Inequalities on the geometric-arithmetic index

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Abstract

Although the notion of geometric-arithmetic index has been introduced in the chemical graph theory these past years, it has already proved to be useful. The objective of the work we present here is twofold: First, obtaining new relations connecting the geometric-arithmetic index with other topological indices; second, to characterize graphs which are extremal with respect to those relations.

1. Introduction

A single number (or a set of numbers) which represents a chemical structure in graph-theoretical terms via the molecular graph is called a *topological descriptor*; besides, if it correlates with a molecular property, it is called *topological index* and it is used to understand physicochemical properties of chemical compounds. The interest of topological indices lies in the fact that they synthesize some of the properties of a molecule usually into a single number, or, in some occasions, a few numbers. With this in mind, hundreds of topological indices have been introduced and studied so far; it is worth noting the seminal work by Wiener in which he used the sum of all shortest-path distances of a (molecular) graph in order to model physical properties of alkanes (see [47]).

Topological indices based on end-vertex degrees of edges have been used for 40 years and some of them are recognized tools in chemical research. Probably, the best known among such descriptors are the Randić connectivity index (R) and the Zagreb indices.

The *first and second Zagreb indices*, denoted by M_1 and M_2 respectively, were introduced by Gutman and Trinajstić in 1972 (see [23]) as

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

where uv stands for the edge of the graph G connecting vertices u and v and d_u is the degree of the vertex u.

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Research on the Zagreb indices is abundant. In the works [19–21] and the references therein one can find details of their mathematical theory and chemical applications.

One can define the *first and second variable Zagreb indices* as (see e.g. [26, 27, 30])

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

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

Variable molecular descriptors were proposed not only as a new way of characterizing heteroatoms in molecules (see [32, 33]), but also as a method to assess the structural differences. For further information see e.g. [34] and [30].

Gutman and Tošović [22] tested the correlation abilities of 20 vertex-degree-based topological indices used in the chemical literature for the case of standard heats of formation and normal boiling points of octane isomers. It is noteworthy that the second variable Zagreb index M_2^α with exponent $\alpha = -1$ (and to a lesser extent with exponent $\alpha = -2$) performs significantly better than the Randić index ($R = M_2^{-0.5}$).

When it comes to the second variable Zagreb index, it has proved to be useful to model the structure-boiling point of benzenoid hydrocarbons (see [31]). Another use of variable Zagreb indices seems to be deriving multi-linear regression models [14]. Several papers discuss the relations between these indices and various properties (see, e.g., [4, 26, 28, 40, 48, 49]).

Note that M_1^2 is the first Zagreb index M_1, M_1^{-1} is the inverse index ID, M_1^3 is the forgotten index F, etc.; also, $M_2^{-1/2}$ is the usual Randić index, M_2^1 is the second Zagreb index M_2, M_2^{-1} is the modified Zagreb index, etc.

The *general sum-connectivity index* was defined by Trinajstić and Zhou in [51] as

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

Observe that χ_1 coincides with the first Zagreb index M_1, $2\chi_{-1}$ with the harmonic index H, $\chi_{-1/2}$ with the sum-connectivity index χ, etc.

The (first) geometric-arithmetic index $GA_1 = GA$ is defined in [45] as

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

Although GA was defined roughly ten years ago, it has been the object of study of many papers. (see, e.g., [10–12, 37, 45] and the references therein). In fact, it is an object highly present in current research (see e.g. [5–7, 9, 18] and [24]). There are other geometric-arithmetic indices, like $Z_{p,q}$ ($Z_{0,1} = GA$), but the results in [12, p.598] show that the GA index gathers the same information on the molecule under study as other $Z_{p,q}$ indices.

The number of possible benzenoid hydrocarbons is huge, although only about 1,000 of them have been identified so far. As an example, there are as many as $5.85 \cdot 10^{21}$ benzenoid hydrocarbons with exactly 35 benzene rings [43]. Therefore, the ability to model their physico-chemical properties can be most helpful in order to foresee characteristics of currently unknown species. When comparing Randić index to the predicting capacity of the GA index the latter is reasonably better (see [12, Table 1]). There is a good linear correlation between the heat of formation of benzenoid hydrocarbons and GA as the graphic in [12, Fig.7] (from [12, Table 2], [41]) shows (with a correlation coefficient equal to 0.972).

Furthermore, in the case of standard enthalpy of vaporization, GA index improves the performance of Randić index by more than 9%. This leads to the belief that one should consider GA indices when researching QSPR/QSAR.

A main topic in the study of topological indices is to find bounds of the indices involving several parameters. The objective of this paper is twofold: First, to obtain new

relations connecting the geometric-arithmetic index with other topological indices; second, to characterize graphs which are extremal with respect to the relations obtained.

Here and hereafter, $G = (V(G), E(G))$ will denote a (non-oriented) finite simple (without multiple edges and loops) graph such that each connected component of G has, at least, an edge. Also, the notation Δ, δ, n, m for the maximum degree, the minimum degree and the cardinality of the set of vertices and edges of G, respectively will be used.

2. Main results

The following result relates the geometric-arithmetic and the first Zagreb indices.

Recall that a (Δ, δ)-*biregular graph* (or simply a biregular graph) is a bipartite graph for which any vertex in one side of the given bipartition has degree Δ and any vertex in the other side of the bipartition has degree δ.

Theorem 2.1. *If G is a graph with maximum degree Δ and minimum degree δ, then*

$$GA(G) \geq \frac{1}{2\Delta} M_1(G), \qquad \text{if } \delta/\Delta \geq t_0,$$

$$GA(G) \geq \frac{2\sqrt{\Delta\delta}}{(\Delta + \delta)^2} M_1(G), \qquad \text{if } \delta/\Delta < t_0, \tag{2.1}$$

where t_0 is the unique solution of the equation $t^3 + 5t^2 + 11t - 1 = 0$ in the interval $(0, 1)$. The equality in the first bound is attained if and only if G is regular; the equality in the second bound is attained if and only if G is a biregular graph.

