d_u+d_v}{2\sqrt{d_u d_v}}\Big)^2 \\ &= \frac{1}{4}\left(\frac{\big(\sqrt{\Delta}+\sqrt{\delta}\,\big)^2}{\sqrt{2\sqrt{\Delta\delta}\,(\Delta+\delta)}}\right)^2 AG(G)^2.\end{aligned}$$

Because

$$\begin{aligned}\sum_{uv\in E(G)} 1 = m, \qquad \sum_{uv\in E(G)} \frac{(d_u+d_v)^2}{4d_u d_v} &= \frac{1}{4}\sum_{uv\in E(G)} \frac{d_u^2+d_v^2}{d_u d_v} + \sum_{uv\in E(G)} \frac{1}{2} \\ &= \frac{1}{4}\,SDD(G) + \frac{1}{2}\,m,\end{aligned}$$

we conclude

$$\frac{m}{4}\big(SDD(G)+2m\big) \le \frac{1}{4}\left(\frac{(\sqrt{\Delta}+\sqrt{\delta}\,)^2}{\sqrt{2\sqrt{\Delta\delta}\,(\Delta+\delta)}}\right)^2 AG(G)^2,$$

$$AG(G) \ge \frac{\sqrt{2\sqrt{\Delta\delta}\,(\Delta+\delta)}}{(\sqrt{\Delta}+\sqrt{\delta}\,)^2}\sqrt{m\big(SDD(G)+2m\big)}\,.$$

If the equality in this bound is attained, then Corollary 2 gives

$$1 = \frac{\Delta+\delta}{2\sqrt{\Delta\delta}}\,.$$

Thus, Corollary 1 gives $\Delta=\delta$, and, so, G is regular.
If G is regular, then

$$\frac{\sqrt{2\sqrt{\Delta\delta}\,(\Delta+\delta)}}{(\sqrt{\Delta}+\sqrt{\delta}\,)^2}\sqrt{m\big(SDD(G)+2m\big)} = \frac{\sqrt{2\delta\,2\delta}}{4\delta}\sqrt{m\big(2m+2m\big)} = m = AG(G).$$

On the other hand, the Cauchy–Schwarz inequality gives

$$AG(G)^2 = \Big(\sum_{uv\in E(G)}\frac{d_u+d_v}{2\sqrt{d_ud_v}}\Big)^2 \le \Big(\sum_{uv\in E(G)}1\Big)\Big(\sum_{uv\in E(G)}\frac{(d_u+d_v)^2}{4d_ud_v}\Big).$$

Because

$$\sum_{uv\in E(G)}1 = m, \qquad \sum_{uv\in E(G)}\frac{(d_u+d_v)^2}{4d_ud_v} = \frac{1}{4}\,SDD(G)+\frac{1}{2}\,m,$$

we conclude

$$AG(G)^2 \le \frac{m}{4}\big(SDD(G)+2m\big).$$

If G is regular or biregular, then

$$\frac{1}{2}\sqrt{m\big(SDD(G)+2m\big)} = \frac{1}{2}\sqrt{m\Big(\Big(\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\Big)m+2m\Big)}$$
$$= \frac{m}{2}\sqrt{\frac{\Delta^2+\delta^2+2\Delta\delta}{\Delta\delta}} = \frac{\Delta+\delta}{2\sqrt{\Delta\delta}}\,m = AG(G).$$

□

The *atom-bond connectivity index* [33] is

$$ABC(G) = \sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_u\,d_v}}\,.$$

Furtula et al. [34] made a generalization of ABC index, defined as

$$ABC_\alpha(G) = \sum_{uv\in E(G)}\left(\frac{d_u+d_v-2}{d_u\,d_v}\right)^\alpha, \quad \text{where } \alpha\in\mathbb{R}.$$

They showed that the ABC_α defined in this way, for $\alpha=-3$, has better predictive power than the original ABC index.

The three following results relate the arithmetic-geometric and the general atom-bond connectivity indices.

Theorem 4. *Let G be a graph with maximum degree Δ and without isolated edges, and $\alpha > 0$. Then*

$$AG(G) \le \frac{(\Delta-1)^{\alpha}(\Delta+1)}{2\Delta^{\alpha+\frac{1}{2}}}\, ABC_{-\alpha}(G),$$

and the equality in the inequality holds if and only if G is a union of stars $S_{\Delta+1}$.

