RELATIONS BETWEEN ARITHMETIC-GEOMETRIC INDEX AND GEOMETRIC-ARITHMETIC INDEX

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The arithmetic-geometric index $AG(G)$ and the geometric-arithmetic index $GA(G)$ of a graph G are defined as $AG(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}}$ and $GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$, where $E(G)$ is the edge set of G, and $d_G(u)$ and $d_G(v)$ are the degrees of vertices u and v, respectively. We study relations between $AG(G)$ and $GA(G)$ for graphs G of given size, minimum degree and maximum degree. We present lower and upper bounds on $AG(G) + GA(G)$, $AG(G) - GA(G)$ and $AG(G) \cdot GA(G)$. All the bounds are sharp.

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1. INTRODUCTION

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex $v \in V(G)$ is the number of edges incident with v. In a regular graph, any two vertices have the same degree. A molecular graph is a connected graph in which each vertex has degree at most 4. A bipartite graph is a graph whose vertices can be partitioned into two partite sets, such that no two vertices in the same set are adjacent. A semiregular bipartite graph is a bipartite graph such that every two vertices in the same partite set have the same degree, and any two vertices from different partite sets have distinct degrees. That graph is called (d_1, d_2)-semiregular bipartite, if the degrees of the vertices are d_1 and d_2.

Degree-based topological indices have been used in mathematical chemistry for several decades. The geometric-arithmetic index

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)}$$

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of a graph G has been introduced by Vukičević and Furtula [17] in 2009. The arithmetic-geometric index

$$AG(G) = \sum_{uv \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) d_G(v)}} = \frac{1}{2} \sum_{uv \in E(G)} \left[\sqrt{\frac{d_G(u)}{d_G(v)}} + \sqrt{\frac{d_G(v)}{d_G(u)}} \right]$$

is even newer, as it was introduced in 2015 ([14]).

A lot of research has been done on both indices. The AG index was investigated for example in [10], [11] and [13], and the GA index in [3], [6], [12] and [15]. Chemical applications of the GA index were studied for instance in [1], [17] and [19], and many interesting results can be found in the survey paper [8]. Degree-based indices were investigated also in [2] and [18].

Relations between the AG index and GA index have been studied by several researchers. Cui et al. [5] and Vujošević et al. [16] showed that $GA(G) \leq AG(G)$ which means that

$$AG(G) - GA(G) \geq 0 \quad \text{and} \quad \frac{AG(G)}{GA(G)} \geq 1.$$

Cui et al. [5] also showed that

$$\frac{AG(G)}{GA(G)} \leq \frac{(n + \delta - 1)^2}{4(n-1)\delta}, \quad \text{thus} \quad \frac{AG(G)}{GA(G)} \leq \frac{n^2}{4(n-1)}$$

for connected graphs with n vertices (and minimum degree δ). The latter result was obtained also by Vujošević et al. [16] who gave lower and upper bounds on $AG(G) + GA(G)$, $AG(G) - GA(G)$, $AG(G) \cdot GA(G)$ and $\frac{AG(G)}{GA(G)}$ for connected graphs G of given order. Gutman [9] showed that

$$AG(G) \cdot GA(G) \leq \frac{1}{8} \frac{(\sqrt{\delta} + \sqrt{\Delta})^4}{(\delta + \Delta)\sqrt{\delta\Delta}} \, m^2$$

for graphs with m edges, minimum degree δ and maximum degree Δ.

Motivated by the works [5], [9] and [16], we study relations between $AG(G)$ and $GA(G)$. We extend known results in the area for graphs G of given size, minimum degree and maximum degree. We present lower and upper bounds on $AG(G) + GA(G)$, $AG(G) - GA(G)$ and $AG(G) \cdot GA(G)$. All the bounds are sharp.

Our first theorem is expressed in terms of $M_1(G)$ and $R_{\frac{1}{2}}(G)$, therefore, we present definitions of those indices too. For $\alpha \in \mathbb{R}$, the general Randić index

$$R_\alpha(G) = \sum_{uv \in E(G)} [d_G(u) d_G(v)]^\alpha,$$

of a graph G was introduced by Bollobás and Erdős [4]. Special cases of the general Randić index have been extensively studied, especially the Randić index and second Zagreb index which are obtained if $\alpha = -\frac{1}{2}$ and $\alpha = 1$, respectively. The first Zagreb index

$$M_1(G) = \sum_{v\in V(G)} [d_G(v)]^2 = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]$$

also belongs to the most well-known topological indices.

2. RESULTS

In Theorem 2.1, Corollary 2.1 and Theorem 2.2, we present bounds on $AG(G) + GA(G)$.

THEOREM 2.1. *Let G be a graph with m edges and maximum degree Δ. Then*

$$AG(G) + GA(G) \geq 2m + \frac{[M_1(G) - 2R_{\frac{1}{2}}(G)]^2}{2m(2\Delta - 1)\sqrt{\Delta(\Delta - 1)}}.$$

The equality holds if and only if G is a regular graph or a $(\Delta, \Delta-1)$-semiregular bipartite graph.

Proof. If G is regular, then for any edge $uv \in E(G)$, we have $d_G(u) = d_G(v) = \Delta$,

$$AG(G) = m\left(\frac{\Delta + \Delta}{2\sqrt{\Delta^2}}\right) = m, \qquad GA(G) = m\left(\frac{2\sqrt{\Delta^2}}{\Delta + \Delta}\right) = m,$$

$$M_1(G) = m(\Delta + \Delta) = 2m\Delta \quad \text{and} \quad R_{\frac{1}{2}}(G) = m\sqrt{\Delta^2} = m\Delta.$$

So $M_1(G) - 2R_{\frac{1}{2}}(G) = 0$ and $AG(G) + GA(G) = 2m = 2m + \frac{[M_1(G)-2R_{\frac{1}{2}}(G)]^2}{2m(2\Delta-1)\sqrt{\Delta(\Delta-1)}}$. Thus, Theorem 2.1 holds for regular graphs.