Proof. Since the function $h(t) = t^3 + 5t^2 + 11t - 1$ is increasing on the interval $[0, 1]$, $h(0) < 0$ and $h(1) > 0$, there exists a unique solution of the equation $t^3 + 5t^2 + 11t - 1 = 0$ in the interval $(0, 1)$. Thus, t_0 is well-defined. Since the coefficients of the polynomial $h(t)$ are rational numbers, and the coefficients of t^3 and t^0 of the polynomial $h(t)$ are 1 and -1, respectively, we have that $t_0 \notin \mathbb{Q}$.

We are going to compute the minimum value of the function $f : [\delta, \Delta] \times [\delta, \Delta] \to \mathbb{R}$ given by

$$f(x, y) = \frac{2\sqrt{xy}}{(x + y)^2}.$$

By symmetry, we can assume that $x \leq y$. We have

$$\frac{\partial f}{\partial x}(x, y) = \frac{x^{-1/2}y^{1/2}(x + y)^2 - 2x^{1/2}y^{1/2}2(x + y)}{(x + y)^4}$$

$$= \frac{x^{-1/2}y^{1/2}(x + y) - 4x^{1/2}y^{1/2}}{(x + y)^3}$$

$$= x^{-1/2}y^{1/2} \frac{x + y - 4x}{(x + y)^3}$$

$$= x^{-1/2}y^{1/2} \frac{y - 3x}{(x + y)^3},$$

$$\frac{\partial f}{\partial y}(x, y) = y^{-1/2}x^{1/2} \frac{x - 3y}{(x + y)^3}.$$

Since $y \geq x \geq \delta > 0$, we have $\partial f/\partial y < 0$. Thus, the minimum value of f is attained on the set $\{(x, \Delta) | \delta \leq x \leq \Delta\}$.

If $\Delta \leq 3\delta$, then $\partial f/\partial x(x, \Delta) < 0$ for every $x > \delta$.

If $\Delta > 3\delta$, then $\partial f/\partial x(x, \Delta) > 0$ for every $\delta \leq x < \Delta/3$ and $\partial f/\partial x(x, \Delta) < 0$ for every $\Delta/3 < x \leq \Delta$.

Thus, we have in both cases

$$f(x,y) \geq \min\{f(\Delta,\Delta), f(\delta,\Delta)\} = \min\Big\{\frac{1}{2\Delta}, \frac{2\sqrt{\Delta\delta}}{(\Delta+\delta)^2}\Big\}.$$

Hence,

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} \geq \min\Big\{\frac{1}{2\Delta}, \frac{2\sqrt{\Delta\delta}}{(\Delta+\delta)^2}\Big\}(d_u + d_v),$$

$$GA(G) \geq \min\Big\{\frac{1}{2\Delta}, \frac{2\sqrt{\Delta\delta}}{(\Delta+\delta)^2}\Big\}M_1(G).$$

In order to prove (2.1), it suffices to show that the inequality

$$\frac{1}{2\Delta} \leq \frac{2\sqrt{\Delta\delta}}{(\Delta+\delta)^2} \tag{2.2}$$

holds if and only if $\delta/\Delta \geq t_0$.

Inequality (2.2) is equivalent to the following statements

$$(\Delta+\delta)^2 \leq 4\Delta\sqrt{\Delta\delta}, \qquad \Big(1+\frac{\delta}{\Delta}\Big)^2 \leq 4\sqrt{\frac{\delta}{\Delta}},$$

$$\Big(1+\frac{\delta}{\Delta}\Big)^4 \leq 16\frac{\delta}{\Delta}, \qquad \frac{\delta^4}{\Delta^4} + 4\frac{\delta^3}{\Delta^3} + 6\frac{\delta^2}{\Delta^2} - 12\frac{\delta}{\Delta} + 1 \leq 0.$$

Since $0 < \delta/\Delta \leq 1$, let us consider the function $g(t) = t^4 + 4t^3 + 6t^2 - 12t + 1$ for $t \in (0,1]$. Since $g(t) = (t-1)(t^3 + 5t^2 + 11t - 1) = (t-1)h(t)$, we have $g(t) \leq 0$ if and only if $t \in [t_0, 1]$. Hence, inequality (2.2) holds if and only if $\delta/\Delta \geq t_0$. Note that this condition is equivalent to $\delta/\Delta > t_0$, since $t_0 \notin \mathbb{Q}$; therefore, the equality in (2.2) is attained if and only if $\delta = \Delta$.

Therefore, (2.1) holds.

If $\delta/\Delta \geq t_0$, then the previous argument gives that f attains its minimum value just at the point (Δ, Δ). Thus, the equality in (2.1) is attained if and only if $(d_u, d_v) = (\Delta, \Delta)$ for every $uv \in E(G)$, i.e., G is regular.

If $\delta/\Delta < t_0$, then f attains its minimum value just at the points (δ, Δ) and (Δ, δ). Therefore, the equality in (2.1) is attained if and only if $\{d_u, d_v\} = \{\delta, \Delta\}$ for every $uv \in E(G)$, i.e., G is biregular. $\qquad\square$

We need the following particular case of Jensen's inequality.