Proof. Note that $(d_u, d_v) \neq (1,1)$, since G does not have isolated edges, hence $\Delta \ge 2$. First of all, we are going to compute the minimum value of

$$W(x,y) = \left(\frac{x+y-2}{xy}\right)^{-\alpha} \frac{2\sqrt{xy}}{x+y} = 2(x+y-2)^{-\alpha}(x+y)^{-1}x^{\alpha+\frac{1}{2}}y^{\alpha+\frac{1}{2}}$$

on $\{1 \le x \le y, 2 \le y \le \Delta\}$. We have

$$\begin{aligned}\frac{\partial W}{\partial x} &= 2y^{\alpha+\frac{1}{2}}\Big[-\alpha(x+y-2)^{-\alpha-1}(x+y)^{-1}x^{\alpha+\frac{1}{2}} - (x+y-2)^{-\alpha}(x+y)^{-2}x^{\alpha+\frac{1}{2}} \\ &\qquad + \left(\alpha+\frac{1}{2}\right)(x+y-2)^{-\alpha}(x+y)^{-1}x^{\alpha-\frac{1}{2}}\Big] \\ &= 2y^{\alpha+\frac{1}{2}}x^{\alpha-\frac{1}{2}}(x+y-2)^{-\alpha-1}(x+y)^{-2}\Big[-\alpha(x+y)x - (x+y-2)x \\ &\qquad + \left(\alpha+\frac{1}{2}\right)(x+y-2)(x+y)\Big] \\ &= 2y^{\alpha+\frac{1}{2}}x^{\alpha-\frac{1}{2}}(x+y-2)^{-\alpha-1}(x+y)^{-2}\Big[\alpha(x+y)(x+y-2-x) \\ &\qquad + (x+y-2)\left(\frac{x+y}{2} - x\right)\Big] \\ &= 2y^{\alpha+\frac{1}{2}}x^{\alpha-\frac{1}{2}}(x+y-2)^{-\alpha-1}(x+y)^{-2}\left[\alpha(x+y)(y-2) + \frac{1}{2}(x+y-2)(y-x)\right] \ge 0,\end{aligned}$$

so, $W(x,y)$ is strictly increasing on $x \in [1,y]$ for every fixed $y \ge 2$ and, so, $W(1,y) \le W(x,y)$. Consider

$$a(y) = W(1,y) = 2(y-1)^{-\alpha}(1+y)^{-1}y^{\alpha+1/2}.$$

Subsequently,

$$\begin{aligned}a'(y) &= 2\Big[-\alpha(y-1)^{-\alpha-1}(y+1)^{-1}y^{\alpha+\frac{1}{2}} - (y-1)^{-\alpha}(y+1)^{-2}y^{\alpha+\frac{1}{2}} \\ &\qquad + \left(\alpha+\frac{1}{2}\right)(y-1)^{-\alpha}(y+1)^{-1}y^{\alpha-\frac{1}{2}}\Big] \\ &= 2(y-1)^{-\alpha-1}(y+1)^{-2}y^{\alpha-\frac{1}{2}}\left[-\alpha(y+1)y - (y-1)y + \left(\alpha+\frac{1}{2}\right)(y-1)(y+1)\right] \\ &= 2(y-1)^{-\alpha-1}(y+1)^{-2}y^{\alpha-\frac{1}{2}}\left[\alpha(y+1)(y-1-y) + (y-1)\left(\frac{y+1}{2} - y\right)\right] \\ &= 2(y-1)^{-\alpha-1}(y+1)^{-2}y^{\alpha-\frac{1}{2}}\left[-\alpha(y+1) - \frac{1}{2}(y-1)^2\right] < 0,\end{aligned}$$

so, w is strictly decreasing on $y \in [2,\Delta]$. Thus, we have $a(\Delta) \le a(y) = W(1,y) \le W(x,y)$ for every $1 \le x \le y$, $2 \le y \le \Delta$ and the equalities hold if and only if $x = 1$ and $y = \Delta$. Therefore,

$$\frac{2\Delta^{\alpha+\frac{1}{2}}}{(\Delta-1)^{\alpha}(\Delta+1)}\,\frac{d_u+d_v}{2\sqrt{d_u d_v}} \le \left(\frac{d_u+d_v-2}{d_u d_v}\right)^{-\alpha} \qquad \text{for every } uv \in E(G),$$

and the equality is attained if and only if $d_u = 1$ and $d_v = \Delta$ or vice versa for each edge $uv \in E(G)$, *i.e.*, every connected component of G is a star $S_{\Delta+1}$. □