Now, we consider graphs G which are not regular. We have

$$\begin{aligned} & AG(G) + GA(G) \\ = & \sum_{uv\in E(G)} \left[\frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u)d_G(v)}} + \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)}\right] \\ = & \sum_{uv\in E(G)} \left[\left(\sqrt{\frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u)d_G(v)}}} - \sqrt{\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)}}\right)^2 + 2\right] \\ = & \ 2m + \sum_{uv\in E(G)} \frac{\left[\sqrt{d_G(u)} - \sqrt{d_G(v)}\right]^4}{2[d_G(u) + d_G(v)]\sqrt{d_G(u)d_G(v)}}. \end{aligned}$$

If $d_G(u) = d_G(v)$, then $\frac{\left[\sqrt{d_G(u)}-\sqrt{d_G(v)}\right]^4}{2[d_G(u)+d_G(v)]\sqrt{d_G(u)d_G(v)}} = 0$, thus

$$AG(G) + GA(G) = 2m + \sum_{\substack{uv \in E(G) \\ d_G(u) \neq d_G(v)}} \frac{\left[\sqrt{d_G(u)} - \sqrt{d_G(v)}\right]^4}{2[d_G(u) + d_G(v)]\sqrt{d_G(u)d_G(v)}}.$$

For $uv \in E(G)$ with $d_G(u) \neq d_G(v)$, at most one of $d_G(u)$, $d_G(v)$ is Δ and the other degree is at most $\Delta - 1$. Therefore

$$AG(G) + GA(G) \geq 2m + \sum_{\substack{uv \in E(G) \\ d_G(u) \neq d_G(v)}} \frac{\left[\sqrt{d_G(u)} - \sqrt{d_G(v)}\right]^4}{2(2\Delta - 1)\sqrt{\Delta(\Delta - 1)}}. \tag{1}$$

By Cauchy-Schwarz inequality, we have

$$\left(\sum_{uv \in E(G)} \left[\sqrt{d_G(u)} - \sqrt{d_G(v)}\right]^2\right)^2 \leq m \sum_{uv \in E(G)} \left[\sqrt{d_G(u)} - \sqrt{d_G(v)}\right]^4. \tag{2}$$

Then

$$\begin{aligned}
& \sum_{\substack{uv \in E(G) \\ d_G(u) \neq d_G(v)}} \left[\sqrt{d_G(u)} - \sqrt{d_G(v)}\right]^4 \\
= & \sum_{uv \in E(G)} \left[\sqrt{d_G(u)} - \sqrt{d_G(v)}\right]^4 \\
\geq & \frac{1}{m} \left(\sum_{uv \in E(G)} \left[d_G(u) + d_G(v) - 2\sqrt{d_G(u)d_G(v)}\right]\right)^2 \\
= & \frac{1}{m} \left[M_1(G) - 2R_{\frac{1}{2}}(G)\right]^2.
\end{aligned}$$

Using this result in (1), we get

$$AG(G) + GA(G) \geq 2m + \frac{[M_1(G) - 2R_{\frac{1}{2}}(G)]^2}{2m(2\Delta - 1)\sqrt{\Delta(\Delta - 1)}}. \tag{3}$$

For a connected graph which is not regular, the equality in (3) holds if and only if we have equalities in (1) and (2). The equality in (1) means that every edge uv with $d_G(u) \neq d_G(v)$ must be incident with one vertex of degree Δ and the other vertex of degree $\Delta - 1$. The equality in (2) means that we have

$$\left[\sqrt{d_G(u)} - \sqrt{d_G(v)}\right]^2 = \left[\sqrt{d_G(u')} - \sqrt{d_G(v')}\right]^2 = \left[\sqrt{\Delta} - \sqrt{\Delta - 1}\right]^2$$

for any two edges $uv, u'v' \in E(G)$. Thus, every edge of G is incident with one vertex of degree Δ and the other vertex of degree $\Delta - 1$. Clearly, G is bipartite, otherwise G would contain an odd cycle and there would be two adjacent vertices having the same degree. Hence G is $(\Delta, \Delta - 1)$-semiregular bipartite graph. □

For connected graphs, the following result was obtained also by Gutman [9].

COROLLARY 2.1. *Let G be a graph with m edges. Then*

$$AG(G) + GA(G) \geq 2m.$$

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

Proof. For regular graphs G, we have $AG(G)+GA(G) = 2m$. For graphs G which are not regular, by (1), we have $AG(G) + GA(G) > 2m$. □

Let G be a graph with maximum degree Δ and minimum degree δ. From the proof of Theorem 4 given in [7], we know that for any two vertices $u, v \in V(G)$,

$$\frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u)d_G(v)}} \leq \frac{\Delta + \delta}{2\sqrt{\Delta\delta}} \tag{4}$$

with equality if and only if $\{d_G(u), d_G(v)\} = \{\delta, \Delta\}$. Note that

$$d_G(u) - 2\sqrt{d_G(u)d_G(v)} + d_G(v) = \left[\sqrt{d_G(u)} - \sqrt{d_G(v)}\right]^2 \geq 0,$$

thus $d_G(u) + d_G(v) \geq 2\sqrt{d_G(u)d_G(v)}$. Consequently,

$$\frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u)d_G(v)}} \geq 1. \tag{5}$$

The equality holds if and only if $d_G(u) = d_G(v)$.

