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Some Properties of the Arithmetic–Geometric Index

Edil D. Molina [1,†], José M. Rodríguez [2,†], José L. Sánchez [1,†] and José M. Sigarreta [1,*,†]

[1] Facultad de Matemáticas, Universidad Autónoma de Guerrero, Carlos E. Adame No.54 Col. Garita, 39650 Acalpulco Gro., Mexico; edil941023@gmail.com (E.D.M.); jlsanchezsantiesteban@gmail.com (J.L.S.)
[2] Departamento de Matemáticas, Universidad Carlos III de Madrid, Avenida de la Universidad 30, 28911 Leganés, Madrid, Spain; jomaro@math.uc3m.es
* Correspondence: josemariasigarretaalmira@hotmail.com; Tel.: +52-744-159-2272
† These authors contributed equally to this work.

Abstract: Recently, the arithmetic–geometric index (AG) was introduced, inspired by the well-known and studied geometric–arithmetic index (GA). In this work, we obtain new bounds on the arithmetic–geometric index, improving upon some already known bounds. In particular, we show families of graphs where such bounds are attained.

Keywords: arithmetic–geometric index; topological index; chemical graph theory

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1. Introduction

In mathematical chemistry, a topological descriptor is a function that associates each molecular graph with a real value, and if it correlates well with some chemical property, it is called a topological index. Since Wiener's work (see [1]), numerous topological indices have been defined and discussed, since the growing interest in their study is due to their several applications in chemistry, for example in QSPR/QSAR research (see [2–4]). For more information on other important applications of topological indices to specific problems in physics, computer science and environment science (see [5–7]). In particular, among the topological descriptors, the most studied from the mathematical point of view due to their practical scope are the so-called vertex-degree-based topological indices. Probably the most studied, with more than 500 papers, is the Randić index defined as

$$R(H) = \sum_{ij \in E(H)} \frac{1}{\sqrt{d_i d_j}},$$

where ij denotes the edge of the graph H and d_i is the degree of the vertex i.

In [8,9], the *variable Zagreb indices* are defined as

$$M_1^\alpha(H) = \sum_{i \in V(H)} d_i^\alpha, \qquad M_2^\alpha(H) = \sum_{ij \in E(H)} (d_i d_j)^\alpha,$$

with $\alpha \in \mathbb{R}$.

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

The *general sum-connectivity index* was defined in [10] as

$$\chi_\alpha(H) = \sum_{ij \in E(H)} (d_i + d_j)^\alpha.$$

Note that $\chi_{-1/2}$ is the sum-connectivity index, $2\chi_{-1}$ is the harmonic index Har, etc.

The *max–min rodeg index* and *min–max rodeg index* were defined in [11] respectively as

$$Mm_{sde}(H) = \sum_{ij \in E(H)} \sqrt{\frac{\max\{d_i, d_j\}}{\min\{d_i, d_j\}}}, \qquad mM_{sde}(H) = \sum_{ij \in E(H)} \sqrt{\frac{\min\{d_i, d_j\}}{\max\{d_i, d_j\}}}.$$

these indices have shown good predictive properties (see [11]).

The *symmetric division deg index* was defined in [11,12] as

$$SDD(H) = \sum_{ij \in E(H)} \frac{d_i^2 + d_j^2}{d_i d_j} = \sum_{ij \in E(H)} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right).$$

It was claimed in [11] that SDD correlates well with the total surface area of polychlorobiphenyls. In the paper [13], the applicability of SDD is tested on a wider empirical basis; also, its prediction ability is compared with other (more often used) topological indices.

The $GA(H)$ is defined in [14] as

$$GA(H) = \sum_{ij \in E(H)} \frac{2\sqrt{d_i d_j}}{d_i + d_j}.$$

There are many papers studying the mathematical and computational properties of the GA index (see, e.g., [14–21] and the references therein).

As an inverse variant of this topological index, in 2015, the *arithmetic–geometric index* was introduced in [22] as

$$AG(H) = \sum_{ij \in E(H)} \frac{d_i + d_j}{2\sqrt{d_i d_j}}.$$

The AG index of some kinds of trees was discussed in the papers [22,23]. Moreover, the AG index of graphene, which is the most conductive and effective material for electromagnetic interference shielding, was computed in [24]. The paper [25] 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 of graphs appeared in [26,27]. The paper [28] studies optimal AG-graphs for several classes graphs, and it includes inequalities involving $GA + AG$ and $GA \cdot AG$. In [29–32], 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. Motivated by these papers, we obtain new bounds of the AG index, improving upon some already known bounds. Furthermore, we show families of graphs where such bounds are attained. Some of these families are regular graphs, and we recall that some regular graphs play an important role in mathematical chemistry; for instance, Isaac graphs are well-known regular graphs that are isomorphic to hydrogen-suppressed molecular graphs [33].

Given a topological index $I(H) = \sum_{ij \in E(H)} f(d_i, d_j)$, we can consider the reciprocal topological index defined as $J(H) = \sum_{ij \in E(H)} 1/f(d_i, d_j)$. It is essential to point out that several important topological indices are associated with the above relationships. For example, the first Zagreb index M_1 and the first modified Zagreb index ${}^mM_1$, the second Zagreb index M_2 and the second modified Zagreb index ${}^mM_2$, the Randić index R and the reciprocal Randić index $M_2^{1/2}$, the max–min rodeg index Mm_{sde} and the min–max rodeg index mM_{sde}, etc.

Inspired by these ideas, the arithmetic–geometric index AG was defined, which is the reciprocal of the well-studied geometric–arithmetic index GA. Although these topological indices are mathematically represented by an inverse relationship, their scope and results from both theoretical and practical points of view are different. In some cases, the reciprocal topological indices have shown better correlation with some physico–chemical properties than their related indices. In the case of the AG index, in order to investigate its predictive power, we used a datum for entropy (S) of octane isomers, and the results are compared with those obtained for the GA index, (see Figure 1). The correlation coefficient obtained for the AG index is $\mathbf{r}_{AG} = -0.927$, while for the GA index, it is $\mathbf{r}_{GA} = 0.912$, so the AG index, in this case, shows better predictive power than the GA index. However, when we used a datum for the boiling point of octane isomers, it turned out that the GA index showed better predictive power than the AG index. After this paper was accepted, Ref. [34] showed that both indices have the same predictive power for many kinds of graphs.