Remark 2. *The argument in the proof of Theorem 4 (with the same hypotheses) allows for obtaining the following lower bound of AG, but it is elementary:*

$$\frac{(2\Delta-2)^{\alpha}}{\Delta^{2\alpha}}\, ABC_{-\alpha}(G) \le AG(G),$$

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

We can improve Theorem 4 when $\delta \ge 2$.

Theorem 5. *Let G be a graph with maximum degree Δ and minimum degree $\delta \ge 2$, and $\alpha > 0$. Afterwards,*

$$AG(G) \le \max\left\{\frac{(2\delta-2)^{\alpha}}{\delta^{2\alpha}}, \frac{(\Delta+\delta-2)^{\alpha}(\Delta+\delta)}{2(\Delta\delta)^{\alpha+\frac{1}{2}}}\right\} ABC_{-\alpha}(G).$$

The equality in the inequality holds if G is regular.

Proof. Consider the notation in the proof of Theorem 4, and the function

$$c(y) = W(\delta, y) = 2\delta^{\alpha+\frac{1}{2}}(y+\delta-2)^{-\alpha}(y+\delta)^{-1}y^{\alpha+\frac{1}{2}},$$

with $2 \le \delta \le y \le \Delta$. The argument in the proof of Theorem 4 gives that $c(y) = W(\delta, y) \le W(x, y)$ for every $\delta \le x \le y \le \Delta$.

We have

$$\begin{aligned} c'(y) &= 2\delta^{\alpha+\frac{1}{2}}\Big[-\alpha(y+\delta-2)^{-\alpha-1}(y+\delta)^{-1}y^{\alpha+\frac{1}{2}} - (y+\delta-2)^{-\alpha}(y+\delta)^{-2}y^{\alpha+\frac{1}{2}} \\ &\qquad + \left(\alpha+\frac{1}{2}\right)(y+\delta-2)^{-\alpha}(y+\delta)^{-1}y^{\alpha-\frac{1}{2}}\Big] \\ &= 2\delta^{\alpha+\frac{1}{2}}(y+\delta-2)^{-\alpha-1}(y+\delta)^{-2}y^{\alpha-\frac{1}{2}}\Big[-\alpha(y+\delta)y - (y+\delta-2)y \\ &\qquad + \left(\alpha+\frac{1}{2}\right)(y+\delta-2)(y+\delta)\Big] \\ &= 2\delta^{\alpha+\frac{1}{2}}(y+\delta-2)^{-\alpha-1}(y+\delta)^{-2}y^{\alpha-\frac{1}{2}}\Big[\alpha(y+\delta)(-y+y+\delta-2) \\ &\qquad + (y+\delta-2)\left(-y+\frac{y+\delta}{2}\right)\Big] \\ &= 2\delta^{\alpha+\frac{1}{2}}(y+\delta-2)^{-\alpha-1}(y+\delta)^{-2}y^{\alpha-\frac{1}{2}}\Big[\alpha(y+\delta)(\delta-2) - \frac{1}{2}(y+\delta-2)(y-\delta)\Big]. \end{aligned}$$

Consider first the case $\delta = 2$. We have

$$\begin{aligned} c'(y) &= 2\delta^{\alpha+\frac{1}{2}}(y+\delta-2)^{-\alpha-1}(y+\delta)^{-2}y^{\alpha-\frac{1}{2}}\Big[\alpha(y+\delta)(\delta-2) - \frac{1}{2}(y+\delta-2)(y-\delta)\Big] \\ &= -\delta^{\alpha+\frac{1}{2}}(y+\delta-2)^{-\alpha}(y+\delta)^{-2}y^{\alpha-\frac{1}{2}}(y-\delta) \le 0. \end{aligned}$$

Thus, $\min_{y\in[\delta,\Delta]} c(y) = c(\Delta)$.