Inequality (4) is used in the proofs of Theorems 2.2, 2.5 and 2.8. Inequality (5) is used in the proofs of Theorems 2.2, 2.4 and 2.5.

THEOREM 2.2. *Let G be a graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$AG(G) + GA(G) \leq \frac{\Delta^2 + \delta^2 + 6\Delta\delta}{2(\Delta + \delta)\sqrt{\Delta\delta}}\, m.$$

The equality holds if and only if G is a regular graph or a (Δ, δ)-semiregular bipartite graph.

Proof. By (4), for any two vertices $u, v \in V(G)$,

$$\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} \le \frac{\Delta+\delta}{2\sqrt{\Delta\delta}}$$

with equality if and only if $\{d_G(u), d_G(v)\} = \{\delta, \Delta\}$. Similarly,

$$-\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)} \le -\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}.$$

By (5),

$$\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} \ge 1 \quad \text{and} \quad 0 < \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)} \le 1.$$

Then

$$0 \le \sqrt{\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}}} - \sqrt{\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}} \le \sqrt{\frac{\Delta+\delta}{2\sqrt{\Delta\delta}}} - \sqrt{\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}}$$

with equality if and only if $\{d_G(u), d_G(v)\} = \{\delta, \Delta\}$. Consequently,

$$\begin{aligned}
& AG(G) + GA(G) \\
= & \sum_{uv\in E(G)} \left[\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} + \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}\right] \\
= & \sum_{uv\in E(G)} \left[\left(\sqrt{\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}}} - \sqrt{\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}}\right)^2 + 2\right] \\
\le & \sum_{uv\in E(G)} \left[\left(\sqrt{\frac{\Delta+\delta}{2\sqrt{\Delta\delta}}} - \sqrt{\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}}\right)^2 + 2\right] \\
= & \sum_{uv\in E(G)} \left[\frac{\Delta+\delta}{2\sqrt{\Delta\delta}} + \frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\right] \\
= & \frac{\Delta^2+\delta^2+6\Delta\delta}{2(\Delta+\delta)\sqrt{\Delta\delta}}\, m.
\end{aligned}$$

The equality holds if and only if $\{d_G(u), d_G(v)\} = \{\delta, \Delta\}$ for every edge $uv \in E(G)$, which means that every edge of G is incident with one vertex of degree Δ and the other vertex of degree δ, so G is a regular graph (if $\Delta = \delta$) or (Δ, δ)-semiregular bipartite graph (if $\Delta > \delta$). □

Let S be the set containing graphs G such that $V(G) = V_1 \cup V_2 \cup \cdots \cup V_p$ $(p \ge 2)$, where

$$V_1 = \{v \in V(G) : d_G(v) = \Delta\},$$

$$
\begin{aligned}
V_2 &= \{v \in V(G) : d_G(v) = r < \Delta\}, \\
V_j &= \left\{v \in V(G) : d_G(v) = \frac{r^{j-1}}{\Delta^{j-2}}\right\},\ j = 3, 4, \ldots, p,
\end{aligned}
$$

and any edge of G is incident with one vertex in V_{k-1} and one vertex in V_k, where $k \in \{2, 3, \ldots, p\}$. We can also write

$$
V_j = \left\{v \in V(G) : d_G(v) = \frac{r^{j-1}}{\Delta^{j-2}}\right\},\ j = 1, 2, \ldots, p.
$$

Clearly, $\frac{r^{j-1}}{\Delta^{j-2}}$ must be an integer for each $j = 1, 2, \ldots, p$, and Δ is the maximum degree of G.

Example 2.3. Let $G \in S$ for $p = 4$, $\Delta = 8$ and $r = 4$. Then $\frac{r^2}{\Delta} = 2$ and $\frac{r^3}{\Delta^2} = 1$. We have $V(G) = V_1 \cup V_2 \cup V_3 \cup V_4$, where

$$
\begin{aligned}
V_1 &= \{v \in V(G) : d_G(v) = 8\}, \qquad V_2 = \{v \in V(G) : d_G(v) = 4\}, \\
V_3 &= \{v \in V(G) : d_G(v) = 2\}, \qquad V_4 = \{v \in V(G) : d_G(v) = 1\}.
\end{aligned}
$$

This graph is presented in Figure 1.

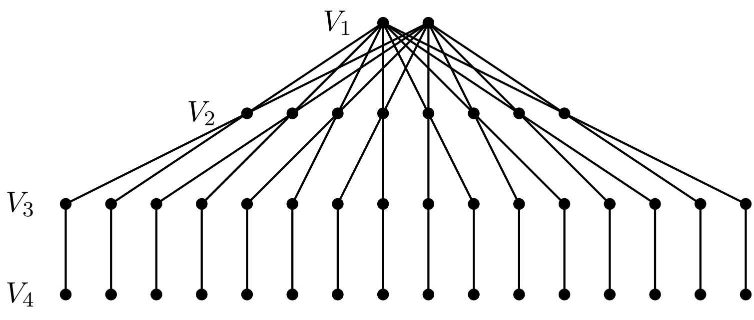

Figure 1 – Graph in S for $p = 4$, $\Delta = 8$ and $r = 4$.

We present the exact value of $AG(G) \cdot GA(G)$ for any graph $G \in S$.

Lemma 2.1. *Let $G \in S$. Then*

$$
AG(G) \cdot GA(G) = m^2,
$$

where m is the number of edges of G.

