Southeast Asian Bulletin of Mathematics (2022) 46: 437–452

Southeast Asian
Bulletin of
Mathematics

Inequalities Involving the Geometric-Arithmetic Index*

Walter Carballosa
Department of Mathematics and Statistics, Florida International University, 11200 SW 8th Street, Miami, Florida 33199, USA
Email: wcarball@fiu.edu

Received 6 March 2020
Accepted 30 April 2022

Communicated by W.S. Cheung

AMS Mathematics Subject Classification(2020): 05C09, 05C92

Abstract. The concept of geometric-arithmetic index GA_1 was introduced in the chemical graph theory recently, but it has shown to be useful. The aim of this paper is to give new inequalities involving the geometric-arithmetic index and characterize extremal graphs with respect to them.

Keywords: Geometric-arithmetic index; Vertex-degree-based topological index.

1. Introduction

A single number, representing a chemical structure in graph-theoretical terms via the molecular graph, is called a topological descriptor and if it is well correlated with a molecular property it is called topological index, which is used to understand physicochemical properties of chemical compounds. Topological indices are interesting since they capture some of the properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes (see [47]).

Topological indices based on end-vertex degrees of edges have been used over 50 years. Among them, several indices are recognized to be useful tools in

*The research was supported by a grant from Agencia Estatal de Investigación, Spain (PID2019-106433GB-I00 /AEI/10.13039/501100011033).

chemical researches. Probably, the best know such descriptors are the Randić connectivity index (R) [36] and the Zagreb indices. The first and second Zagreb indices, denoted by M_1 and M_2, respectively, and introduced by Gutman and Trinajstić in 1972 (see [20]), are defined 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 denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u.

There is a vast amount of research on the Zagreb indices. For details of their chemical applications and mathematical theory see [16, 17, 18], and the references therein.

In [23, 24, 29], the *first and second variable Zagreb indices* are defined as

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

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

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 [11] as

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

The concept of variable molecular descriptors was proposed as a new way of characterizing heteroatoms in molecules (see [33, 34]), but also to assess the structural differences (e.g., the relative role of carbon atoms of acyclic and cyclic parts in alkylcycloalkanes [35]). The idea behind the variable molecular descriptors is that the variables are determined during the regression so that the standard error of estimate for a particular studied property is as small as possible (see, e.g., [29]).

In the paper of Gutman and Tošović [19], the correlation abilities of 20 vertex-degree-based topological indices occurring in the chemical literature were tested for the case of standard heats of formation and normal boiling points of octane isomers. It is remarkable to realize 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 ($R = M_2^{-0.5}$).

The second variable Zagreb index has been used in the structure-boiling point modeling of benzenoid hydrocarbons [31]. Besides, variable Zagreb indices exhibit a potential applicability for deriving multi-linear regression models [10].

Various properties and relations of these indices are discussed in several papers (see, e.g., [3, 4, 5, 9, 24, 25, 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 Zhou and Trinajstić in [51] as

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

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

The first geometric-arithmetic index GA_1 is defined in [44] as

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

Although GA_1 was introduced in 2009, there are many papers dealing with this index (see, e.g., [6, 7, 8, 15, 21, 26, 27, 30, 32, 37, 38, 39, 40, 44] and the references therein). There are other geometric-arithmetic indices, like $Z_{p,q}$ ($Z_{0,1} = GA_1$), but the results in [7, p. 598] show that the GA_1 index gathers the same information on observed molecule as other $Z_{p,q}$ indices.

Although only about 1000 benzenoid hydrocarbons are known, the number of possible benzenoid hydrocarbons is huge. For instance, the number of possible benzenoid hydrocarbons with 35 benzene rings is $5.85 \cdot 10^{21}$ [43]. Therefore, modeling their physico-chemical properties is important in order to predict properties of currently unknown species. The predicting ability of the GA_1 index compared with Randić index is reasonably better (see [7, Table 1]). The graphic in [7, Fig. 7] (from [7, Table 2], [41]) shows that there exists a good linear correlation between GA_1 and the heat of formation of benzenoid hydrocarbons (the correlation coefficient is equal to 0.972).

Furthermore, the improvement in prediction with GA_1 index comparing to Randić index in the case of standard enthalpy of vaporization is more than 9%. That is why one can think that GA_1 index should be considered in the QSPR/QSAR researches.