Now, assume that $\delta \ge 3$. Let us consider the second degree polynomial

$$P(y) = \alpha(y+\delta)(\delta-2) - \frac{1}{2}(y+\delta-2)(y-\delta).$$

Because

$$P(0) = \alpha\delta(\delta-2) - \frac{1}{2}(\delta-2)(-\delta) = \left(\alpha + \frac{1}{2}\right)\delta(\delta-2) \geq 0,$$

there exists at least a non-positive zero of P. Hence, there exists at most a zero of P in the interval $[\delta, \Delta]$. Additionally, $P(\delta) = 2\delta(\delta-2) > 0$.

Thus, there exists, at most, a zero of c' in the interval $[\delta, \Delta]$ and $c'(\delta) > 0$. Consequently,

$$\min_{y\in[\delta,\Delta]} c(y) = \min\left\{c(\delta),\, c(\Delta)\right\},$$

for every $\delta \geq 3$ and, so, for every $\delta \geq 2$. Therefore,

$$\begin{aligned} W(x,y) &\geq W(\delta,y) \geq c(y) \geq \min\left\{c(\delta),\, c(\Delta)\right\} \\ &= \min\left\{\delta^{2\alpha}(2\delta-2)^{-\alpha},\, 2(\Delta\delta)^{\alpha+\frac{1}{2}}(\Delta+\delta-2)^{-\alpha}(\Delta+\delta)^{-1}\right\}, \end{aligned}$$

for every $\delta \leq x \leq y \leq \Delta$ and, by symmetry, for every $\delta \leq x, y \leq \Delta$. Consequently,

$$\min\left\{\frac{\delta^{2\alpha}}{(2\delta-2)^{\alpha}},\, \frac{2(\Delta\delta)^{\alpha+\frac{1}{2}}}{(\Delta+\delta-2)^{\alpha}(\Delta+\delta)}\right\}\frac{d_u+d_v}{2\sqrt{d_ud_v}} \leq \left(\frac{d_u+d_v-2}{d_ud_v}\right)^{-\alpha}$$

for every $uv \in E(G)$, and

$$AG(G) \leq \max\left\{\frac{(2\delta-2)^{\alpha}}{\delta^{2\alpha}},\, \frac{(\Delta+\delta-2)^{\alpha}(\Delta+\delta)}{2(\Delta\delta)^{\alpha+\frac{1}{2}}}\right\}ABC_{-\alpha}(G).$$

If G is regular, thus $\Delta = \delta$ and

$$\begin{aligned} &\max\left\{\frac{(2\delta-2)^{\alpha}}{\delta^{2\alpha}},\, \frac{(\Delta+\delta-2)^{\alpha}(\Delta+\delta)}{2(\Delta\delta)^{\alpha+\frac{1}{2}}}\right\}ABC_{-\alpha}(G) \\ &\max\left\{\frac{(2\delta-2)^{\alpha}}{\delta^{2\alpha}},\, \frac{(2\delta-2)^{\alpha}2\delta}{2\delta^{2\alpha+1}}\right\}\frac{\delta^{2\alpha}}{(2\delta-2)^{\alpha}}\, m = m = AG(G), \end{aligned}$$

and the equality in the inequality holds. □

Now, we relate the arithmetic-geometric and general atom-bond connectivity indices with parameter greater than or equal to $1/2$.