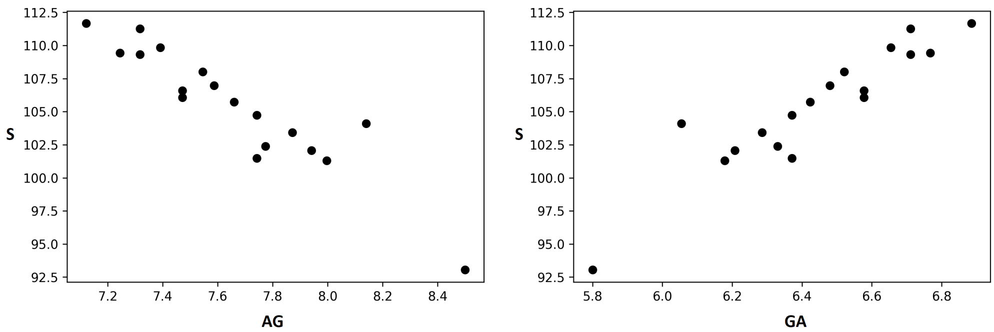

Figure 1. Graphs showing correlation between S and AG, S and GA respectively.

The arithmetic–geometric index was proposed recently and few important papers have been published on the subject. In this paper, we find several new mathematical properties (that cannot be obtained from the GA index), especially bounds that improve those already known.

Throughout this work, $H = (V(H), E(H))$ denotes a finite simple graph with at least an edge in each connected component of H. We denote by m, n, δ, Δ the cardinality of the set of edges $E(H)$ and vertices $V(H)$, and the minimum and maximum degree of H, respectively.

2. Relationships between AG and Other Important Topological Indices

One can check that the following lemma holds:

Lemma 1. *Let f be the function $f(x,y) = \frac{x+y}{2\sqrt{xy}}$ defined on the rectangle $[a,b] \times [a,b]$ with $a > 0$. Then:*

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

The following inequalities for graphs H, 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 $GA(H) \cdot AG(H) \ge m^2$ and $GA(H) \le m$, see [15,16]. The upper bound in (1) appears in [31].

The following result shows the relationship between the AG index and the Randić index that correlates well with several physico–chemical properties. For this reason, it is one of the most studied indices, with innumerable applications in chemistry and pharmacology.

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

$$AG(H) \le m + \frac{\left(\sqrt{\Delta}-\sqrt{\delta}\right)^2}{2} R(H).$$

The equality in the bound is attained if and only if H is regular or biregular.

Proof. Note that:

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

$$AG(H) = m + \sum_{ij \in E(H)} \frac{\left(\sqrt{d_i} - \sqrt{d_j}\,\right)^2}{2\sqrt{d_i d_j}}.$$

Since:

$$\sum_{ij \in E(H)} \frac{\left(\sqrt{d_i} - \sqrt{d_j}\,\right)^2}{2\sqrt{d_i d_j}} \le \frac{\left(\sqrt{\Delta} - \sqrt{\delta}\,\right)^2}{2} \sum_{ij \in E(H)} \frac{1}{\sqrt{d_i d_j}},$$

we have:

$$AG(H) \le m + \frac{\left(\sqrt{\Delta} - \sqrt{\delta}\,\right)^2}{2} R(H).$$

The bound is tight if and only if:

$$\left(\sqrt{d_i} - \sqrt{d_j}\right)^2 = \left(\sqrt{\Delta} - \sqrt{\delta}\,\right)^2$$

for every $ij \in E(H)$, and this happens if and only if $d_i = \Delta$ and $d_j = \delta$, or vice versa, for every $ij \in E(H)$, so H is regular if $\Delta = \delta$ or is otherwise biregular. □

The following theorem shows a relationship between the index AG and the index M_2^{-a}, the second variable Zagreb index.

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

$$AG(H) \le K_a M_2^{-a}(H),$$

with:

$$K_a := \begin{cases} \delta^{2a}, & \text{if } a \le -1/2, \\ \max\left\{\delta^{2a},\, \frac{1}{2}(\delta + \Delta)(\delta\Delta)^{a-1/2}\right\}, & \text{if } -1/2 < a \le 0, \\ \max\left\{\Delta^{2a},\, \frac{1}{2}(\delta + \Delta)(\delta\Delta)^{a-1/2}\right\}, & \text{if } 0 < a < 1/2, \\ \Delta^{2a}, & \text{if } a \ge 1/2. \end{cases}$$

The equality in the bound is attained for some fixed $a \notin (-1/2, 1/2)$ if and only if H is a regular graph.

Proof. Let us optimize the function $g : [\delta, \Delta] \times [\delta, \Delta] \to (0, \infty)$ defined as

$$g(x,y) = \frac{\frac{x+y}{2\sqrt{xy}}}{(xy)^{-a}} = \frac{1}{2}\,(xy)^{a-1/2}(x+y) = \frac{1}{2}\,x^{a+1/2}y^{a-1/2} + \frac{1}{2}\,x^{a-1/2}y^{a+1/2}.$$

If $a \ge 1/2$, then $a + 1/2 > a - 1/2 \ge 0$ and g strictly increases in each variable. Thus:

$$g(x,y) \le g(\Delta, \Delta) = \Delta^{2a}$$

and the bound is tight if and only if $x = y = \Delta$. Therefore:

$$AG(H) \le \Delta^{2a} M_2^{-a}(H).$$

Let us now consider the case $-1/2 \le a < 1/2$. Since g is a symmetric function, we can also assume that $x \le y$. We have:

$$\begin{aligned}\frac{\partial g}{\partial x}(x,y) &= \frac{1}{2}(1/2+a)x^{a-1/2}y^{a-1/2} + \frac{1}{2}(a-1/2)x^{a-3/2}y^{a+1/2} \\ &= \frac{1}{2}\,x^{a-3/2}y^{a-1/2}\big((1/2+a)x + (a-1/2)y\big), \\ \frac{\partial g}{\partial y}(x,y) &= \frac{1}{2}\,y^{a-3/2}x^{a-1/2}\big((1/2+a)y + (a-1/2)x\big).\end{aligned}$$