A main topic in the study of topological indices is to find bounds of the indices involving several parameters. The main aim of this paper is to obtain new inequalities involving the geometric-arithmetic index GA_1 and characterize graphs extremal with respect to them.

Throughout this paper, we use $G = (V(G), E(G))$ to denote a (non-oriented) finite simple (without multiple edges and loops) graph without isolated vertices. We denote by Δ, δ, n, m the maximum degree, the minimum degree, and the cardinality of the set of vertices and edges of G, respectively.

2. Inequalities Involving the Geometric-Arithmetic Index

Theorem 2.1. *If G is a graph with m edges, maximum degree Δ and minimum degree δ, then*
$$GA_1(G) \ge m - \frac{1}{2}\left(\sqrt{\Delta} - \sqrt{\delta}\,\right)^2 H(G),$$
and the equality is attained if and only if G is regular graph or bipartite.

Proof. We have
$$\begin{aligned} GA_1(G) + \sum_{uv\in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2}{d_u + d_v} &= \sum_{uv\in E(G)} \left(\frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} + \frac{\left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2}{d_u + d_v} \right) \\ &= \sum_{uv\in E(G)} 1 = m. \end{aligned}$$
So since
$$\sum_{uv\in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2}{d_u + d_v} \le \frac{1}{2} \sum_{uv\in E(G)} \frac{2\left(\sqrt{\Delta} - \sqrt{\delta}\,\right)^2}{d_u + d_v} = \frac{1}{2}\left(\sqrt{\Delta} - \sqrt{\delta}\,\right)^2 H(G),$$
we conclude
$$GA_1(G) \ge m - \frac{1}{2}\left(\sqrt{\Delta} - \sqrt{\delta}\,\right)^2 H(G).$$

Moreover, if the equality is attained, then $\left|\sqrt{d_u} - \sqrt{d_v}\,\right| = \sqrt{\Delta} - \sqrt{\delta}$ for every $uv \in E(G)$; thus, $\{d_u, d_v\} = \{\Delta, \delta\}$ for every $uv \in E(G)$, and G is a regular or bipartite graph. Note that if $\{d_u, d_v\} \ne \{\Delta, \delta\}$ for some $uv \in E(G)$, then the equality fails. Moreover, if G is connected and bipartite, then vertices in each part have the same degree. ■

The following well-known result provides a converse of Cauchy-Schwarz inequality (see, e.g., [28, Lemma 3.4]).

Lemma 2.2. *If $a_j, b_j \ge 0$ and $\omega b_j \le a_j \le \Omega b_j$ for $1 \le j \le k$, then*
$$\Big(\sum_{j=1}^k a_j^2\Big)^{1/2} \Big(\sum_{j=1}^k b_j^2\Big)^{1/2} \le \frac{1}{2}\left(\sqrt{\frac{\Omega}{\omega}} + \sqrt{\frac{\omega}{\Omega}}\right) \sum_{j=1}^k a_j b_j.$$
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 $1 \le j \le k$.

The following Kober's inequalities appear in [22] (see also [50, Lemma 1]).

Lemma 2.3. *If $a_j > 0$ for $1 \le j \le k$, then*
$$\sum_{j=1}^k a_j + k(k-1)\Big(\prod_{j=1}^k a_j\Big)^{1/k} \le \Big(\sum_{j=1}^k \sqrt{a_j}\Big)^2 \le (k-1)\sum_{j=1}^k a_j + k\Big(\prod_{j=1}^k a_j\Big)^{1/k}.$$

Now we can apply these lemmas above to obtain some relations of the Geometric-Arithmetic index, GA_1, with the multiplicative versions of the Zagred indices, Π_1,Π_2 and Π_1^*.

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

$$GA_1(G) \le M_2^{1/2}(G)\, H(G) - 2m(m-1)\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}}\,,$$

$$GA_1(G) \ge \frac{4\Delta\delta}{(m-1)(\Delta+\delta)^2}\, M_2^{1/2}(G)\, H(G) - \frac{2m}{m-1}\,\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}}\,.$$

The equality in the first bound is attained for every regular graph; the equality in the second bound is attained if and only if G is regular.