Proof. Any edge uv of G is incident with one vertex in V_{k-1} and one vertex in V_k, where $k \in \{2, 3, \ldots, p\}$.

$$
\frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) d_G(v)}} = \frac{\frac{r^{k-2}}{\Delta^{k-3}} + \frac{r^{k-1}}{\Delta^{k-2}}}{2\sqrt{\frac{r^{k-2}}{\Delta^{k-3}} \frac{r^{k-1}}{\Delta^{k-2}}}} = \frac{\frac{r^{k-2}}{\Delta^{k-2}}(\Delta + r)}{2\,\frac{r^{k-2}}{\Delta^{k-2}}\sqrt{\Delta r}} = \frac{\Delta + r}{2\sqrt{\Delta r}}.
$$

Hence

$$\begin{aligned} AG(G)\cdot GA(G) &= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} \sum_{uv\in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)} \\ &= m\left(\frac{\Delta+r}{2\sqrt{\Delta r}}\right) m\left(\frac{2\sqrt{\Delta r}}{\Delta+r}\right) \\ &= m^2. \end{aligned}$$

□

We give a lower bound on $AG(G)\cdot GA(G)$ for a graph G of given size.

THEOREM 2.4. *Let G be a graph with m edges. Then*

$$AG(G)\cdot GA(G) \geq m^2.$$

If G is connected, then the equality holds if and only if G is a regular graph or $G \in S$.

Proof. For the i-th edge $uv \in E(G)$, let $\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} = x_i$, where $i = 1, 2, \dots, m$, since $|E(G)| = m$. By (5), we know that the rational numbers $x_i \geq 1$. We can assume that $x_1 \geq x_2 \geq \cdots \geq x_m \geq 1$. Thus, we have

$$\begin{aligned} AG(G)\cdot GA(G) &= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} \sum_{uv\in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)} \\ &= \sum_{k=1}^{m} x_k \sum_{k=1}^{m} \frac{1}{x_k} \\ &= m + \sum_{1\leq i<j\leq m} \left(\frac{x_i}{x_j}+\frac{x_j}{x_i}\right) \\ &= m + \sum_{1\leq i<j\leq m} \left[\left(\sqrt{\frac{x_i}{x_j}}-\sqrt{\frac{x_j}{x_i}}\right)^2 + 2\right] \\ &= m^2 + \sum_{1\leq i<j\leq m} \left(\sqrt{\frac{x_i}{x_j}}-\sqrt{\frac{x_j}{x_i}}\right)^2 \qquad (6) \\ &\geq m^2. \end{aligned}$$

It remains to find the extremal graphs. If $AG(G)\cdot GA(G) = m^2$, then $x_1 = x_2 = \cdots = x_m$. We consider two cases.

Case 1: $x_1 = x_2 = \cdots = x_m = 1$.

For any edge $uv \in E(G)$, we have $\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} = 1$, which implies that $\left[\sqrt{d_G(u)} - \sqrt{d_G(v)}\right]^2 = 0$. Thus $d_G(u) = d_G(v)$. Since G is connected, all the vertices of G have the same degree, so G is a regular graph. Clearly, for a regular graph G, we have $AG(G) = GA(G) = m$ and hence $AG(G) \cdot GA(G) = m^2$.

Case 2: $x_1 = x_2 = \cdots = x_m > 1$.

Note that for any two edges $v_1v_2, v_1v_3 \in E(G)$, we have

$$\frac{d_G(v_1) + d_G(v_2)}{2\sqrt{d_G(v_1)d_G(v_2)}} = \frac{d_G(v_1) + d_G(v_3)}{2\sqrt{d_G(v_1)d_G(v_3)}},$$

which implies that

$$\left[d_G(v_1) - \sqrt{d_G(v_2)d_G(v_3)}\right]\left[\sqrt{d_G(v_2)} - \sqrt{d_G(v_3)}\right] = 0. \tag{7}$$

Let w be any vertex of maximum degree in G. So $d_G(w) = \Delta$. Let u and u' be any two vertices adjacent to w in G. So $wu, wu' \in E(G)$. By (7), we obtain

$$\left[\Delta - \sqrt{d_G(u)d_G(u')}\right]\left[\sqrt{d_G(u)} - \sqrt{d_G(u')}\right] = 0.$$

Since $x_i > 1$ $(1 \le i \le m)$, we have $d_G(u) < \Delta$ and $d_G(u') < \Delta$. (If, say, $d_G(u) = \Delta$, then $\frac{d_G(w)+d_G(u)}{2\sqrt{d_G(w)d_G(u)}} = 1$, a contradiction). Hence $d_G(u) = d_G(u') < \Delta$ for any two neighbors u, u' of w in G. Let $d_G(u) = r$ for any vertex u adjacent to w. Let z $(\neq w)$ be a vertex adjacent to u. So $uw, uz \in E(G)$. By (7), we have

$$\left[r - \sqrt{\Delta d_G(z)}\right]\left[\sqrt{\Delta} - \sqrt{d_G(z)}\right] = 0.$$

We obtain

$$d_G(z) = \Delta \ \text{ or } \ d_G(z) = \frac{r^2}{\Delta}.$$

If G contains a vertex z of degree $\frac{r^2}{\Delta}$, then z has at least one neighbor of degree r and one can easily show that any other vertex adjacent to z has degree r or $\frac{r^3}{\Delta^2}$. In general, if G contains a vertex z' of degree $\frac{r^{j-1}}{\Delta^{j-2}}$, then z' has at least one neighbor of degree $\frac{r^{j-2}}{\Delta^{j-3}}$ and any other vertex adjacent to z' has degree $\frac{r^{j-2}}{\Delta^{j-3}}$ or $\frac{r^j}{\Delta^{j-1}}$, where $j \ge 3$ is an integer. Since G is connected, it follows that $G \in S$. By Lemma 2.1, for $G \in S$, we have $AG(G) \cdot GA(G) = m^2$. □

We obtain an upper bound on $AG(G) \cdot GA(G)$.