Assume first that $0 < a < 1/2$. Thus, $a + 1/2 > 0$ and:

$$(1/2+a)y + (a-1/2)x \ge (1/2+a)x + (a-1/2)x = 2ax > 0$$

and thus, $\partial g/\partial y > 0$. Therefore, the maximum value of g is attained on $\{\delta \le x \le \Delta,\ y = \Delta\}$. Since:

$$\frac{\partial g}{\partial x}(\Delta,\Delta) = \frac{1}{2}\,\Delta^{2a-2}\big((a+1/2)\Delta + (a-1/2)\Delta\big) = a\Delta^{2a-1} > 0,$$

and $\partial g/\partial x(x,\Delta) = 0$ at most once when $x \in [\delta,\Delta]$, we have:

$$\begin{aligned}\max_{x,y\in[\delta,\Delta]} g(x,y) = \max_{x\in[\delta,\Delta]} g(x,\Delta) &= \max\big\{g(\delta,\Delta),\ g(\Delta,\Delta)\big\} \\ &= \max\Big\{\frac{1}{2}\,(\Delta\delta)^{a-1/2}(\Delta+\delta),\ \Delta^{2a}\Big\}.\end{aligned}$$

Assume now that $-1/2 < a \le 0$. We have $a + 1/2 > 0$ and:

$$(1/2+a)x + (a-1/2)y \le (1/2+a)y + (a-1/2)y = 2ay \le 0$$

and thus, $\partial g/\partial x \le 0$. Therefore, the maximum value of g is attained on $\{x = \delta,\ \delta \le y \le \Delta\}$. Since:

$$\frac{\partial g}{\partial y}(\Delta,\Delta) = \frac{1}{2}\,\Delta^{2a-2}\big((a+1/2)\Delta + (a-1/2)\Delta\big) = a\Delta^{2a-1} > 0,$$

and $\partial g/\partial y(\delta,y) = 0$ at most once when $y \in [\delta,\Delta]$, we have:

$$\begin{aligned}\max_{x,y\in[\delta,\Delta]} g(x,y) = \max_{y\in[\delta,\Delta]} g(\delta,y) &= \max\big\{g(\delta,\delta),\ g(\delta,\Delta)\big\} \\ &= \max\Big\{\frac{1}{2}\,(\Delta\delta)^{a-1/2}(\Delta+\delta),\ \delta^{2a}\Big\}.\end{aligned}$$

Finally, assume that $a \le -1/2$. Hence, $a - 1/2 < a + 1/2 \le 0$ and g strictly decreases in each variable. Thus:

$$g(x,y) \le g(\delta,\delta) = \delta^{2a}$$

and the bound is tight if and only if $x = y = \delta$. Therefore:

$$AG(H) \le \delta^{2a} M_2^{-a}(H).$$

The properties of the function g give that the bound is tight for some fixed $a \ge 1/2$ (respectively, $a \le -1/2$) if and only if $d_i = d_j = \Delta$ (respectively, $d_i = d_j = \delta$) for every $ij \in E(H)$, and this happens if and only if H is a regular graph. □

Remark 1. *The proof of Theorem 2 allows us to obtain that:*

$$C_a M_2^{-a}(H) \le AG(H),$$

with:

$$C_a := \begin{cases} \Delta^{2a}, & \text{if } a \le 0, \\ \delta^{2a}, & \text{if } a > 0. \end{cases}$$

However, this inequality is direct, since:

$$AG(H) \ge m = \sum_{ij \in E(H)} \frac{(d_i d_j)^a}{(d_i d_j)^a} \ge C_a \sum_{ij \in E(H)} \frac{1}{(d_i d_j)^a} = C_a M_2^{-a}(H).$$

Theorem 2 has the following result for the Randić, reciprocal Randić and modified Zagreb indices.

Corollary 1. *If H is a graph with a maximum degree Δ and minimum degree δ, then:*

$$\begin{aligned} AG(H) &\le \delta^{-2} M_2(H), \\ AG(H) &\le \Delta\, R(H), \\ AG(H) &\le \delta^{-1} M_2^{1/2}(H), \\ AG(H) &\le \Delta^2 M_2^{-1}(H). \end{aligned}$$

The following result shows a relationship between the $AG(H)$ index and the $\chi_\beta(H)$ index, which for different values of b generalizes the indices M_1, Har, χ ($b = 1$, $b = -1$, $b = -1/2$, respectively).

Theorem 3. *If H is a graph with minimum degree δ and maximum degree Δ, and $b \in \mathbb{R}$, then:*

$$AG(H) \le B_b\, \chi_b(H),$$

with:

$$B_b := \begin{cases} \max\left\{\frac{1}{2}\,(\Delta\delta)^{-1/2}(\Delta+\delta)^{1-b},\ (2\Delta)^{-b}\right\}, & \text{if } b < 0, \\ \max\left\{\frac{1}{2}\,(\Delta\delta)^{-1/2}(\Delta+\delta)^{1-b},\ (2\delta)^{-b}\right\}, & \text{if } 0 \le b < 1/2, \\ (2\delta)^{-b}, & \text{if } b \ge 1/2. \end{cases}$$

The equality in the bound is attained for some fixed $b \ge 1/2$ if and only if H is a regular graph.

Proof. For each $b < 1/2$, let us define:

$$a = \frac{b}{2b-2} \in \left(\frac{-1}{2}, \frac{1}{2}\right).$$

Let us consider the function: $g : [\delta, \Delta] \times [\delta, \Delta] \to (0, \infty)$ defined as

$$g(x,y) = \frac{1}{2}\,(xy)^{a-1/2}(x+y) = \frac{1}{2}\,x^{a+1/2}y^{a-1/2} + \frac{1}{2}\,x^{a-1/2}y^{a+1/2}\,.$$

Since g is a symmetric function, we can assume $x \le y$. We have:

$$\begin{aligned} \frac{\partial g}{\partial x}(x,y) &= \frac{1}{2}(1/2+a)x^{a-1/2}y^{a-1/2} + \frac{1}{2}(a-1/2)x^{a-3/2}y^{a+1/2} \\ &= \frac{1}{2}\,x^{a-3/2}y^{a-1/2}\big((1/2+a)x + (a-1/2)y\big), \\ \frac{\partial g}{\partial y}(x,y) &= \frac{1}{2}\,y^{a-3/2}x^{a-1/2}\big((1/2+a)y + (a-1/2)x\big). \end{aligned}$$