Theorem 6. *If G is a graph with minimum degree $\delta \geq 2$ and maximum degree Δ, and $\beta \geq 1/2$, then*

$$AG(G) \leq \left(\frac{\Delta^2}{2\Delta-2}\right)^{\beta} ABC_{\beta}(G),$$

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

Proof. Define $\alpha = -\beta \leq -1/2$. As in the proof of Theorem 4, let us consider

$$W(x,y) = \left(\frac{x+y-2}{xy}\right)^{-\alpha}\frac{2\sqrt{xy}}{x+y} = 2(x+y-2)^{-\alpha}(x+y)^{-1}x^{\alpha+\frac{1}{2}}y^{\alpha+\frac{1}{2}}$$

on $\{2 \le \delta \le x \le y \le \Delta\}$. We have

$$\frac{\partial W}{\partial x} = 2y^{\alpha+\frac{1}{2}} x^{\alpha-\frac{1}{2}} (x+y-2)^{-\alpha-1} (x+y)^{-2} \left[\alpha(x+y)(y-2) + \frac{1}{2}(x+y-2)(y-x) \right]$$
$$\le 2y^{\alpha+\frac{1}{2}} x^{\alpha-\frac{1}{2}} (x+y-2)^{-\alpha-1} (x+y)^{-2} \left[-\frac{1}{2}(x+y)(y-2) + \frac{1}{2}(x+y-2)(y-x) \right]$$
$$= 2y^{\alpha+\frac{1}{2}} x^{\alpha-\frac{1}{2}} (x+y-2)^{-\alpha-1} (x+y)^{-2} \left[-\frac{1}{2}(x-2) - (y-x) \right] \le 0,$$

on $\{\delta \le x \le y \le \Delta\}$. Hence, $W(y,y) \le W(x,y)$ when $\delta \le x \le y \le \Delta$. We define now

$$b(y) = W(y,y) = 2^{-\alpha} \left(\frac{y-1}{y^2} \right)^{-\alpha}.$$

Subsequently,

$$b'(y) = \alpha 2^{-\alpha} \left(\frac{y-1}{y^2} \right)^{-\alpha-1} \frac{y-2}{y^3} \le 0.$$

Consequently, b is a strictly decreasing function on $\delta \le y \le \Delta$, and

$$W(\Delta,\Delta) = b(\Delta) \le b(y) = W(y,y) \le W(x,y)$$

when $\delta \le x \le y \le \Delta$. Hence, by symmetry,

$$\left(\frac{2\Delta-2}{\Delta^2} \right)^{\beta} = W(\Delta,\Delta) \le W(x,y)$$

for each $\delta \le x, y \le \Delta$, and

$$\left(\frac{2\Delta-2}{\Delta^2} \right)^{\beta} \frac{d_u+d_v}{2\sqrt{d_u d_v}} \le \left(\frac{d_u+d_v-2}{d_u d_v} \right)^{\beta} \qquad \text{for every } uv \in E(G),$$

$$\left(\frac{2\Delta-2}{\Delta^2} \right)^{\beta} AG(G) \le ABC_{\beta}(G).$$

□

Remark 3. *The arguments in the proof of Theorem 6 (with the same hypotheses) allow to obtain the following lower bound of AG, but it is elementary:*

$$\left(\frac{\delta^2}{2\delta-2} \right)^{\beta} ABC_{\beta}(G) \le AG(G),$$

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

3. General Bounds on the AG Index

In this section we obtain additional lower bounds of AG improving the lower bound in (1), which do not involve other topological indices. The two following bounds involve m and the minimum degree.

Theorem 7. *If G is a graph with m edges, minimum degree δ, maximum degree $\delta+1$, and α is the number of edges uv with $d_u \ne d_v$, then α is an even integer and*

$$AG(G) = m + \alpha \left(\frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} - 1 \right).$$

Proof. Let $D = \{uv \in E(G) : \ d_u \neq d_v\}$, then α is the cardinality of D. Because δ is the minimum degree of G and $\delta + 1$ is its maximum degree, if $uv \in D$, then $d_u = \delta$ and $d_v = \delta + 1$ or vice versa and, therefore,

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

If $uv \in D^c$, then $d_u = d_v = \delta$ or $d_u = d_v = \delta + 1$, and therefore

$$\frac{d_u + d_v}{2\sqrt{d_u d_v}} = 1.$$

Because there are exactly α edges in D and $m - \alpha$ edges in D^c, we have

$$\begin{aligned} AG(G) &= \sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}} \\ &= \sum_{uv \in D^c} \frac{d_u + d_v}{2\sqrt{d_u d_v}} + \sum_{uv \in D} \frac{d_u + d_v}{2\sqrt{d_u d_v}} \\ &= \sum_{uv \in D^c} 1 + \sum_{uv \in D} \frac{2\delta + 1}{2\sqrt{\delta(\delta + 1)}} \\ &= m - \alpha + \alpha \frac{2\delta + 1}{2\sqrt{\delta(\delta + 1)}} . \end{aligned}$$

Assume, for contradiction, that α is an odd integer.