Lemma 2.2. *If f is a convex function in an interval I and $x_1, \ldots, x_m \in I$, then*

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

Theorem 2.3. *If G is a graph with m edges, maximum degree Δ and minimum degree δ, then*

$$GA(G) \geq \frac{m^2}{\Delta H(G)}, \qquad \text{if } \delta/\Delta \geq t_0,$$

$$GA(G) \geq \frac{4\sqrt{\Delta\delta}\, m^2}{(\Delta+\delta)^2 H(G)}, \qquad \text{if } \delta/\Delta < t_0, \tag{2.3}$$

where t_0 is the unique solution of the equation $t^3 + 5t^2 + 11t - 1 = 0$ in the interval $(0,1)$. The equality in the first bound is attained if and only if G is regular; the equality in the second bound is attained if and only if G is a biregular graph.

Proof. The argument in the proof of Theorem 2.1 gives

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

for every $uv \in E(G)$. Since $f(x) = 1/x$ is a convex function in $\mathbb{R}_+$, Lemma 2.2 gives

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

$$\leq \frac{1}{2m} \left(\min\left\{ \frac{1}{2\Delta} , \frac{2\sqrt{\Delta\delta}}{(\Delta + \delta)^2} \right\} \right)^{-1} \sum_{uv \in E(G)} \frac{2}{d_u + d_v}$$

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

The argument in the proof of Theorem 2.1 gives

$$\min\left\{ \frac{1}{2\Delta} , \frac{2\sqrt{\Delta\delta}}{(\Delta + \delta)^2} \right\} = \frac{1}{2\Delta} , \qquad \text{if } \delta/\Delta \geq t_0,$$

$$\min\left\{ \frac{1}{2\Delta} , \frac{2\sqrt{\Delta\delta}}{(\Delta + \delta)^2} \right\} = \frac{2\sqrt{\Delta\delta}}{(\Delta + \delta)^2} , \qquad \text{if } \delta/\Delta < t_0,$$

Thus, (2.3) holds.

If the graph is regular or biregular, then we have, respectively,

$$\frac{m^2}{\Delta H(G)} = \frac{m^2}{\Delta m/\Delta} = m = GA(G),$$

$$\frac{4\sqrt{\Delta\delta}\, m^2}{(\Delta + \delta)^2 H(G)} = \frac{4\sqrt{\Delta\delta}\, m^2}{(\Delta + \delta)^2 \, 2m/(\Delta + \delta)} = \frac{2\sqrt{\Delta\delta}}{\Delta + \delta} m = GA(G).$$

If the equality in the first bound in (2.3) is attained, then the argument in the proof of Theorem 2.1 gives that G is regular.

If the equality in the second bound in (2.3) is attained, then the equality in the proof of Theorem 2.1 gives that G is biregular. $\qquad\square$

Theorem 2.4. *If G is a graph with m edges and minimum degree δ, then*

$$GA(G) \geq m - \frac{M_1(G) - 2M_2^{1/2}(G)}{2\delta} ,$$

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

Proof. We have

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

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

Since

$$\sum_{uv \in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\right)^2}{d_u + d_v} \leq \frac{1}{2\delta} \sum_{uv \in E(G)} \left(\sqrt{d_u} - \sqrt{d_v}\right)^2$$

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

we conclude

$$GA(G) \geq m - \frac{M_1(G) - 2M_2^{1/2}(G)}{2\delta} .$$

If G is regular, then

$$m - \frac{M_1(G) - 2M_2^{1/2}(G)}{2\delta} = m - \frac{2\delta m - 2\delta m}{2\delta} = m = GA(G).$$

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

Remark 2.5. Since $M_1(G) - 2M_2^{1/2}(G) = \sum_{uv \in E(G)}(\sqrt{d_u} - \sqrt{d_v})^2$, we have $M_1(G) - 2M_2^{1/2}(G) \geq 0$.

Theorem 2.6. *If $\alpha > 0$ and G is a graph with m edges and minimum degree δ, then*

$$GA(G) \geq 2\delta m^{(\alpha+1)/\alpha}\chi_\alpha(G)^{-1/\alpha},$$

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

Proof. Let us define $p = (\alpha + 1)/\alpha > 1$. Hölder inequality gives

$$m = \sum_{uv \in E(G)} \Big(\frac{\sqrt{d_u d_v}}{d_u + d_v}\Big)^{1/p}\Big(\frac{d_u + d_v}{\sqrt{d_u d_v}}\Big)^{1/p}$$

$$\leq \Big(\sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{d_u + d_v}\Big)^{1/p}\Big(\sum_{uv \in E(G)}\Big(\frac{d_u + d_v}{\sqrt{d_u d_v}}\Big)^{1/(p-1)}\Big)^{(p-1)/p},$$

$$m^p \leq \frac{1}{2}GA(G)\Big(\frac{1}{\delta^{1/(p-1)}}\chi_{1/(p-1)}(G)\Big)^{p-1} = \frac{1}{2\delta}GA(G)\chi_{1/(p-1)}(G)^{p-1}.$$

The result follows from this inequality and the equality $p - 1 = 1/\alpha$.

If the graph is regular, then

$$2\delta m^{(\alpha+1)/\alpha}\chi_\alpha(G)^{-1/\alpha} = 2\delta m^{1/\alpha}m((2\delta)^\alpha m)^{-1/\alpha} = m = GA(G).$$

If the equality is attained, then the previous argument gives $\sqrt{d_u d_v} = \delta$ for every $uv \in E(G)$. Thus, $d_u = \delta$ for every $u \in V(G)$, and G is a regular graph. □

As a consequence of Theorem 2.6, we obtain the following result appearing in [36, Theorem 3.7].