Proof. The first inequality in Lemma 2.3 and Cauchy-Schwarz inequality give

$$\begin{aligned}
&\sum_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{d_u+d_v} + m(m-1)\Big(\prod_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{d_u+d_v}\Big)^{1/m} \\
&\le \Big(\sum_{uv\in E(G)} \frac{(d_u d_v)^{1/4}}{(d_u+d_v)^{1/2}}\Big)^2 \\
&\le \sum_{uv\in E(G)} (d_u d_v)^{1/2} \sum_{uv\in E(G)} \frac{1}{d_u+d_v} = M_2^{1/2}(G)\,\frac{1}{2}\,H(G), \\
&\quad GA_1(G) + 2m(m-1)\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}} \le M_2^{1/2}(G)\, H(G).
\end{aligned}$$

Since

$$\frac{(d_u d_v)^{1/4}}{\frac{1}{(d_u+d_v)^{1/2}}} = (d_u d_v)^{1/4}(d_u+d_v)^{1/2}$$

and

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

Lemma 2.2 gives

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

This inequality and Lemma 2.3 give

$$(m-1)\sum_{uv\in E(G)}\frac{\sqrt{d_ud_v}}{d_u+d_v}+m\Big(\prod_{uv\in E(G)}\frac{\sqrt{d_ud_v}}{d_u+d_v}\Big)^{1/m}$$
$$\geq\Big(\sum_{uv\in E(G)}\frac{(d_ud_v)^{1/4}}{(d_u+d_v)^{1/2}}\Big)^2\geq\frac{2\Delta\delta}{(\Delta+\delta)^2}\,M_2^{1/2}(G)\,H(G),$$
$$(m-1)GA_1(G)+2m\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}}\geq\frac{4\Delta\delta}{(\Delta+\delta)^2}\,M_2^{1/2}(G)\,H(G).$$

If G is a regular graph, then

$$M_2^{1/2}(G)\,H(G)-2m(m-1)\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}}$$
$$=\Delta m\frac{m}{\Delta}-2m(m-1)\frac{(\Delta^{2m})^{1/(2m)}}{((2\Delta)^m)^{1/m}}=m=GA_1(G),$$
$$\frac{4\Delta\delta}{(m-1)(\Delta+\delta)^2}\,M_2^{1/2}(G)\,H(G)-\frac{2m}{m-1}\,\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}}$$
$$=\frac{4\Delta^2}{(m-1)4\Delta^2}\,\Delta m\frac{m}{\Delta}-\frac{2m}{m-1}\,\frac{(\Delta^{2m})^{1/(2m)}}{((2\Delta)^m)^{1/m}}=m=GA_1(G).$$

If the equality in the second bound is attained, then Lemma 2.2 gives $\sqrt{2}\,\delta=\sqrt{2}\,\Delta$, i.e., G is regular. ∎

Theorem 2.5. *If G is a graph with m edges, then*

$$GA_1(G)\geq 2m\,\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}},$$

and the equality is attained if G is either a regular graph or a bipartite graph where vertices in each part have the same degree.

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

$$\frac{1}{2m}\,GA_1(G)=\frac{1}{m}\sum_{uv\in E(G)}\frac{\sqrt{d_ud_v}}{d_u+d_v}\geq\Big(\prod_{uv\in E(G)}\frac{\sqrt{d_ud_v}}{d_u+d_v}\Big)^{1/m}$$
$$=\frac{\Big(\prod_{uv\in E(G)}d_ud_v\Big)^{1/(2m)}}{\Big(\prod_{uv\in E(G)}(d_u+d_v)\Big)^{1/m}}=\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}}.$$

If G is a regular graph or a bipartite graph where vertices in each part have the same degree, then

$$2m\,\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}}=2m\,\frac{((\Delta\delta)^m)^{1/(2m)}}{((\Delta+\delta)^m)^{1/m}}=\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\,m=GA_1(G),$$

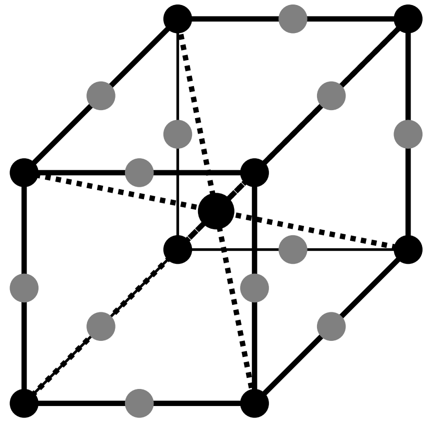

Figure 1: A graph that attains the equality in Theorem 2.5.