Let G_1 be a subgraph of G induced by the n_1 vertices with degree δ in $V(G)$, and denote by m_1 the number of edges of G_1. Handshaking Lemma gives $n_1\delta - \alpha = 2m_1$. Because α is an odd integer, δ is also an odd integer. Thus, $\delta + 1$ is an even integer.

Let G_2 be a subgraph of G that is induced by the n_2 vertices with degree $\delta + 1$ in $V(G)$, and denote, by m_2, the number of edges of G_2. Handshaking Lemma gives $n_2(\delta + 1) - \alpha = 2m_2$, a contradiction, since α is an odd integer and $\delta + 1$ is an even integer.

Thus, we conclude that α is an even integer. □

Theorem 8. *If G is a connected graph with m edges, minimum degree δ and maximum degree $\delta + 1$, then*

$$AG(G) \geq m + \frac{2\delta + 1}{\sqrt{\delta(\delta + 1)}} - 2 ,$$

and the equality is attained for each δ.

Proof. Let α be the number of edges $uv \in E(G)$ with $d_u \neq d_v$. Theorem 7 gives that α is an even integer. Because G is a connected graph, we have $\alpha \neq 0$ and so, $\alpha \geq 2$. Since

$$\frac{2\delta + 1}{2\sqrt{\delta(\delta + 1)}} > 1$$

and $\alpha \geq 2$, Theorem 7 gives

$$\begin{aligned} AG(G) &= m + \alpha \left(\frac{2\delta + 1}{2\sqrt{\delta(\delta + 1)}} - 1 \right) \\ &\geq m + 2 \left(\frac{2\delta + 1}{2\sqrt{\delta(\delta + 1)}} - 1 \right) \\ &= m - 2 + \frac{2\delta + 1}{\sqrt{\delta(\delta + 1)}} . \end{aligned}$$

Given a fixed δ, let us consider the complete graphs $K_{\delta+1}$ and $K_{\delta+2}$ with $\delta+1$ and $\delta+2$ vertices, respectively. Fix $u_1, u_2 \in V(K_{\delta+1})$ and $v_1, v_2 \in V(K_{\delta+2})$, and denote by $K'_{\delta+1}$ and $K'_{\delta+2}$ the graphs obtained from $K_{\delta+1}$ and $K_{\delta+2}$ by deleting the edges u_1u_2 and v_1v_2, respectively. Let Γ_δ be the graph with $V(\Gamma_\delta) = V(K'_{\delta+1}) \cup V(K'_{\delta+2})$ and $E(\Gamma_\delta) = E(K'_{\delta+1}) \cup E(K'_{\delta+2}) \cup \{u_1v_1\} \cup \{u_2v_2\}$. Thus, Γ_δ has $\delta^2+2\delta+1$ edges, minimum degree δ, maximum degree $\delta+1$, and Theorem 7 give

$$AG(\Gamma_\delta) = \delta^2 + 2\delta - 1 + \frac{2\delta+1}{\sqrt{\delta(\delta+1)}}.$$

Hence, the equality is attained for each δ. □

A *chemical graph* is a graph with $\Delta \le 4$.

Corollary 3. *If G is a connected chemical graph with m edges, minimum degree δ, and maximum degree $\delta+1$, then Then*

$$AG(G) \ge m - 2 + \frac{7\sqrt{3}}{6}.$$

Furthermore, the equality in the bound is attained.