Corollary 2.7. *If G is a graph with m edges and minimum degree δ, then*

$$GA(G) \geq \frac{2\delta m^2}{M_1(G)},$$

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

Theorem 2.8. *If $p \geq 2$ and G is a graph with m edges and minimum degree δ, then*

$$GA(G) \geq 2\,\delta^{1/2}m^p M_1^{(2p-1)/(2p-2)}(G)^{1-p}.$$

Proof. Hölder inequality gives

$$m = \sum_{uv \in E(G)} \Big(\frac{\sqrt{d_u d_v}}{d_u + d_v}\Big)^{1/p}\Big(\frac{d_u + d_v}{\sqrt{d_u d_v}}\Big)^{1/p}$$

$$\leq \Big(\sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{d_u + d_v}\Big)^{1/p}\Big(\sum_{uv \in E(G)}\Big(\sqrt{\frac{d_u}{d_v}} + \sqrt{\frac{d_v}{d_u}}\Big)^{1/(p-1)}\Big)^{(p-1)/p}.$$

Since $p \geq 2$, we have $0 < 1/(p-1) \leq 1$ and so

$$m^p \leq \Big(\sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{d_u + d_v}\Big)\Big(\sum_{uv \in E(G)}\Big(\Big(\frac{d_u}{d_v}\Big)^{1/(2p-2)} + \Big(\frac{d_v}{d_u}\Big)^{1/(2p-2)}\Big)\Big)^{p-1}.$$

Since

$$\sum_{uv \in E(G)} \left(\left(\frac{d_u}{d_v} \right)^{1/(2p-2)} + \left(\frac{d_v}{d_u} \right)^{1/(2p-2)} \right) \le \delta^{-1/(2p-2)} \sum_{uv \in E(G)} (d_u^{1/(2p-2)} + d_v^{1/(2p-2)})$$

$$= \delta^{-1/(2p-2)} \sum_{u \in V(G)} d_u^{1/(2p-2)} d_u$$

$$= \delta^{-1/(2p-2)} M_1^{(2p-1)/(2p-2)}(G),$$

we have

$$m^p \le \frac{1}{2} GA(G) \left(\delta^{-1/(2p-2)} M_1^{(2p-1)/(2p-2)}(G) \right)^{p-1}$$

$$= \frac{1}{2} \delta^{-1/2} GA(G) M_1^{(2p-1)/(2p-2)}(G)^{p-1}.$$

$\square$

We will need the following elementary result. We include a proof for the sake of completeness.

Lemma 2.9. *Let $f : [a, b] \to \mathbb{R}$ be a C^2 function such that $f' = gh$ for some C^1 functions g, h with $g \ge 0$ and $h' \ge 0$ on $[a, b]$. Then $\max_{t \in [a,b]} f(t) = \max\{f(a), f(b)\}$.*

Proof. If $h \ge 0$, then $f' \ge 0$ and $\max_{t \in [a,b]} f(t) = f(b) = \max\{f(a), f(b)\}$.

If $h \le 0$, then $f' \le 0$ and $\max_{t \in [a,b]} f(t) = f(a) = \max\{f(a), f(b)\}$.

Otherwise, $h(a) < 0$ and $h(b) > 0$ since $h' \ge 0$ on $[a, b]$. Thus, there exists $t_0 \in (a, b)$ such that $h(t_0) = 0$. Since $h' \ge 0$ on $[a, b]$, we have $h \le 0$ on $[a, t_0]$ and $h \ge 0$ on $[t_0, b]$. Hence, f is non-increasing on $[a, t_0]$ and non-decreasing on $[t_0, b]$, and the conclusion holds. $\square$

Theorem 2.10. *Let G be a graph with maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$GA(G) \ge \delta^{-2\alpha} M_2^\alpha(G), \qquad \text{if } \alpha \le -1/2,$$

$$GA(G) \ge \min\left\{ \delta^{-2\alpha}, \frac{2}{(\Delta\delta)^{\alpha-1/2}(\Delta + \delta)} \right\} M_2^\alpha(G), \qquad \text{if } -1/2 < \alpha \le 0,$$

$$GA(G) \ge \min\left\{ \Delta^{-2\alpha}, \frac{2}{(\Delta\delta)^{\alpha-1/2}(\Delta + \delta)} \right\} M_2^\alpha(G), \qquad \text{if } 0 < \alpha < 1/2,$$

$$GA(G) \ge \Delta^{-2\alpha} M_2^\alpha(G), \qquad \text{if } \alpha \ge 1/2.$$

Every bound is attained for every regular graph G. Furthermore, the bounds in the first and fourth cases are attained if and only if G is regular.

Proof. We are going to compute the maximum value of the function $f : [\delta, \Delta] \times [\delta, \Delta] \to \mathbb{R}$ given by

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

If $\alpha \le -1/2$, then f is a decreasing function in each variable, and so, $f(x, y) \le f(\delta, \delta) = 2\delta^{2\alpha}$ and

$$M_2^\alpha(G) \le \delta^{2\alpha} GA(G).$$

If $\alpha \ge 1/2$, then f is an increasing function in each variable, and so, $f(x, y) \le f(\Delta, \Delta) = 2\Delta^{2\alpha}$ and

$$M_2^\alpha(G) \le \Delta^{2\alpha} GA(G).$$

Let us consider the case $-1/2 < \alpha < 1/2$. We have

$$\frac{\partial f}{\partial x}(x, y) = (\alpha + 1/2)x^{\alpha-1/2}y^{\alpha-1/2} + (\alpha - 1/2)x^{\alpha-3/2}y^{\alpha+1/2}$$

$$= x^{\alpha-3/2}y^{\alpha-1/2}((\alpha + 1/2)x + (\alpha - 1/2)y),$$

$$\frac{\partial f}{\partial y}(x, y) = y^{\alpha-3/2}x^{\alpha-1/2}((\alpha + 1/2)y + (\alpha - 1/2)x).$$

By symmetry, we can assume that $x \leq y$.