and the equality holds. ■

Note that the equality in the theorem above is attained if and only if $\sqrt{d_u d_v}/(d_u + d_v)$ is constant for every $uv \in E(G)$, and so the geometric mean is equal to the arithmetic mean. Since $\frac{\sqrt{d_u\, d_v}}{d_u+d_v}$ is a 0-homogenous expression we have for instance, $\frac{\sqrt{2\cdot 4}}{2+4} = \frac{\sqrt{4\cdot 8}}{4+8}$. Then the equality in Theorem 2.5 might be attained for some graphs with degree sequence involving more than two values. For instance, the equality is attained for a graph G obtained from a cube graph Q_3 by adding a new vertex v connected to every vertices in $V(Q_3)$, and then applying edge-subdivision to every edge in $E(Q_3)$, see Figure 1. Note that G has one vertex with degree 8, eight vertices with degree 4 and twelve vertices with degree 2 such that the edges join vertices with either degrees 8 and 4, or degrees 4 and 2.

Also, given different integers $d_1, \ldots, d_k$, if G_i is any d_i-regular graph, then the equality in Theorem 2.5 is attained by the union $G = \cup_{i=1}^{k} G_i$.

In the same paper, where Zagreb indices were introduced, the *forgotten topological index* (or *F-index*) is defined as

$$F(G) = \sum_{u \in V(G)} d_u^3 = \sum_{uv \in E(G)} (d_u^2 + d_v^2).$$

Both the forgotten topological index and the first Zagreb index were employed in the formulas for total π-electron energy in [20], as a measure of branching extent of the carbon-atom skeleton of the underlying molecule.

The *Albertson index* is defined in [1] (see [2]) as

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

This index is also known as *third Zagreb index* (see [13]) and *misbalance deg index* (see [45, 46]). This is a significant predictor of standard enthalpy of vaporization for octane isomers (see [45]).

Theorem 2.6. *If G is a graph with maximum degree Δ and minimum degree δ, then*
$$GA_1(G) \geq \frac{F(G)}{2\Delta^2} - \frac{(\Delta-\delta)Alb(G)}{2\Delta\delta}\,,$$
and the equality is attained if and only if G is regular.

Proof. Since
$$\frac{d_u^2+d_v^2}{2\Delta} \leq \frac{d_u^2+d_v^2}{d_u+d_v} = \frac{2d_ud_v}{d_u+d_v} + \frac{(d_u-d_v)^2}{d_u+d_v} \leq \frac{2\Delta\sqrt{d_ud_v}}{d_u+d_v} + \frac{(d_u-d_v)^2}{d_u+d_v}\,,$$
for every $uv \in E(G)$, we have
$$\frac{F(G)}{2\Delta} \leq \Delta\, GA_1(G) + \sum_{uv\in E(G)} \frac{(d_u-d_v)^2}{d_u+d_v}\,.$$

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
$$\frac{F(G)}{2\Delta} \leq \Delta\, GA_1(G) + \frac{(\Delta-\delta)Alb(G)}{2\delta}\,.$$

If the graph is regular, then
$$\frac{F(G)}{2\Delta^2} - \frac{(\Delta-\delta)Alb(G)}{2\Delta\delta} = \frac{F(G)}{2\Delta^2} = \frac{2\Delta^2 m}{2\Delta^2} = m = GA_1(G).$$

The first 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. ■

The following lemma, that will be useful, is the well-known Jensen's inequality.

Lemma 2.7. *For a real convex function φ, numbers $x_1, x_2, \ldots, x_n$ in its domain, and positive weights $a_1, a_2, \ldots, a_n$, we have*
$$\varphi\left(\frac{\sum a_i x_i}{\sum a_i}\right) \leq \frac{\sum a_i \varphi(x_i)}{\sum a_i}\,,$$
and the inequality is reversed if φ is concave, which is
$$\varphi\left(\frac{\sum a_i x_i}{\sum a_i}\right) \geq \frac{\sum a_i \varphi(x_i)}{\sum a_i}\,.$$

Equality holds if and only if $x_1 = x_2 = \cdots = x_n$ *or* φ *is linear on a domain containing* $x_1, x_2, \cdots, x_n$.