Assume first that $0 < a < 1/2$. Thus, $1/2 + a > 0$ and:

$$(1/2+a)y + (a-1/2)x \ge (1/2+a)x + (a-1/2)x = 2ax > 0$$

and thus, $\partial g/\partial y > 0$. Therefore, the maximum value of g is attained on $\{\delta \le x \le \Delta,\ y = \Delta\}$. Since:

$$\frac{\partial g}{\partial x}(\Delta,\Delta) = \frac{1}{2}\,\Delta^{2a-2}\big((a+1/2)\Delta + (a-1/2)\Delta\big) = a\Delta^{2a-1} > 0,$$

and $\partial g/\partial x(x,\Delta) = 0$ at most once when $x \in [\delta,\Delta]$, we have:

$$\begin{aligned}\max_{x,y\in[\delta,\Delta]} g(x,y) &= \max_{x\in[\delta,\Delta]} g(x,\Delta) = \max\big\{g(\delta,\Delta),\, g(\Delta,\Delta)\big\}\\ &= \max\Big\{\frac{1}{2}\,(\Delta\delta)^{a-1/2}(\Delta+\delta),\, \Delta^{2a}\Big\}.\end{aligned}$$

Assume now that $-1/2 < a \le 0$. We have $a + 1/2 > 0$ and:

$$(1/2+a)x + (a-1/2)y \le (1/2+a)y + (a-1/2)y = 2ay \le 0$$

and thus, $\partial g/\partial x \le 0$. Therefore, the maximum value of g is attained on $\{x = \delta,\ \delta \le y \le \Delta\}$. Since:

$$\frac{\partial g}{\partial y}(\Delta,\Delta) = \frac{1}{2}\,\Delta^{2a-2}\big((a+1/2)\Delta + (a-1/2)\Delta\big) = a\Delta^{2a-1} > 0,$$

and $\partial g/\partial y(\delta,y) = 0$ at most once when $y \in [\delta,\Delta]$, we have:

$$\begin{aligned}\max_{x,y\in[\delta,\Delta]} g(x,y) &= \max_{y\in[\delta,\Delta]} g(\delta,y) = \max\big\{g(\delta,\delta),\, g(\delta,\Delta)\big\}\\ &= \max\Big\{\frac{1}{2}\,(\Delta\delta)^{a-1/2}(\Delta+\delta),\, \delta^{2a}\Big\}.\end{aligned}$$

Define:

$$C_a := \begin{cases} \max\big\{\delta^{2a},\, \tfrac{1}{2}(\delta+\Delta)(\delta\Delta)^{a-1/2}\big\}, & \text{if } -1/2 < a \le 0,\\ \max\big\{\Delta^{2a},\, \tfrac{1}{2}(\delta+\Delta)(\delta\Delta)^{a-1/2}\big\}, & \text{if } 0 < a < 1/2,\end{cases}$$

we have:

$$\begin{aligned}(xy)^{a-1/2}(x+y) &\le 2C_a,\\ (xy)^{1/(2b-2)}(x+y) &\le 2C_a.\end{aligned}$$

Since $b < 1/2$, we have $1 - b > 0$ and:

$$\frac{1}{2}\,(xy)^{-1/2}(x+y)^{1-b} \le \frac{1}{2}\,(2C_a)^{1-b}.$$

If $0 \le b < 1/2$, then $-1/2 < a \le 0$ and:

$$\begin{aligned}\frac{1}{2}\,(2C_a)^{1-b} &= \frac{1}{2}\Big(2\max\Big\{\frac{1}{2}\,(\Delta\delta)^{a-1/2}(\Delta+\delta),\, \delta^{2a}\Big\}\Big)^{1-b}\\ &= \frac{1}{2}\Big(2\max\Big\{\frac{1}{2}\,(\Delta\delta)^{1/(2b-2)}(\Delta+\delta),\, \delta^{b/(b-1)}\Big\}\Big)^{1-b}\\ &= \max\Big\{\frac{1}{2}\,(\Delta\delta)^{-1/2}(\Delta+\delta)^{1-b},\, (2\delta)^{-b}\Big\} = B_b.\end{aligned}$$

If $b < 0$, then $0 < a < 1/2$ and:

$$\begin{aligned}\frac{1}{2}\,(2C_a)^{1-b} &= \frac{1}{2}\Big(2\max\Big\{\frac{1}{2}\,(\Delta\delta)^{a-1/2}(\Delta+\delta),\, \Delta^{2a}\Big\}\Big)^{1-b}\\ &= \frac{1}{2}\Big(2\max\Big\{\frac{1}{2}\,(\Delta\delta)^{1/(2b-2)}(\Delta+\delta),\, \Delta^{b/(b-1)}\Big\}\Big)^{1-b}\\ &= \max\Big\{\frac{1}{2}\,(\Delta\delta)^{-1/2}(\Delta+\delta)^{1-b},\, (2\Delta)^{-b}\Big\} = B_b.\end{aligned}$$

If $b \ge 1/2$, then the function $A : [\delta, \Delta] \times [\delta, \Delta] \to \mathbb{R}$ defined as

$$A(x,y) = 2\sqrt{xy}\,(x+y)^{b-1}$$

satisfies:

$$\begin{aligned}
\frac{\partial A}{\partial x}(x,y) &= x^{-1/2}y^{1/2}(x+y)^{b-1} + 2x^{1/2}y^{1/2}(b-1)(x+y)^{b-2} \\
&= x^{-1/2}y^{1/2}(x+y)^{b-2}\big(x+y+(2b-2)x\big)^{b-2} \\
&= x^{-1/2}y^{1/2}(x+y)^{b-2}\big((2b-1)x+y\big)^{b-2} \\
&\ge x^{-1/2}y^{b-3/2}(x+y)^{b-2} > 0, \\
\frac{\partial A}{\partial y}(x,y) &= y^{-1/2}x^{1/2}(x+y)^{b-2}\big((2b-1)y+x\big)^{b-2} \\
&\ge y^{-1/2}x^{b-3/2}(x+y)^{b-2} > 0.
\end{aligned}$$

Thus, A is a strictly increasing function in each variable and thus:

$$2\sqrt{xy}\,(x+y)^{b-1} = A(x,y) \ge A(\delta,\delta) = (2\delta)^b,$$

with equality if and only if $x = y = \delta$. Hence:

$$\begin{aligned}
(2\delta)^b\,\frac{x+y}{2\sqrt{xy}} &\le (x+y)^b \qquad \forall\, x,y \in [\delta,\Delta], \\
\frac{d_i+d_j}{2\sqrt{d_id_j}} &\le (2\delta)^{-b}(d_i+d_j)^b \qquad \forall\, ij \in E(H), \\
AG(H) &\le B_b\,\chi_b(H),
\end{aligned}$$

and the equality in this last inequality is attained if and only if $d_i = d_j = \delta$ for every $ij \in E(H)$, i.e., H is a regular graph. □

Remark 2. *The proof of Theorem 3 allows us to obtain that:*

$$A_b\,\chi_b(H) \le AG(H),$$

with:

$$A_b := \begin{cases} (2\delta)^{-b}, & \text{if } b < 0, \\ (2\Delta)^{-b}, & \text{if } b \ge 0. \end{cases}$$

However, this inequality is direct, since:

$$AG(H) \ge m = \sum_{ij\in E(H)} \frac{(d_i+d_j)^b}{(d_i+d_j)^b} \ge A_b \sum_{ij\in E(H)} (d_i+d_j)^b = A_b\,\chi_b(H).$$

Theorem 3 has the following consequence for the first Zagreb, harmonic and sum-connectivity indices.