Assume now $-1/2 < \alpha \leq 0$. Thus, $(\alpha + 1/2)x + (\alpha - 1/2)y \leq (\alpha + 1/2)y + (\alpha - 1/2)y = 2\alpha y \leq 0$ and so, $\partial f/\partial x \leq 0$. Therefore, the maximum value of f is attained on the set $\{x = \delta, \, \delta \leq y \leq \Delta\}$.

Since the function $(\alpha + 1/2)y + (\alpha - 1/2)\delta$ is increasing on $y \in [\delta, \Delta]$ and $\partial f/\partial y(\delta, y)$ and $(\alpha + 1/2)y + (\alpha - 1/2)\delta$ have the same sign, Lemma 2.9 gives $f(\delta, y) \leq \max\{f(\delta, \delta), f(\delta, \Delta)\}$. Thus,

$$f(x, y) \leq \max\left\{2\delta^{2\alpha}, (\Delta\delta)^{\alpha-1/2}(\Delta + \delta)\right\}.$$

Finally, assume $0 < \alpha < 1/2$. Thus, $(\alpha + 1/2)y + (\alpha - 1/2)x \geq (\alpha + 1/2)x + (\alpha - 1/2)x = 2\alpha x > 0$ and so, $\partial f/\partial y > 0$. Therefore, the maximum value of f is attained on the set $\{y = \Delta, \, \delta \leq x \leq \Delta\}$.

Since the function $(\alpha + 1/2)x + (\alpha - 1/2)\Delta$ is increasing on $x \in [\delta, \Delta]$ and $\partial f/\partial x(x, \Delta)$ and $(\alpha + 1/2)x + (\alpha - 1/2)\Delta$ have the same sign, Lemma 2.9 gives $f(x, \Delta) \leq \max\{f(\delta, \Delta), f(\Delta, \Delta)\}$. Therefore,

$$f(x, y) \leq \max\left\{2\Delta^{2\alpha}, (\Delta\delta)^{\alpha-1/2}(\Delta + \delta)\right\}.$$

This finishes the proof of the inequalities.

If the graph is regular, then

$$\frac{2}{(\Delta\delta)^{\alpha-1/2}(\Delta + \delta)} = \delta^{-2\alpha} = \Delta^{-2\alpha}$$

and

$$\Delta^{-2\alpha}M_2^{\alpha}(G) = \Delta^{-2\alpha}\Delta^{2\alpha}m = GA(G).$$

The properties of the function f give that, in the first and fourth cases, each equality is attained if and only if either $d_u = d_v = \delta$ for every $uv \in E(G)$ or $d_u = d_v = \Delta$ for every $uv \in E(G)$, and so, G is regular. $\square$

Theorem 2.10 has the following consequence for the Randić, second Zagreb and reciprocal Randić indices.

Corollary 2.11. *Let G be a graph with maximum degree Δ and minimum degree δ. Then*

$$GA(G) \geq \delta R(G),$$

$$GA(G) \geq \Delta^{-2}M_2(G),$$

$$GA(G) \geq \Delta^{-1}M_2^{1/2}(G).$$

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

Note that the first inequality in Corollary 2.11 appears in [39, Theorem 6].

3. Other bounds

The *Albertson index* is defined in [2] (see also [3]) as

$$Alb(G) = \sum_{uv \in E(G)} |d_u - d_v|.$$

This index is also known as *third Zagreb index* (see [16]) and *misbalance deg index* (see [46] and [44]). This is a significant predictor of standard enthalpy of vaporisation for octane isomers (see [46]). This index is much used as a measure of non-regularity of a graph.

Theorem 3.1. *If G is a graph with m edges and minimum degree δ, then*

$$GA(G) \geq m - \frac{1}{2\delta} \, Alb(G),$$

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

Proof. We have seen in the proof of Theorem 2.4 that

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

We have

$$|\sqrt{d_u} - \sqrt{d_v}||\sqrt{d_u} - \sqrt{d_v}| \leq |\sqrt{d_u} - \sqrt{d_v}|(\sqrt{d_u} + \sqrt{d_v}),$$

$$\sum_{uv \in E(G)} (\sqrt{d_u} - \sqrt{d_v})^2 \leq \sum_{uv \in E(G)} |d_u - d_v| = Alb(G).$$

Hence,

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

$$\geq m - \frac{1}{2\delta} \sum_{uv \in E(G)} (\sqrt{d_u} - \sqrt{d_v})^2 \geq m - \frac{1}{2\delta} \, Alb(G).$$

If G is regular, then $GA(G) = m$ and $Alb(G) = 0$ and so, the equality 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 so, G is a regular graph. $\square$

Theorem 3.2. *If G is a graph with maximum degree Δ and minimum degree δ, then*

$$Alb(G) \leq \frac{\Delta^2 - \delta^2}{2\sqrt{\Delta\delta}} \, GA(G),$$

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

Proof. We have

$$\frac{|d_u - d_v|}{\frac{2\sqrt{d_u d_v}}{d_u + d_v}} = \frac{|d_u - d_v|(d_u + d_v)}{2\sqrt{d_u d_v}} = \frac{|d_u^2 - d_v^2|}{2\sqrt{d_u d_v}} = \frac{1}{2}\left| \sqrt{\frac{d_u^3}{d_v}} - \sqrt{\frac{d_v^3}{d_u}} \right|$$

$$\leq \frac{1}{2}\left(\sqrt{\frac{\Delta^3}{\delta}} - \sqrt{\frac{\delta^3}{\Delta}} \right) = \frac{\Delta^2 - \delta^2}{2\sqrt{\Delta\delta}},$$

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

If G is a regular or biregular graph, then

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

If the equality is attained, then the previous argument gives that $\{d_u, d_v\} = \{\Delta, \delta\}$ for every $uv \in E(G)$; thus, G is a regular or biregular graph. $\square$

The following well-known result provides a converse of Cauchy-Schwarz inequality (see, e.g., [29, Lemma 3.4]).