THEOREM 2.5. *Let G be a graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$AG(G) \cdot GA(G) \le m^2 + \frac{m_1(m_1-1)}{2} \frac{\left[(\Delta+\delta)\sqrt{\Delta(\Delta-1)} - (2\Delta-1)\sqrt{\Delta\delta}\right]^2}{(2\Delta-1)(\Delta+\delta)\Delta\sqrt{(\Delta-1)\delta}} + \frac{\left(\sqrt{\Delta}-\sqrt{\delta}\right)^4}{\sqrt{\Delta\delta}}(m-m_1)m_1,$$

where m_1 is the number of edges $uv \in E(G)$ with $d_G(u) \neq d_G(v)$. The equality holds if G is a regular graph or a $(\Delta, \Delta-1)$-semiregular bipartite graph.

Proof. For a regular graph G, we have $m_1 = 0$ and $AG(G) \cdot GA(G) = m^2$. So the equality holds in Theorem 2.5.

Let us consider graphs G which are not regular. Since m_1 is the number of edges $uv \in E(G)$ with $d_G(u) \neq d_G(v)$, we have $1 \le m_1 \le m$. For the i-th edge $uv \in E(G)$, let $\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} = x_i$, where $i = 1, 2, \ldots, m$. By (5), we can assume that $x_1 \ge x_2 \ge \cdots \ge x_{m_1} > 1 = x_{m_1+1} = x_{m_1+2} = \cdots = x_m$. From (6), we obtain

$$\begin{aligned} & AG(G) \cdot GA(G) \\ = \; & m^2 + \sum_{1\le i<j\le m_1} \left(\sqrt{\frac{x_i}{x_j}} - \sqrt{\frac{x_j}{x_i}}\right)^2 + \sum_{m_1+1\le i<j\le m} \left(\sqrt{\frac{x_i}{x_j}} - \sqrt{\frac{x_j}{x_i}}\right)^2 \\ & + \sum_{\substack{1\le i\le m_1 \\ m_1+1\le j\le m}} \left(\sqrt{\frac{x_i}{x_j}} - \sqrt{\frac{x_j}{x_i}}\right)^2 \\ = \; & m^2 + \sum_{1\le i<j\le m_1} \left(\sqrt{\frac{x_i}{x_j}} - \sqrt{\frac{x_j}{x_i}}\right)^2 + (m-m_1)\sum_{i=1}^{m_1}\left(\sqrt{x_i} - \frac{1}{\sqrt{x_i}}\right)^2, \end{aligned} \tag{8}$$

since

$$\sum_{m_1+1\le i<j\le m} \left(\sqrt{\frac{x_i}{x_j}} - \sqrt{\frac{x_j}{x_i}}\right)^2 = 0$$

and

$$\sum_{\substack{1\le i\le m_1 \\ m_1+1\le j\le m}} \left(\sqrt{\frac{x_i}{x_j}} - \sqrt{\frac{x_j}{x_i}}\right)^2 = (m-m_1)\sum_{i=1}^{m_1}\left(\sqrt{x_i} - \frac{1}{\sqrt{x_i}}\right)^2.$$

For $uv \in E(G)$ with $d_G(u) > d_G(v)$, we have $d_G(u) - d_G(v) \ge 1$ and $d_G(u)d_G(v) \le \Delta(\Delta-1)$ as Δ is the maximum degree in G. Thus

$$\frac{1}{\Delta(\Delta-1)} \le \frac{[d_G(u)-d_G(v)]^2}{d_G(u)d_G(v)}.$$

Then

$$\frac{1}{\Delta(\Delta-1)} + 4 \le \frac{d_G(u)}{d_G(v)} + \frac{d_G(v)}{d_G(u)} + 2,$$

which gives

$$\frac{(2\Delta-1)^2}{\Delta(\Delta-1)} \le \left(\sqrt{\frac{d_G(u)}{d_G(v)}}+\sqrt{\frac{d_G(v)}{d_G(u)}}\right)^2,$$

and consequently,

$$\frac{2\Delta-1}{\sqrt{\Delta(\Delta-1)}} \le \sqrt{\frac{d_G(u)}{d_G(v)}}+\sqrt{\frac{d_G(v)}{d_G(u)}} = \frac{d_G(u)+d_G(v)}{\sqrt{d_G(u)d_G(v)}}.$$

Thus, for $1 \le i \le m_1$,

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

by (4). Then

$$\left(\sqrt{x_i}-\frac{1}{\sqrt{x_i}}\right)^2 \le \left(\sqrt{\frac{\Delta+\delta}{2\sqrt{\Delta\delta}}}-\sqrt{\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}}\right)^2 = \frac{(\sqrt{\Delta}-\sqrt{\delta})^4}{2(\Delta+\delta)\sqrt{\Delta\delta}}. \tag{9}$$

For $x_i \ge x_j$, where $1 \le i < j \le m_1$, we obtain

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

which gives

$$\sqrt{\frac{x_i}{x_j}}-\sqrt{\frac{x_j}{x_i}} \le \sqrt{\frac{(\Delta+\delta)\sqrt{\Delta(\Delta-1)}}{(2\Delta-1)\sqrt{\Delta\delta}}}-\sqrt{\frac{(2\Delta-1)\sqrt{\Delta\delta}}{(\Delta+\delta)\sqrt{\Delta(\Delta-1)}}}$$

and hence

$$\left(\sqrt{\frac{x_i}{x_j}}-\sqrt{\frac{x_j}{x_i}}\right)^2 \le \frac{\left[(\Delta+\delta)\sqrt{\Delta(\Delta-1)}-(2\Delta-1)\sqrt{\Delta\delta}\right]^2}{(2\Delta-1)(\Delta+\delta)\Delta\sqrt{(\Delta-1)\delta}}. \tag{10}$$