Corollary 2. *Let H be a graph with minimum degree δ and maximum degree Δ. Then:*

$$\begin{aligned}
AG(H) &\le \frac{1}{2\delta}\,M_1(H), \\
AG(H) &\le \frac{1}{2}\max\left\{\frac{1}{2}\,(\Delta\delta)^{-1/2}(\Delta+\delta)^2,\, 2\Delta\right\} Har(H), \\
AG(H) &\le \max\left\{\frac{1}{2}\,(\Delta\delta)^{-1/2}(\Delta+\delta)^{3/2},\, (2\Delta)^{1/2}\right\} \chi(H).
\end{aligned}$$

The following result relates AG and SDD indices.

Theorem 4. *Let H be a graph with m edges, minimum degree δ and maximum degree Δ. Then:*

$$\frac{\sqrt{\Delta\delta}}{\Delta+\delta}\Big(\frac{1}{2}\,SDD(H)+m\Big) \le AG(H) \le \frac{1}{4}\,SDD(H)+\frac{1}{2}\,m.$$

The equality in the lower bound is attained if H is a regular or biregular graph. The equality in the upper bound is attained if and only if each connected component of H is a regular graph.

Proof. Lemma 1 gives:

$$\begin{aligned}\frac{\Delta+\delta}{\sqrt{\Delta\delta}}\,AG(H) &= \sum_{ij\in E(H)} \frac{\Delta+\delta}{\sqrt{\Delta\delta}}\,\frac{d_i+d_j}{2\sqrt{d_id_j}} \ge \frac{1}{2}\sum_{ij\in E(H)}\left(\frac{d_i+d_j}{\sqrt{d_id_j}}\right)^2\\ &= \frac{1}{2}\sum_{ij\in E(H)}\left(\sqrt{\frac{d_i}{d_j}}+\sqrt{\frac{d_j}{d_i}}\right)^2 = \frac{1}{2}\sum_{ij\in E(H)}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)+\frac{1}{2}\sum_{ij\in E(H)}2\\ &= \frac{1}{2}\,SDD(H)+m.\end{aligned}$$

If H is a regular or biregular graph, then:

$$\begin{aligned}\frac{\sqrt{\Delta\delta}}{\Delta+\delta}\Big(\frac{1}{2}\,SDD(H)+m\Big) &= \frac{1}{2}\,\frac{\sqrt{\Delta\delta}}{\Delta+\delta}\Big(\Big(\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\Big)m+2m\Big)\\ &= \frac{1}{2}\,\frac{\sqrt{\Delta\delta}}{\Delta+\delta}\Big(\frac{\Delta^2+\delta^2+2\Delta\delta}{\Delta\delta}\Big)m = \frac{\Delta+\delta}{2\sqrt{\Delta\delta}}\,m = AG(H).\end{aligned}$$

Lemma 1 gives:

$$\begin{aligned}AG(H) &= \sum_{ij\in E(H)} \frac{d_i+d_j}{2\sqrt{d_id_j}} \le \frac{1}{4}\sum_{ij\in E(H)}\left(\frac{d_i+d_j}{\sqrt{d_id_j}}\right)^2\\ &= \frac{1}{4}\sum_{ij\in E(H)}\left(\sqrt{\frac{d_i}{d_j}}+\sqrt{\frac{d_j}{d_i}}\right)^2 = \frac{1}{4}\sum_{ij\in E(H)}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)+\frac{1}{4}\sum_{ij\in E(H)}2\\ &= \frac{1}{4}\,SDD(H)+\frac{1}{2}\,m.\end{aligned}$$

If the equality in this bound is attained, then Lemma 1 gives $d_i = d_j$ for every $ij \in E(H)$ and so, each connected component of H is a regular graph.

If each connected component of H is a regular graph, then:

$$\frac{1}{4}\,SDD(H)+\frac{1}{2}\,m = \frac{1}{4}\big(2m+2m\big) = m = AG(H).$$

□

It is easy to check that $SDD(H) \ge 2m$ and thus, Theorem 4 has the following consequence.

Corollary 3. *Let H be a graph. Then:*

$$AG(H) \le \frac{1}{2}\,SDD(H).$$

The inequality in Corollary 3 appears in [30, Theorem 10] for connected graphs. (Note that the definition of SDD in [30] is slightly different.) Our argument gives it for general graphs, and Theorem 4 improves this inequality.

We present here elementary relations between AG, Mm_{sde} and Mm_{sde} indices.

Proposition 1. *If H is a graph, then:*

$$AG(H) = \frac{1}{2}\, Mm_{sde}(H) + \frac{1}{2}\, mM_{sde}(H), \qquad AG(H) \le Mm_{sde}(H).$$

The equality in the bound is attained if and only if each connected component of H is a regular graph.

Proof. We have:

$$\begin{aligned} AG(H) &= \sum_{ij\in E(H)} \frac{d_i + d_j}{2\sqrt{d_i d_j}} = \frac{1}{2} \sum_{ij\in E(H)} \left(\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}} \right) \\ &= \frac{1}{2} \sum_{ij\in E(H)} \left(\sqrt{\frac{\max\{d_i, d_j\}}{\min\{d_i, d_j\}}} + \sqrt{\frac{\min\{d_i, d_j\}}{\max\{d_i, d_j\}}} \right) \\ &= \frac{1}{2}\, Mm_{sde}(H) + \frac{1}{2}\, mM_{sde}(H). \end{aligned}$$

In addition:

$$AG(H) = \sum_{ij\in E(H)} \frac{1}{2} \left(\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}} \right) \le \sum_{ij\in E(H)} \sqrt{\frac{\max\{d_i, d_j\}}{\min\{d_i, d_j\}}} = Mm_{sde}(H).$$

The bound is tight if and only if:

$$\sqrt{\frac{d_i}{d_j}} = \sqrt{\frac{d_j}{d_i}} = \sqrt{\frac{\max\{d_i, d_j\}}{\min\{d_i, d_j\}}}$$

for every $ij \in E(H)$, i.e., $d_i = d_j$ for every $ij \in E(H)$, and this happens if and only if each connected component of H is a regular graph. □

3. A General Bound of the AG Index

In this section. we find and show optimal inequalities, which do not involve other topological indices, for the topological index AG as a function of graph invariants such as the number of edges and the minimum and maximum degree.