Proof. Because G is a chemical graph, we have $1 \le \delta \le 3$. Since

$$\min_{1\le\delta\le3} \frac{2\delta+1}{\sqrt{\delta(\delta+1)}} = \min\left\{\frac{3}{\sqrt{2}}, \frac{5}{\sqrt{6}}, \frac{7}{\sqrt{12}}\right\} = \frac{7\sqrt{3}}{6},$$

Theorem 8 gives the desired inequality.
The graph Γ_3 in the proof of Theorem 8 provides that the equality is attained. □

We need some definitions. Let G be a graph with maximum degree Δ and minimum degree $\delta < \Delta - 1$. We denote, by $\alpha_0, \alpha_1, \alpha_2,$, the cardinality of the subsets of edges

$$\begin{aligned}
A_0 &= \{uv \in E(G) : d_u = \delta, d_v = \Delta\},\\
A_1 &= \{uv \in E(G) : d_u = \delta, \delta < d_v < \Delta\},\\
A_2 &= \{uv \in E(G) : d_u = \Delta, \delta < d_v < \Delta\},
\end{aligned}$$

respectively.
We need the following result ([28], Theorem 5).

Lemma 4. *If G is a graph with m edges, maximum degree Δ, and minimum degree $\delta < \Delta - 1$, then*

$$AG(G) \le \frac{\Delta+\delta}{2\sqrt{\Delta\delta}}\, m - \alpha_1\left(\frac{\Delta+\delta}{2\sqrt{\Delta\delta}} - \frac{\delta+\Delta-1}{2\sqrt{\delta(\Delta-1)}}\right) - \alpha_2\left(\frac{\Delta+\delta}{2\sqrt{\Delta\delta}} - \frac{\Delta+\delta+1}{2\sqrt{\Delta(\delta+1)}}\right),$$

$$AG(G) \ge m + \alpha_0\left(\frac{\Delta+\delta}{2\sqrt{\Delta\delta}} - 1\right) + \alpha_1\left(\frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} - 1\right) + \alpha_2\left(\frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 1\right).$$

We are going to use Lemma 4 to obtain the following lower bound of AG involving m and the minimum and maximum degree.

Theorem 9. *Let G be a connected graph with m edges, maximum degree Δ and minimum degree $\delta < \Delta - 1$. Subsequently,*

$$AG(G) \ge m + \min\left\{\frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 2,\ \frac{\Delta+\delta}{2\sqrt{\Delta\delta}} - 1\right\}.$$

The equality in the bound is attained.

Proof. Because G is connected, we have two possibilities: $A_0 \neq \emptyset$, or $A_1 \neq \emptyset$ and $A_2 \neq \emptyset$.

In the first case, $\alpha_0 \geq 1$ and, since

$$\frac{d_u + d_v}{2\sqrt{d_u d_v}} \geq 1,$$

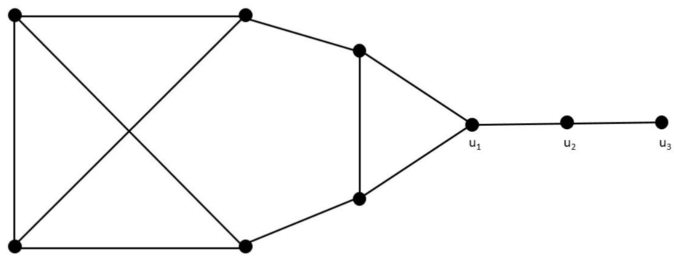
Lemma 4 gives

$$\begin{aligned} AG(G) &\geq m + \alpha_0 \left(\frac{\Delta + \delta}{2\sqrt{\Delta\delta}} - 1 \right) + \alpha_1 \left(\frac{2\delta + 1}{2\sqrt{\delta(\delta+1)}} - 1 \right) + \alpha_2 \left(\frac{2\Delta - 1}{2\sqrt{\Delta(\Delta-1)}} - 1 \right) \\ &\geq m + \frac{\Delta + \delta}{2\sqrt{\Delta\delta}} - 1 \,. \end{aligned}$$

In the second case, $\alpha_1, \alpha_2 \geq 1$ and Lemma 4 give

$$\begin{aligned} AG(G) &\geq m + \alpha_0 \left(\frac{\Delta + \delta}{2\sqrt{\Delta\delta}} - 1 \right) + \alpha_1 \left(\frac{2\delta + 1}{2\sqrt{\delta(\delta+1)}} - 1 \right) + \alpha_2 \left(\frac{2\Delta - 1}{2\sqrt{\Delta(\Delta-1)}} - 1 \right) \\ &\geq m + \frac{2\delta + 1}{2\sqrt{\delta(\delta+1)}} + \frac{2\Delta - 1}{2\sqrt{\Delta(\Delta-1)}} - 2 \,. \end{aligned}$$

Let G be the graph in the figure.