Using (10) and (9) in (8), we obtain

$$\begin{aligned} AG(G)\cdot GA(G) \le m^2 &+ \frac{m_1(m_1-1)}{2}\frac{\left[(\Delta+\delta)\sqrt{\Delta(\Delta-1)}-(2\Delta-1)\sqrt{\Delta\delta}\right]^2}{(2\Delta-1)(\Delta+\delta)\Delta\sqrt{(\Delta-1)\delta}} \\ &+ \frac{\left(\sqrt{\Delta}-\sqrt{\delta}\right)^4}{\sqrt{\Delta\delta}}(m-m_1)m_1, \end{aligned}$$

For a $(\Delta, \Delta-1)$-semiregular bipartite graph G, we have $m_1 = m$ and $\delta = \Delta - 1$. We have $AG(G) = \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}}m$ and $GA(G) = \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}m$, hence $AG(G)\cdot GA(G) = m^2$. So the equality holds in Theorem 2.5. □

Lemma 2.2 is used in the proof of Theorem 2.7.

LEMMA 2.2. *There is no connected graph G with an edge $v_1v_2 \in E(G)$ such that $d_G(v_2) = d_G(v_1) + 1$ and $d_G(u) = d_G(v)$ for all the other edges $uv \in E(G)$.*

Proof. Assume to the contrary that there is a connected graph G with an edge $v_1v_2 \in E(G)$ such that $d_G(v_2) = d_G(v_1)+1$ and $d_G(u) = d_G(v)$ for all the other edges $uv \in E(G)$. Then the degree of any vertex in G is Δ and $\Delta - 1$. So $d_G(v_1) = \Delta - 1$ and $d_G(v_2) = \Delta$.

Note that v_1v_2 is a cut edge (otherwise if v_1v_2 is not a cut edge, then there exists a path $v_1u_1u_2 \ldots u_tv_2$ for $t \geq 1$ in G such that $\Delta-1 = d_G(v_1) = d_G(u_1) = \cdots = d_G(u_t) = d_G(v_2) = \Delta$, a contradiction). Suppose that $G-v_1v_2 = G_1 \cup G_2$, where $v_1 \in V(G_1)$ and $v_2 \in V(G_2)$. Then $d_G(v) = \Delta - 1$ for every $v \in V(G_1)$ and $d_G(v) = \Delta$ for every $v \in V(G_2)$. Let $|E(G_1)| = m_1$ and $|E(G_2)| = m_2$. Then

$$\sum_{v \in V(G_1)} d_{G_1}(v) = (\Delta - 2) + (\Delta - 1)(|V(G_1)| - 1) = (\Delta - 1)|V(G_1)| - 1 = 2m_1$$

and

$$\sum_{v \in V(G_2)} d_{G_2}(v) = (\Delta - 1) + \Delta(|V(G_2)| - 1) = \Delta|V(G_2)| - 1 = 2m_2,$$

which means that both, $(\Delta - 1)|V(G_1)|$ and $\Delta|V(G_2)|$ are odd. However, that is not possible, since $\Delta - 1$ or Δ is even. We have a contradiction. $\square$

Remark 2.6. Having Lemma 2.2, it is natural to ask whether

• there is any connected graph G with an edge $v_1v_2 \in E(G)$ such that $d_G(v_2) = d_G(v_1) + 2$ and $d_G(u) = d_G(v)$ for all the other edges $uv \in E(G)$;

• there is any connected graph G with two edges $v_1v_2, v_1'v_2' \in E(G)$ (possibly sharing a vertex) such that $d_G(v_2) = d_G(v_1)+1$ and $d_G(v_2') = d_G(v_1')+1$, and $d_G(u) = d_G(v)$ for all the other edges $uv \in E(G)$.

The answers are given in Figures 2, 3 and 4.

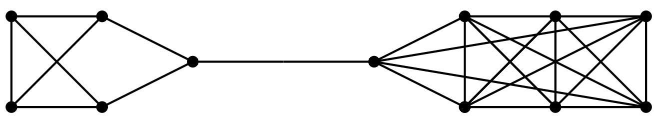

Figure 2 – Graph H_1.

In Figure 2, we present the graph H_1 with an edge $v_1v_2 \in E(G)$ such that $d_G(v_2) = d_G(v_1) + 2$ and $d_G(u) = d_G(v)$ for all the other edges $uv \in E(G)$.

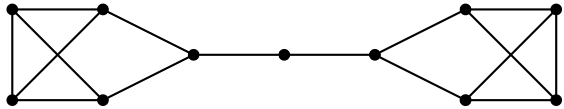

Figure 3 – Graph H_2.

In Figure 3, we present the graph H_2 with two edges $v_1v_2, v_1v_2' \in E(G)$ such that $\{d_G(v_1), d_G(v_2)\} = \{d_G(v_1), d_G(v_2')\} = \{\Delta-1, \Delta\}$ and $d_G(u) = d_G(v)$ for all the other edges $uv \in E(G)$.

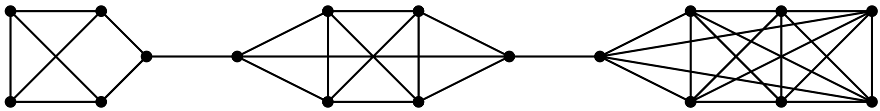

Figure 4 – Graph H_3.