We will need the following definitions. Given a graph H 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

$$\begin{aligned} A_0 &= \{ij \in E(H) : d_i = \delta, d_j = \Delta\}, \\ A_1 &= \{ij \in E(H) : d_i = \delta, \delta < d_i < \Delta\}, \\ A_2 &= \{ij \in E(H) : d_i = \Delta, \delta < d_j < \Delta\}, \end{aligned}$$

respectively.

Theorem 5. *Let H be a graph with maximum degree Δ, minimum degree $\delta < \Delta - 1$ and m edges. Then:*

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

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

Proof. Let us consider the function $g(t) = \frac{1+t^2}{2t}$ on the interval $(0, \infty)$. We have $g'(t) = \frac{t^2-1}{2t^2}$, therefore $g'(t) < 0$ for $t \in (0,1)$ and $g'(t) > 0$ for $t \in (1, \infty)$. Then, g decreases on $(0,1]$ and g increases on $[1, \infty)$.

From the above argument, it follows that the function:

$$\frac{\delta + d_j}{2\sqrt{\delta d_j}} = g\left(\left(\frac{d_j}{\delta}\right)^{1/2}\right)$$

is increasing in $d_j \in (\delta, \Delta)$ and thus:

$$\frac{\delta + (\delta+1)}{2\sqrt{\delta(\delta+1)}} \le \frac{\delta + d_j}{2\sqrt{\delta d_j}} \le \frac{\delta + \Delta - 1}{2\sqrt{\delta(\Delta-1)}},$$

for every $ij \in A_1$.

In a similar way, the function:

$$\frac{\Delta + d_j}{2\sqrt{\Delta d_j}} = g\left(\left(\frac{d_j}{\Delta}\right)^{1/2}\right)$$

is decreasing in $d_j \in (\delta, \Delta)$ and thus:

$$\frac{\Delta + (\Delta-1)}{2\sqrt{\Delta(\Delta-1)}} \le \frac{\Delta + d_j}{2\sqrt{\Delta d_j}} \le \frac{\Delta + \delta + 1}{2\sqrt{\Delta(\delta+1)}},$$

for every $ij \in A_2$.

Since:

$$1 \le \frac{d_i + d_j}{2\sqrt{d_i d_j}} \le \frac{\Delta + \delta}{2\sqrt{\Delta\delta}}$$

for every $ij \in E(H)$, we have:

$$\begin{aligned} AG(H) &= \sum_{ij \in E(H) \setminus A_0 \cup A_1 \cup A_2} \frac{d_i + d_j}{2\sqrt{d_i d_j}} + \sum_{ij \in A_0} \frac{d_i + d_j}{2\sqrt{d_i d_j}} + \sum_{ij \in A_1} \frac{d_i + d_j}{2\sqrt{d_i d_j}} + \sum_{ij \in A_2} \frac{d_i + d_j}{2\sqrt{d_i d_j}} \\ &= \sum_{ij \in E(H) \setminus A_0 \cup A_1 \cup A_2} \frac{d_i + d_j}{2\sqrt{d_i d_j}} + \sum_{ij \in A_0} \frac{\Delta + \delta}{2\sqrt{\Delta\delta}} + \sum_{ij \in A_1} \frac{\delta + d_j}{2\sqrt{\delta d_j}} + \sum_{ij \in A_2} \frac{\Delta + d_j}{2\sqrt{\Delta d_j}}, \end{aligned}$$

therefore:

$$AG(H) \ge m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{\Delta + \delta}{2\sqrt{\Delta\delta}} + \alpha_1 \frac{2\delta + 1}{2\sqrt{\delta(\delta+1)}} + \alpha_2 \frac{2\Delta - 1}{2\sqrt{\Delta(\Delta-1)}},$$

and:

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

□

Lemma 2. *If* $v(t) = \frac{1+t}{2\sqrt{t}}$*, then:* (1) $v(t) \le \frac{1}{8}(1-t)^2 + 1$ *for every* $t \in [1, \infty)$,

(2) $v(t) \ge \frac{1}{16}(1-t)^2 + 1$ *for every* $t \in (0, 1.945]$.

Proof. We have for every $s \in [1, \infty)$ and $t = s^2 \in [1, \infty)$:

$$
\begin{aligned}
(s-1)^3(s^2+3s+4) &\geq 0, \\
s^5 - 2s^3 - 4s^2 + 9s - 4 &\geq 0, \\
4(s^2+1) &\leq s\big(8 + (1-s^2)^2\big), \\
v(t) = \frac{t+1}{2\sqrt{t}} &\leq \frac{1}{8}(1-t)^2 + 1.
\end{aligned}
$$

Let $s_1 = 1.39485...$ be the unique real solution of $s^3 + 2s^2 + s - 8 = 0$ in the interval $(0, \infty)$. We have for every $s \in [0, s_1]$ and $t = s^2 \in (0, 1.945] \subset (0, s_1^2]$:

$$
\begin{aligned}
(s-1)^2(s^3+2s^2+s-8) &\leq 0, \\
s^5 - 2s^3 - 8s^2 + 17s - 8 &\leq 0, \\
8(s^2+1) &\geq s\big(16 + (1-s^2)^2\big), \\
v(t) = \frac{1+t}{2\sqrt{t}} &\geq \frac{1}{16}(1-t)^2 + 1.
\end{aligned}
$$

□

Proposition 2. *Let H be a graph with maximum degree Δ, minimum degree $\delta < \Delta - 1$ and m edges.*

1. *If δ is an even integer, then:*

$$
AG(H) \geq m + \min\left\{ \frac{\Delta+\delta}{2\sqrt{\Delta\delta}} + \frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} - 2,\ \frac{2\delta+1}{\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 3 \right\}.
$$

2. *If Δ is an even integer, then:*

$$
AG(H) \geq m + \min\left\{ \frac{\Delta+\delta}{2\sqrt{\Delta\delta}} + \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 2,\ \frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{\sqrt{\Delta(\Delta-1)}} - 3 \right\}.
$$

3. *If δ and Δ are even integers, then:*

$$
AG(H) \geq m + \frac{2\delta+1}{\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{\sqrt{\Delta(\Delta-1)}} - 4.
$$

Proof. Assume first that δ is an even integer.