Lemma 3.3. *If $a_j, b_j \geq 0$ and $\omega b_j \leq a_j \leq \Omega b_j$ for $1 \leq j \leq k$, then*

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

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

Multiplicative versions of the first and the second Zagreb indices, Π_1 and Π_2, were first considered in [42], defined as

$$\Pi_1(G) = \prod_{u \in V(G)} d_u^2, \qquad \Pi_2(G) = \prod_{uv \in E(G)} d_u d_v.$$

Also, the multiplicative sum-Zagreb index Π_1^* was introduced in [15] as

$$\Pi_1^*(G) = \prod_{uv \in E(G)} (d_u + d_v).$$

Theorem 3.4. *If G is a graph with m edges, maximum degree Δ and minimum degree δ, then*

$$GA(G) \ge \frac{m}{\Delta} \Pi_1(G)^{\delta/(4m)},$$

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

Proof. The multiplicative version of the first Zagreb index satisfies

$$\Pi_1(G) = \prod_{u \in V(G)} d_u^2 = \prod_{uv \in E(G)} d_u^{2/d_u} d_v^{2/d_v} \le \Big(\prod_{uv \in E(G)} d_u d_v \Big)^{2/\delta}.$$

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

$$\frac{1}{m} GA(G) = \frac{1}{m} \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \ge \Big(\prod_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \Big)^{1/m}$$

$$\ge \Big(\frac{1}{\Delta^m} \prod_{uv \in E(G)} \sqrt{d_u d_v} \Big)^{1/m} = \frac{1}{\Delta} \Big(\Big(\prod_{uv \in E(G)} d_u d_v \Big)^{2/\delta} \Big)^{\delta/(4m)}$$

$$\ge \frac{1}{\Delta} \Pi_1(G)^{\delta/(4m)}.$$

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

If the graph is regular, then

$$\frac{m}{\Delta} \Pi_1(G)^{\delta/(4m)} = \frac{m}{\Delta} \Big(\prod_{uv \in E(G)} \Delta^{2/\Delta} \Delta^{2/\Delta} \Big)^{\Delta/(4m)} = m = GA(G).$$

$\square$

Theorem 3.5. *If $\alpha > 0$ and G is a graph with m edges and maximum degree Δ, then*

$$GA(G) \ge \frac{m^{(2\alpha+1)/(2\alpha)}}{\Delta \, M_2^{-\alpha}(G)^{1/(2\alpha)}},$$

and the equality is attained for some α if and only if G is regular.

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

$$\frac{1}{m} GA(G) = \frac{1}{m} \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \ge \Big(\prod_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \Big)^{1/m}$$

$$\ge \Big(\frac{1}{\Delta^m} \prod_{uv \in E(G)} \sqrt{d_u d_v} \Big)^{1/m},$$

$$GA(G)^{2\alpha} \ge \Big(\frac{m}{\Delta} \Big)^{2\alpha} \Big(\prod_{uv \in E(G)} (d_u d_v)^\alpha \Big)^{1/m}.$$

Using the fact that the harmonic mean is at most the geometric mean, we deduce

$$GA(G)^{2\alpha} \geq \left(\frac{m}{\Delta}\right)^{2\alpha}\left(\prod_{uv \in E(G)}(d_u d_v)^{\alpha}\right)^{1/m}$$

$$\geq \left(\frac{m}{\Delta}\right)^{2\alpha}\frac{m}{\sum_{uv \in E(G)}(d_u d_v)^{-\alpha}} = \left(\frac{m}{\Delta}\right)^{2\alpha}\frac{m}{M_2^{-\alpha}(G)}.$$

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

If the graph is regular, then

$$\frac{m^{(2\alpha+1)/(2\alpha)}}{\Delta\, M_2^{-\alpha}(G)^{1/(2\alpha)}} = \frac{m^{1/(2\alpha)}m}{\Delta(\Delta^{-2\alpha}m)^{1/(2\alpha)}} = m = GA(G).$$

$\square$

We need the following result in [35, Theorem 3.3].

Lemma 3.6. *If G is a graph with maximum degree Δ and minimum degree δ, then*

$$\frac{\delta^{\alpha}}{2}\, M_1^{\alpha+1}(G) \leq M_2^{\alpha}(G) \leq \frac{\Delta^{\alpha}}{2}\, M_1^{\alpha+1}(G) \qquad \text{if } \alpha > 0,$$

$$\frac{\Delta^{\alpha}}{2}\, M_1^{\alpha+1}(G) \leq M_2^{\alpha}(G) \leq \frac{\delta^{\alpha}}{2}\, M_1^{\alpha+1}(G) \qquad \text{if } \alpha < 0,$$

and the equality holds for some α if and only if G is regular.

Corollary 3.7. *If $\alpha > 0$ and G is a graph with m edges, maximum degree Δ and minimum degree δ, then*

$$GA(G) \geq \frac{2^{1/(2\alpha)}\delta^{1/2}m^{(2\alpha+1)/(2\alpha)}}{\Delta\, M_1^{1-\alpha}(G)^{1/(2\alpha)}},$$

and the equality holds for some α if and only if G is regular.