In Figure 4, we present the graph H_3 with two edges $v_1v_2, v_1'v_2' \in E(G)$ such that $\{d_G(v_1), d_G(v_2)\} = \{\Delta-2, \Delta-1\}$ and $\{d_G(v_1'), d_G(v_2')\} = \{\Delta-1, \Delta\}$, and $d_G(u) = d_G(v)$ for all the other edges $uv \in E(G)$.

Bounds on $AG(G) - GA(G)$ are given in Theorems 2.7 and 2.8.

THEOREM 2.7. *Let G be a connected graph with maximum degree Δ and minimum degree δ.*

If $\Delta = \delta + 1$, then

$$AG(G) - GA(G) \geq \frac{1}{(2\Delta - 1)\sqrt{\Delta(\Delta - 1)}}.$$

The equality holds if and only if G contains exactly two edges $uv \in E(G)$ such that $d_G(u) \neq d_G(v)$.

If $\Delta \neq \delta + 1$, then

$$AG(G) - GA(G) \geq \frac{\Delta - \delta}{2(2\Delta - 1)\sqrt{\Delta(\Delta - 1)}}.$$

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

Proof. We distinguish two cases.

Case 1: $\Delta = \delta + 1$.

For any edge $uv \in E(G)$ with $d_G(u) = d_G(v)$, we have

$$\frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u)d_G(v)}} = 1 = \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)}.$$

For any edge $uv \in E(G)$ with $d_G(u) \neq d_G(v)$, we have $\{d_G(u), d_G(v)\} = \{\Delta - 1, \Delta\}$, so

$$\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} = \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} \quad \text{and} \quad \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)} = \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}.$$

By Lemma 2.2, there exist at least two edges $uv \in E(G)$ such that $d_G(u) \neq d_G(v)$, thus

$$\begin{aligned} AG(G) - GA(G) &= \sum_{uv \in E(G)} \left[\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} - \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)} \right] \\ &= \sum_{\substack{uv \in E(G) \\ d_G(v_i) \neq d_G(v_j)}} \left[\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} - \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)} \right] \\ &= \sum_{\substack{uv \in E(G) \\ d_G(u) \neq d_G(v)}} \left[\frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \right] \\ &\geq 2 \left[\frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \right] \\ &= \frac{1}{(2\Delta-1)\sqrt{\Delta(\Delta-1)}}. \end{aligned}$$

The equality holds if and only if G contains exactly two edges $uv \in E(G)$ such that $d_G(u) \neq d_G(v)$ (which means that $\{d_G(u), d_G(v)\} = \{\Delta - 1, \Delta\}$).

Case 2: $\Delta \neq \delta + 1$.

For a regular graph G, we have $\delta = d_G(u) + d_G(v) = \Delta$ and

$$\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} = 1 = \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}$$

for any edge $uv \in E(G)$. Thus $AG(G) = m$, $GA(G) = m$ and

$$AG(G) - GA(G) = 0 = \frac{\Delta - \delta}{2(2\Delta-1)\sqrt{\Delta(\Delta-1)}}.$$

Hence, the equality holds in Theorem 2.7.

Now we consider graphs G which are not regular. So $\Delta \geq \delta + 2$. There exists an edge $uv \in E(G)$ such that $d_G(u) = \delta \leq \Delta - 2$ and $d_G(v) \leq \Delta$. Then

$$[d_G(u) + d_G(v)]\sqrt{d_G(u)d_G(v)} \leq 2(\Delta-1)\sqrt{\Delta(\Delta-2)} < (2\Delta-1)\sqrt{\Delta(\Delta-1)}.$$

For all the other edges $uv \in E(G)$ such that $d_G(u) \neq d_G(v)$, we have $[d_G(u) + d_G(v)]\sqrt{d_G(u)d_G(v)} \leq (2\Delta - 1)\sqrt{\Delta(\Delta - 1)}$. Thus

$$\begin{aligned} AG(G) - GA(G) &= \sum_{\substack{uv\in E(G)\\ d_G(u)\neq d_G(v)}} \left[\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}} - \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}\right] \\ &= \sum_{\substack{uv\in E(G)\\ d_G(u)\neq d_G(v)}} \frac{[d_G(u)-d_G(v)]^2}{2(d_G(u)+d_G(v))\sqrt{d_G(u)d_G(v)}} \\ &> \sum_{\substack{uv\in E(G)\\ d_G(u)\neq d_G(v)}} \frac{[d_G(u)-d_G(v)]^2}{2(2\Delta-1)\sqrt{\Delta(\Delta-1)}}. \qquad (11) \end{aligned}$$

Since G is connected, G contains a path $v_1v_2\ldots v_p$, where $d_G(v_1) = \Delta$, $d_G(v_p) = \delta$, $p \geq 2$ and $\delta < d_G(v_i) < \Delta$ for $2 \leq i \leq p-1$. Let r be the number of edges v_iv_{i+1} such that $d_G(v_i) \neq d_G(v_{i+1})$, where $1 \leq i \leq p-1$. We denote the degrees of the vertices $v_1, v_2, \ldots, v_p$ by

$$\Delta = d_1, \underbrace{d_2, \ldots, d_2}_{t_2}, \underbrace{d_3, \ldots, d_3}_{t_3}, \ldots, \underbrace{d_r, \ldots, d_r}_{t_r}, d_{r+1} = \delta,$$

respectively, where $d_1 \neq d_2 \neq d_3 \neq \ldots \neq d_r \neq d_{r+1}$. Note that for any integer n, we have $n^2 \geq |n|$. Then

$$\begin{aligned} \sum_{\substack{uv\in E(G)\\ d_G(u)\neq d_G(v)}} [d_G(u)-d_G(v)]^2 &\geq \sum_{i=1}^{p-1}[d_G(v_i)-d_G(v_{i+1})]^2 \\ &\geq \sum_{i=1}^{p-1}|d_G(v_i)-d_G(v_{i+1})| \\ &\geq (d_1-d_2)+(d_2-d_3)+\cdots+(d_r-d_{r+1}) \\ &= \Delta-\delta. \end{aligned}$$

Consequently, by (11), for graphs which are not regular, we obtain

$$AG(G) - GA(G) > \frac{\Delta-\delta}{2(2\Delta-1)\sqrt{\Delta(\Delta-1)}}.$$

□

THEOREM 2.8. *Let G be a graph with m edges, maximum degree Δ and minimum degree δ. Then*

$$AG(G) - GA(G) \leq \frac{(\Delta-\delta)^2}{2(\Delta+\delta)\sqrt{\Delta\delta}}\, m.$$

The equality holds if and only if G is a regular graph or a (Δ, δ)-semiregular bipartite graph.