Let H_1 be the subgraph of H induced by the n_1 vertices with degree δ in $V(H)$, and denote by m_1 the cardinality of the set of edges of H_1. Handshaking Lemma gives $n_1\delta - \alpha_0 - \alpha_1 = 2m_1$. Since δ is an even integer, $\alpha_0 + \alpha_1$ is also an even integer; since each component of H is a connected graph, we have $\alpha_0 + \alpha_1 \geq 1$ and so, $\alpha_0 + \alpha_1 \geq 2$.

If $\alpha_0 \geq 2$, then Theorem 5 gives:

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

If $\alpha_0 = 1$, then $\alpha_1 \geq 1$ and Theorem 5 gives:

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

If $\alpha_0 = 0$, then $\alpha_1 \geq 2$ and $\alpha_2 \geq 1$, and Theorem 5 gives:

$$\begin{aligned} AG(H) &\geq m + \alpha_0\left(\frac{\delta+\Delta}{2\sqrt{\delta\Delta}} - 1\right) + \alpha_1\left(\frac{1+2\delta}{2\sqrt{(\delta+1)\delta}} - 1\right) + \alpha_2\left(\frac{2\Delta-1}{2\sqrt{(\Delta-1)\Delta}} - 1\right) \\ &\geq m + \frac{2\delta+1}{\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 3. \end{aligned}$$

Since Lemma 1 gives:

$$\frac{\Delta+\delta}{2\sqrt{\Delta\delta}} \geq \frac{2\delta+1}{2\sqrt{\delta(\delta+1)}},$$

we have:

$$AG(H) \geq m + \min\left\{\frac{\delta+\Delta}{2\sqrt{\delta\Delta}} + \frac{2\delta+1}{2\sqrt{(\delta+1)\delta}} - 2,\ \frac{2\delta+1}{\sqrt{(\delta+1)\delta}} + \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 3\right\}.$$

Assume now that Δ is an even integer. Let H_2 be the subgraph of H induced by the n_2 vertices with a degree Δ in $V(H)$, and denote by m_2 the cardinality of the set of edges of H_2. Handshaking Lemma gives $n_2\Delta - \alpha_0 - \alpha_2 = 2m_2$. Since Δ is an even integer, $\alpha_0 + \alpha_2$ is also an even integer; since each component of H is a connected graph, we have $\alpha_0 + \alpha_2 \geq 1$ and thus, $\alpha_0 + \alpha_2 \geq 2$.

If $\alpha_0 \geq 2$, then Theorem 5 gives:

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

If $\alpha_0 = 1$, then $\alpha_2 \geq 1$ and Theorem 5 gives:

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

If $\alpha_0 = 0$, then $\alpha_2 \geq 2$ and $\alpha_1 \geq 1$, and Theorem 5 gives:

$$\begin{aligned} AG(H) &\geq m + \alpha_0\left(\frac{\delta+\Delta}{2\sqrt{\delta\Delta}} - 1\right) + \alpha_1\left(\frac{1+2\delta}{2\sqrt{(\delta+1)\delta}} - 1\right) + \alpha_2\left(\frac{2\Delta-1}{2\sqrt{(\Delta-1)\Delta}} - 1\right) \\ &\geq m + \frac{1+2\delta}{2\sqrt{(\delta+1)\delta}} + \frac{2\Delta-1}{\sqrt{\Delta(\Delta-1)}} - 3. \end{aligned}$$

Since:

$$\frac{\Delta+\delta}{2\sqrt{\Delta\delta}} \geq \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}},$$

we have:

$$AG(H) \geq m + \min\left\{ \frac{\Delta+\delta}{2\sqrt{\Delta\delta}} + \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 2,\ \frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{\sqrt{\Delta(\Delta-1)}} - 3 \right\}.$$

Finally, assume that δ and Δ are even integers. The previous arguments give $\alpha_0 + \alpha_1 \geq 2$ and $\alpha_0 + \alpha_2 \geq 2$.

If $\alpha_0 \geq 2$, then Theorem 5 gives:

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

If $\alpha_0 = 1$, then $\alpha_1, \alpha_2 \geq 1$ and Theorem 5 gives:

$$\begin{aligned} AG(H) &\geq m + \alpha_0\left(\frac{\delta+\Delta}{2\sqrt{\delta\Delta}} - 1\right) + \alpha_1\left(\frac{1+2\delta}{2\sqrt{(\delta+1)\delta}} - 1\right) + \alpha_2\left(\frac{2\Delta-1}{2\sqrt{(\Delta-1)\Delta}} - 1\right) \\ &\geq m + \frac{\Delta+\delta}{2\sqrt{\Delta\delta}} + \frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 3. \end{aligned}$$

If $\alpha_0 = 0$, then $\alpha_1, \alpha_2 \geq 2$, and Theorem 5 gives:

$$\begin{aligned} AG(H) &\geq m + \alpha_0\left(\frac{\Delta+\delta}{2\sqrt{\Delta\delta}} - 1\right) + \alpha_1\left(\frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} - 1\right) + \alpha_2\left(\frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 1\right) \\ &\geq m + \frac{2\delta+1}{\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{\sqrt{\Delta(\Delta-1)}} - 4. \end{aligned}$$

We claim now:

$$1 + \frac{\delta+\Delta}{2\sqrt{\delta\Delta}} \geq \frac{1+2\delta}{2\sqrt{(\delta+1)\delta}} + \frac{2\Delta-1}{2\sqrt{(\Delta-1)\Delta}}.$$