Proof. Theorem 3.5 and Lemma 3.6 give

$$GA(G) \geq \frac{m^{(2\alpha+1)/(2\alpha)}}{\Delta\, M_2^{-\alpha}(G)^{1/(2\alpha)}} \geq \frac{m^{(2\alpha+1)/(2\alpha)}}{\Delta\left(\frac{1}{2}\,\delta^{-\alpha}M_1^{1-\alpha}(G)\right)^{1/(2\alpha)}} = \frac{2^{1/(2\alpha)}\delta^{1/2}m^{(2\alpha+1)/(2\alpha)}}{\Delta\, M_1^{1-\alpha}(G)^{1/(2\alpha)}}.$$

If the graph is regular, then

$$\frac{2^{1/(2\alpha)}\delta^{1/2}m^{(2\alpha+1)/(2\alpha)}}{\Delta\, M_1^{1-\alpha}(G)^{1/(2\alpha)}} = \frac{2^{1/(2\alpha)}\delta^{1/2}m^{1/(2\alpha)}m}{\delta(\delta^{-\alpha}\delta n)^{1/(2\alpha)}} = \frac{2^{1/(2\alpha)}\delta^{1/2}m^{1/(2\alpha)}m}{\delta\,\delta^{-1/2}(2m)^{1/(2\alpha)}} = m = GA(G).$$

If the equality holds, then we have the equality in Theorem 3.5, and thus the graph is regular. $\square$

Theorem 3.8. *If G is a graph, then*

$$GA(G) \geq \frac{2M_2^{1/4}(G)^2}{M_1(G)},$$

and the equality is attained if G is a regular or biregular graph.

Proof. Cauchy-Schwarz inequality gives

$$M_2^{1/4}(G)^2 = \left(\sum_{uv \in E(G)}\frac{(d_u d_v)^{1/4}}{(d_u + d_v)^{1/2}}(d_u + d_v)^{1/2}\right)^2 \leq \left(\sum_{uv \in E(G)}\frac{\sqrt{d_u d_v}}{d_u + d_v}\right)\left(\sum_{uv \in E(G)}(d_u + d_v)\right)$$

$$= \frac{1}{2}\,GA(G)M_1(G).$$

If G is regular or biregular, then

$$\frac{2M_2^{1/4}(G)^2}{M_1(G)} = \frac{2\left((\Delta\delta)^{1/4}m\right)^2}{(\Delta+\delta)m} = \frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\,m = GA(G).$$

$\square$

The following technical result appears in [36, Corollary 2.3].

Lemma 3.9. *Let g be the function $g(x,y) = \frac{2\sqrt{xy}}{x+y}$ with $0 < a \le x, y \le b$. Then*

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

The equality in the lower bound is attained if and only if either $x = a$ and $y = b$, or $x = b$ and $y = a$, and the equality in the upper bound is attained if and only if $x = y$. Besides, $g(x,y) = g(x',y')$ if and only if x/y is equal to either x'/y' or y'/x'.

As a consequence of Lemma 3.9 we obtain the following bounds for the geometric-arithmetic index [10] (see also [12, p.609-610]).

Proposition 3.10. *If G is a graph with m edges, maximum degree Δ and minimum degree δ, then*

$$\frac{2m\sqrt{\Delta\delta}}{\Delta+\delta} \le GA(G) \le m. \tag{3.1}$$

The equality in the first inequality is attained if and only if G is regular or biregular. The equality in the second inequality is attained if and only if G is regular.

The *forgotten topological index* (or *F-index*) was introduced in [23], at the same time as Zagreb indices. There, it was defined as

$$F(G) = \sum_{u \in V(G)} d_u^3.$$

As the first Zagreb index it was used when finding the total π-electron energy (see [23]). It was thought to assess the extent of the branching of the carbon-atom skeleton of the associated molecule. Recently, when Furtula and Gutman ([17]) showed that the acetic factor and the entropy could be predicted similarly by either the F-index or the first Zagreb index, attention was finally given to the former. Both of them yield correlation coefficients greater than 0.95. Besides, [17] pointed out that the F-index could be employed to predict the logarithm of the octanol-water partition coefficient (see also [1]) very accuarately. For more bounds of the F-index see, e.g., [1, 8, 38].

We report a mistake in the lower bound of GA in [39, Theorem 5]. By using the argument in the proof of that theorem, we obtain the following inequality involving the forgotten topological index.

Theorem 3.11. *If G is a graph with maximum degree Δ and minimum degree δ, then*

$$GA(G) \ge \frac{4\Delta^2\delta^2\sqrt{\left(F(G) + 2M_2(G)\right)M_2^{-1}(G)}}{(\Delta+\delta)^2(\Delta^2+\delta^2)},$$

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

Proof. We have by Lemma 3.9

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

for every $uv \in E(G)$. Hence,

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

Moreover,

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

$$= \sum_{u \in V(G)} d_u^3 + 2M_2(G)$$

$$= F(G) + 2M_2(G).$$

Since

$$\delta^2 \leq \frac{(d_u + d_v)/2}{1/\sqrt{d_u d_v}} = \frac{d_u + d_v}{2} \sqrt{d_u d_v} \leq \Delta^2,$$

Lemma 3.3 gives

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

$$= \frac{\Delta\delta\sqrt{(F(G) + 2M_2(G)) M_2^{-1}(G)}}{\Delta^2 + \delta^2},$$

and the desired inequality follows.