We have $m = 12$, $\Delta = 3$, $\delta = 1$, $A_0 = \emptyset$, $\alpha_0 = 0$, $A_1 = \{u_2 u_3\}$, $\alpha_1 = 1$, $A_2 = \{u_1 u_2\}$ and $\alpha_2 = 1$. Additionally, if $uv \notin A_0 \cup A_1 \cup A_2$, then $d_u = d_v$. Thus,

$$\begin{aligned} AG(G) &= \sum_{uv \in E(G) \setminus A_0 \cup A_1 \cup A_2} \frac{d_u + d_v}{2\sqrt{d_u d_v}} + \sum_{uv \in A_0} \frac{\Delta + \delta}{2\sqrt{\Delta\delta}} + \sum_{uv \in A_1} \frac{\delta + d_v}{2\sqrt{\delta d_v}} + \sum_{uv \in A_2} \frac{\Delta + d_v}{2\sqrt{\Delta d_v}} \\ &= 10 + \frac{2\delta + 1}{2\sqrt{\delta(\delta+1)}} + \frac{2\Delta - 1}{2\sqrt{\Delta(\Delta-1)}} = 10 + \frac{3}{2\sqrt{2}} + \frac{5}{2\sqrt{6}} \approx 12.0813 \end{aligned}$$

The lower bound is

$$\begin{aligned} & m + \min \left\{ \frac{2\delta + 1}{2\sqrt{\delta(\delta+1)}} + \frac{2\Delta - 1}{2\sqrt{\Delta(\Delta-1)}} - 2, \ \frac{\Delta + \delta}{2\sqrt{\Delta\delta}} - 1 \right\} \\ & 12 + \min \left\{ \frac{3}{2\sqrt{2}} + \frac{5}{2\sqrt{6}} - 2, \ \frac{2}{\sqrt{3}} - 1 \right\} \\ & \approx 12 + \min\{0.0813, \ 0.1547\} = 12.0813 \end{aligned}$$

and so, this graph attains the equality in the inequality. □

4. Conclusions

Topological indices have become a useful tool for the study of theoretical and practical problems in different areas of science. An important line of research that is associated with topological indices is to find optimal bounds and relations between known topological indices. In particular, to obtain bounds for the topological indices that are associated with invariant parameters of a graph.

We have the following nine results for the arithmetic-geometric index AG:

- An upper and lower bound of AG based on the first and second variable Zagreb indices (Theorem 1).
- An upper bound of AG that is based on the second variable Zagreb index M_2^a (Theorem 2).
- An upper and lower bound of AG based on SDD (Theorem 3).
- An upper bound of AG based on the general atom-bond connectivity index ABC_a (Theorem 4).
- Another upper bound of AG based on the general atom-bond connectivity index ABC_a for graphs with minimum degree $\delta \geq 2$ (Theorem 5).
- A further upper bound of AG based on the general atom-bond connectivity index ABC_a for graphs with minimum degree $\delta \geq 2$ (Theorem 6).
- An exact formula of AG based on the number of edges m and the minimum degree δ if the maximum degree is $\delta + 1$ (Theorem 7).
- A lower bound of AG based on the number of edges m and the minimum degree δ if the maximum degree is $\delta + 1$ (Theorem 8). We provide a family of graphs for which the equality is attained.
- A lower bound of AG that is based on the number of edges m, the minimum degree δ, and the maximum degree Δ (Theorem 9). We provide a graph for which the equality is attained.

Because the arithmetic-geometric index is useful from a practical point of view, to know extremal graphs for each bound involving this index allows for detecting chemical compounds that could satisfy desirable properties. Hence, these extremal graphs should correspond to molecules with a extremal value of a desired property correlated well with this index.

In the case of centrality indices, the generalization of degree has turned out to be a useful approach: the role of a more interconnected node can differ from a node that is connected to nodes having a lower degree [35]. We would like to purpose as a direction for future research to study similar problems for centrality indices.

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