Assuming that this inequality holds, we have:

$$m + \frac{\delta+\Delta}{\sqrt{\delta\Delta}} - 2 \geq m + \frac{\delta+\Delta}{2\sqrt{\delta\Delta}} + \frac{1+2\delta}{2\sqrt{(\delta+1)\delta}} + \frac{2\Delta-1}{2\sqrt{(\Delta-1)\Delta}} - 3,$$

$$m + \frac{\Delta+\delta}{2\sqrt{\Delta\delta}} + \frac{2\delta+1}{2\sqrt{(\delta+1)\delta}} + \frac{2\Delta-1}{2\sqrt{(\Delta-1)\Delta}} - 3 \geq m + \frac{1+2\delta}{\sqrt{(\delta+1)\delta}} + \frac{2\Delta-1}{\sqrt{(\Delta-1)\Delta}} - 4,$$

and we conclude:

$$AG(H) \geq m + \frac{1+2\delta}{\sqrt{(\delta+1)\delta}} + \frac{2\Delta-1}{\sqrt{\Delta(\Delta-1)}} - 4.$$

Thus, it suffices to prove the claim.

$$\begin{aligned} 1 + \frac{\delta+\Delta}{2\sqrt{\delta\Delta}} &\geq \frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}}, \\ 1 + v\left(\frac{\Delta}{\delta}\right) &\geq v\left(\frac{1+\delta}{\delta}\right) + v\left(\frac{\Delta}{\Delta-1}\right), \end{aligned}$$

where $v(t) = \frac{1+t}{2\sqrt{t}}$ is the function in Lemma 2. Since v is an increasing function in $[1, \infty)$ and $\Delta \geq \delta + 2$, we have:

$$v\Big(\frac{2+\delta}{\delta}\Big) \leq v\Big(\frac{\Delta}{\delta}\Big), \qquad v\Big(\frac{\Delta}{\Delta-1}\Big) \leq v\Big(\frac{2+\delta}{1+\delta}\Big).$$

Hence, it suffices to show:

$$1 + v\Big(\frac{2+\delta}{\delta}\Big) \geq v\Big(\frac{1+\delta}{\delta}\Big) + v\Big(\frac{2+\delta}{1+\delta}\Big), \tag{2}$$

for every $\delta \geq 1$.

Note that (2) holds for $\delta = 1, 2$. Let us prove that it holds for $\delta \geq 3$. Note that:

$$\frac{1/8}{(\delta+1)^2} \leq \frac{1/8}{\delta^2}, \qquad 2 + \frac{1/8}{\delta^2} + \frac{1/8}{(\delta+1)^2} \leq 2 + \frac{1/4}{\delta^2}.$$

Since $\delta \geq 3$, we have:

$$\frac{2+\delta}{\delta} \leq \frac{5}{3} < 1.945, \qquad \frac{1+\delta}{\delta} > 1, \qquad \frac{2+\delta}{1+\delta} > 1.$$

Thus, Lemma 2 gives:

$$\begin{aligned} v\Big(\frac{1+\delta}{\delta}\Big) + v\Big(\frac{2+\delta}{1+\delta}\Big) &\leq 1 + \frac{1}{8}\Big(\frac{1+\delta}{\delta} - 1\Big)^2 + 1 + \frac{1}{8}\Big(\frac{2+\delta}{1+\delta} - 1\Big)^2 \\ &= 2 + \frac{1/8}{\delta^2} + \frac{1/8}{(\delta+1)^2} \leq 2 + \frac{1/4}{\delta^2} \\ &= 1 + 1 + \frac{1}{16}\Big(1 - \frac{2+\delta}{\delta}\Big)^2 \leq 1 + v\Big(\frac{2+\delta}{\delta}\Big). \end{aligned}$$

These inequalities give (2) for $\delta \geq 3$, and the proof is finished. □

Finally, we show that the bound in Proposition 2 (3) is tight: let us consider the complete graphs K_5 and K_3, and fix $u_1, u_2 \in V(K_5)$ and $v_1, v_2 \in V(K_3)$. Denote by K_5^* the graph obtained from K_5 by deleting the edge u_1u_2. Let Γ be the graph with $V(\Gamma) = V(K_5^*) \cup V(K_3)$ and $E(\Gamma) = E(K_5^*) \cup E(K_3) \cup \{u_1v_1\} \cup \{u_2v_2\}$. Thus, Γ has a maximum degree $\Delta = 4$, minimum degree $\delta = 2$, $\alpha_0 = 0$, $\alpha_1 = 2$, $\alpha_2 = 2$; in addition, if $ij \notin A_0 \cup A_1 \cup A_2$, then $d_i = d_j$, if $ij \in A_1$, then $\{d_i, d_j\} = \{\delta, \delta+1\}$, and if $ij \in A_2$, then $\{d_i, d_j\} = \{\Delta, \Delta - 1\}$. Then, we have:

$$AG(\Gamma) = m + \frac{2\delta+1}{\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{\sqrt{\Delta(\Delta-1)}} - 4.$$

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 associated with topological indices is that of determining optimal bounds and relations between known topological indices—particularly to obtain bounds for the topological indices associated with the invariant parameters of a graph.

Ref. [35] proves that many upper bounds of GA are not useful, and shows the importance of obtaining upper bounds of GA that are less than m. In a similar way, it is important to find lower bounds of AG greater than m.

With this aim, we obtain in this paper several new lower bounds of AG, which are greater than m for graphs with a maximum degree Δ and minimum degree $\delta < \Delta - 1$:

1. If δ is an even integer, then:

$$AG(H) \geq m + \min\left\{ \frac{\Delta+\delta}{2\sqrt{\Delta\delta}} + \frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} - 2,\ \frac{2\delta+1}{\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 3 \right\}.$$

2. If Δ is an even integer, then:

$$AG(H) \geq m + \min\left\{ \frac{\Delta+\delta}{2\sqrt{\Delta\delta}} + \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 2,\ \frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{\sqrt{\Delta(\Delta-1)}} - 3 \right\}.$$

3. If δ and Δ are even integers, then:

$$AG(H) \geq m + \frac{2\delta+1}{\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{\sqrt{\Delta(\Delta-1)}} - 4.$$

We obtain several inequalities relating AG with other topological indices, as

$$\frac{\sqrt{\Delta\delta}}{\Delta+\delta}\left(\frac{1}{2}SDD(H) + m\right) \leq AG(H) \leq \frac{1}{4}SDD(H) + \frac{1}{2}m.$$

This result improves the following bound already known in the literature:

$$AG(H) \leq \frac{1}{2}SDD(H).$$

Moreover, we find families of graphs where the bounds are attained.

Furthermore, we show that at least for entropy, the AG index has better predictive power than GA, while for other physicochemical properties, the GA index has better predictive power than AG.

We think that it would be interesting to obtain for the geometric–arithmetic index some results similar to those included in this work for the AG index.

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