If the graph is regular, then

$$\frac{4\Delta^2\delta^2\sqrt{(F(G) + 2M_2(G)) M_2^{-1}(G)}}{(\Delta + \delta)^2(\Delta^2 + \delta^2)} = \frac{\sqrt{(2\Delta^2 m + 2\Delta^2 m)m/\Delta^2}}{2} = m = GA(G).$$

If the equality is attained, then Lemma 3.3 gives $\delta^2 = \Delta^2$ and G is a regular graph. $\square$

Theorem 3.12. *If G is a graph with maximum degree Δ and minimum degree δ, then*

$$GA(G) \geq \frac{F(G)}{2\Delta^2} - \frac{(\Delta - \delta)Alb(G)}{2\Delta\delta},$$

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

Proof. Since

$$\frac{d_u^2 + d_v^2}{2\Delta} \leq \frac{d_u^2 + d_v^2}{d_u + d_v} = \frac{2d_u d_v}{d_u + d_v} + \frac{(d_u - d_v)^2}{d_u + d_v} \leq \frac{2\Delta\sqrt{d_u d_v}}{d_u + d_v} + \frac{(d_u - d_v)^2}{d_u + d_v},$$

for every $uv \in E(G)$, we have

$$\frac{F(G)}{2\Delta} \leq \Delta\, GA(G) + \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u + d_v}.$$

Since

$$\sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u + d_v} \leq \frac{\Delta - \delta}{2\delta} \sum_{uv \in E(G)} |d_u - d_v| = \frac{\Delta - \delta}{2\delta} Alb(G),$$

we conclude

$$\frac{F(G)}{2\Delta} \leq \Delta\, GA(G) + \frac{(\Delta - \delta)Alb(G)}{2\delta}.$$

If the graph is regular, then

$$\frac{F(G)}{2\Delta^2} - \frac{(\Delta - \delta)Alb(G)}{2\Delta\delta} = \frac{F(G)}{2\Delta^2} = \frac{2\Delta^2 m}{2\Delta^2} = m = GA(G).$$

The previous argument gives that if the bound 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 regular. $\qquad\square$

The following Kober's inequality appears in [25] (see also [50, Lemma 1]).

Lemma 3.13. *If $a_j > 0$ for $1 \le j \le k$, then*

$$\Big(\sum_{j=1}^{k} \sqrt{a_j} \Big)^2 \ge \sum_{j=1}^{k} a_j + k(k-1) \Big(\prod_{j=1}^{k} a_j \Big)^{1/k}.$$

A family of degree–based structure–descriptors, named *Adriatic indices*, was put forward in [44, 46]. Twenty of them were selected as significant predictors. One of them, the *inverse sum indeg* index, *ISI*, was singled out in [44] as a significant predictor of total surface area of octane isomers. This index is defined as

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

In the last years there is an increasing interest in the mathematical properties of this index.

Theorem 3.14. *If G is a graph with m edges and maximum degree Δ, then*

$$GA(G) \ge \sqrt{\frac{2}{\Delta} \Big(ISI(G) + m(m-1) \frac{\Pi_2(G)^{1/m}}{\Pi_1^*(G)^{1/m}} \Big)},$$

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

Proof. Lemma 3.13 gives

$$ISI(G) + m(m-1) \frac{\Pi_2(G)^{1/m}}{\Pi_1^*(G)^{1/m}}$$

$$= \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v} + m(m-1) \Big(\prod_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v} \Big)^{1/m} \le \Big(\sum_{uv \in E(G)} \frac{(d_u d_v)^{1/2}}{(d_u + d_v)^{1/2}} \Big)^2$$

$$= \Big(\frac{1}{\sqrt{2}} \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \Big(\frac{d_u + d_v}{2} \Big)^{1/2} \Big)^2 \le \frac{\Delta}{2} GA(G)^2.$$

If G is regular, then

$$\sqrt{\frac{2}{\Delta} \Big(ISI(G) + m(m-1) \frac{\Pi_2(G)^{1/m}}{\Pi_1^*(G)^{1/m}} \Big)}$$

$$= \sqrt{\frac{2}{\Delta} \Big(\frac{\Delta m}{2} + m(m-1) \frac{(\Delta^{2m})^{1/m}}{((2\Delta)^m)^{1/m}} \Big)} = m = GA(G).$$

If the equality is attained, then the previous argument gives $d_u + d_v = 2\Delta$ for every $uv \in E(G)$, i.e., $d_u = \Delta$ for every $u \in V(G)$ and so, G is a regular graph. $\qquad\square$

We need the following Diaz-Metcalf inequality [13].

Lemma 3.15. *If a_j and b_j are real numbers such that $ha_j \le b_j \le Ha_j$ for $1 \le j \le m$, then*

$$\sum_{j=1}^{m} b_j^2 + hH \sum_{j=1}^{m} a_j^2 \le (h+H) \sum_{j=1}^{m} a_j b_j,$$

where equality holds if and only if $b_j = ha_j$ or $b_j = Ha_j$ for $1 \le j \le m$.

Theorem 3.16. *If G is a graph with maximum degree Δ and minimum degree δ, then*

$$GA(G) \geq \frac{M_2(G) + 4\Delta^2\delta^2\chi_{-2}(G)}{\Delta^2 + \delta^2},$$

and the equality is attained if and only if each connected component of G is δ-regular or Δ-regular. In particular, if G is connected, then the equality is attained if and only if G is regular.

Proof. If we define

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

then

$$4\delta^2 \leq b_j/a_j = 2\sqrt{d_u d_v}\,(d_u + d_v) \leq 4\Delta^2,$$

and so, Lemma 3.15 gives

$$4\sum_{uv \in E(G)} d_u d_v + 16\Delta^2\delta^2 \sum_{uv \in E(G)} \frac{1}{(d_u + d_v)^2} \leq (4\Delta^2 + 4\delta^2) \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v},$$

$$M_2(G) + 4\Delta^2\delta^2\chi_{-2}(G) \leq (\Delta^2 + \delta^2)GA(G).$$

By Lemma 3.15, the equality is attained if and only if $2\sqrt{d_u d_v}\,(d_u + d_v) = 4\delta^2$ or $2\sqrt{d_u d_v}\,(d_u + d_v) = 4\Delta^2$ for each $uv \in E(G)$, and this is equivalent to $d_u = d_v = \delta$ or $d_u = d_v = \Delta$ for each $uv \in E(G)$, i.e., each connected component of G is δ-regular or Δ-regular. $\qquad\square$

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