Proof. By (4), for any two vertices $u, v \in V(G)$,

$$\frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u)d_G(v)}} \leq \frac{\Delta + \delta}{2\sqrt{\Delta\delta}}$$

with equality if and only if $\{d_G(u), d_G(v)\} = \{\delta, \Delta\}$. Similarly,

$$-\frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)} \leq -\frac{2\sqrt{\Delta\delta}}{\Delta + \delta}.$$

Then

$$\begin{aligned} AG(G) - GA(G) &= \sum_{uv \in E(G)} \left[\frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u)d_G(v)}} - \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)} \right] \\ &\leq \sum_{v_i v_j \in E(G)} \left[\frac{\Delta + \delta}{2\sqrt{\Delta\delta}} - \frac{2\sqrt{\Delta\delta}}{\Delta + \delta} \right] \\ &= \frac{(\Delta - \delta)^2}{2(\Delta + \delta)\sqrt{\Delta\delta}}\, m. \end{aligned}$$

The equality holds if and only if $\{d_G(u), d_G(v)\} = \{\delta, \Delta\}$ for every edge $uv \in E(G)$, which means that every edge of G is incident with one vertex of degree Δ and the other vertex of degree δ, so G is a regular graph (if $\Delta = \delta$) or (Δ, δ)-semiregular bipartite graph (if $\Delta > \delta$). □

3. CONCLUSION

In Section 2, we presented relations between the AG index and GA index by studying $AG(G) + GA(G)$, $AG(G) \cdot GA(G)$ and $AG(G) - GA(G)$. Let us apply our results to polycyclic aromatic systems and in more general, to any molecular graphs.

The number of edges of a graph G is denoted by m, minimum degree by δ and maximum degree by Δ. In Corollary 2.1, we showed that

$$AG(G) + GA(G) \geq 2m.$$

For connected graphs, this result was obtained also in [9]. In Theorem 2.2, we obtained the bound

$$AG(G) + GA(G) \leq \frac{\Delta^2 + \delta^2 + 6\Delta\delta}{2(\Delta + \delta)\sqrt{\Delta\delta}}\, m.$$

We use $\delta = 1$ and $\Delta = 4$ to obtain the upper bound

$$AG(G) + GA(G) \leq 2.05\, m$$

for molecular graphs. For polycyclic aromatic systems, we have $\delta = 2$ and $\Delta = 3$, so

$$AG(G) + GA(G) \leq 2.00042\, m.$$

Thus $AG(G) + GA(G)$ is close to $2m$ for molecular graphs and polycyclic aromatic systems (such as benzenoids, phenylenes, fluoranthenes).

Let us investigate $AG(G) \cdot GA(G)$. Gutman [9] showed that

$$AG(G) \cdot GA(G) \leq \frac{1}{8} \frac{(\sqrt{\delta} + \sqrt{\Delta})^4}{(\delta + \Delta)\sqrt{\delta\Delta})} \, m^2,$$

with equality if and only if G is regular. Using $\delta = 1$ and $\Delta = 4$, we obtain

$$AG(G) \cdot GA(G) \leq 1.0125\, m^2$$

for molecular graphs. Using $\delta = 2$ and $\Delta = 3$, we have

$$AG(G) \cdot GA(G) \leq 1.000104\, m^2$$

for polycyclic aromatic systems. Note that in Theorem 2.5, we presented an upper bound on $AG(G) \cdot GA(G)$, which is sharp also for $(\Delta, \Delta - 1)$-semiregular bipartite graphs G.

In Theorem 2.4, we obtained the bound

$$AG(G) \cdot GA(G) \geq m^2$$

and we presented all the connected graphs satisfying the equality $AG(G) \cdot GA(G) = m^2$. From the previous inequalities, it follows that even for molecular graphs and polycyclic aromatic systems, $AG(G) \cdot GA(G)$ is very close to m^2.

Finally, we consider $AG(G) - GA(G)$. In Theorem 2.8, we obtained the bound

$$AG(G) - GA(G) \leq \frac{(\Delta - \delta)^2}{2(\Delta + \delta)\sqrt{\Delta\delta}} \, m.$$

Using $\delta = 1$ and $\Delta = 4$, we obtain

$$AG(G) - GA(G) \leq 0.45\, m$$

for molecular graphs. Using $\delta = 2$ and $\Delta = 3$, we have

$$AG(G) - GA(G) \leq 0.041\, m$$

for polycyclic aromatic systems. In Section 1, we presented the bound

$$AG(G) - GA(G) \geq 0$$

given in [5] and [16]. Hence, $AG(G) - GA(G)$ is close to 0 for polycyclic aromatic systems. Let us mention that we improved the bound $AG(G) - GA(G) \geq 0$ for connected graphs with given δ and Δ by presenting sharp lower bounds on $AG(G) - GA(G)$ in Theorem 2.7.

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