Theorem 2.8. *Let* G *be a graph with* m *edges, maximum degree* Δ *and minimum degree* δ, *and let* t_0 *be the unique real root of the equation* $t^3 - t^2 - t - 1 = 0$. *Then*

$$GA_1(G) \geq \begin{cases} \frac{m^2}{\Delta\, H(G)} & \text{if } \Delta/\delta \leq t_0^4, \\ \frac{4\sqrt{\Delta\delta}\, m^2}{(\Delta+\delta)^2 H(G)} & \text{if } \Delta/\delta \geq t_0^4. \end{cases}$$

The equality holds in the first bound if G *is regular. The equality holds in the second bound if* G *is a bipartite graph where vertices in each part have the same degree.*

Proof. Since $f(x) = 1/x$ is a convex function in $\mathbb{R}_+$, Lemma 2.7 gives

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

$$\frac{m^2}{GA_1(G)} \leq H(G) \max_{x,y\in[\delta,\Delta]} g(x,y),$$

where

$$g(x,y) = \frac{(x+y)^2}{4\sqrt{xy}} = \frac{1}{4}\big(x^{3/4}y^{-1/4} + y^{3/4}x^{-1/4}\big)^2.$$

Since

$$\begin{aligned} \frac{\partial g}{\partial x} &= \frac{1}{2}\big(x^{3/4}y^{-1/4} + y^{3/4}x^{-1/4}\big)\Big(\frac{3}{4}x^{-1/4}y^{-1/4} - \frac{1}{4}y^{3/4}x^{-5/4}\Big) \\ &= \frac{1}{8}\big(x^{3/4}y^{-1/4} + y^{3/4}x^{-1/4}\big)x^{-5/4}y^{-1/4}(3x - y), \\ \frac{\partial g}{\partial y} &= \frac{1}{8}\big(y^{3/4}x^{-1/4} + x^{3/4}y^{-1/4}\big)y^{-5/4}x^{-1/4}(3y - x), \end{aligned}$$

we have

$$\begin{aligned} \max_{y\in[\delta,\Delta]} g(x,y) &= \max\big\{g(x,\delta),\, g(x,\Delta)\big\}, \\ \max_{x\in[\delta,\Delta]} g(x,y) &= \max\big\{g(\delta,y),\, g(\Delta,y)\big\}, \\ \max_{x,y\in[\delta,\Delta]} g(x,y) &= \max\big\{g(\delta,\delta),\, g(\delta,\Delta),\, g(\Delta,\delta),\, g(\Delta,\Delta)\big\}. \end{aligned}$$

Since $g(x,x) = x$ is an increasing function and $g(x,y) = g(y,x)$, we have

$$\max_{x,y\in[\delta,\Delta]} g(x,y) = \max\big\{g(\Delta,\Delta),\, g(\Delta,\delta)\big\} = \max\Big\{\Delta,\, \frac{(\Delta+\delta)^2}{4\sqrt{\Delta\delta}}\Big\}.$$

The function $f(t) = t^3 - t^2 - t - 1$ has derivative $f'(t) = 3t^2 - 2t - 1 = (3t+1)(t-1)$. It is easy to check that $f(t)$ has a unique real zero $t_0 > 1$ and $f(t) \geq 0$ if and only if $t \geq t_0$.

Thus, the function $F(t) = t^4 - 2t^3 + 1 = (t^3 - t^2 - t - 1)(t - 1)$ satisfies $F(t) \geq 0$ if $t \geq t_0$ and $F(t) \leq 0$ if $1 \leq t \leq t_0$. Consequently, we have

$$\begin{aligned} t^4 + 1 &\geq 2t^3, && \text{if } t \geq t_0, \\ x^4 + y^4 &\geq 2x^3 y, && \text{if } x/y \geq t_0, \\ \Delta + \delta &\geq 2\Delta^{3/4}\delta^{1/4}, && \text{if } \Delta/\delta \geq t_0^4, \\ \frac{(\Delta+\delta)^2}{4\sqrt{\Delta\delta}} &\geq \Delta, && \text{if } \Delta/\delta \geq t_0^4. \end{aligned}$$

In a similar way, we obtain

$$\frac{(\Delta+\delta)^2}{4\sqrt{\Delta\delta}} \leq \Delta, \qquad \text{if } \Delta/\delta \leq t_0^4.$$

If the graph is regular, then $H(G) = m/\Delta$, $GA_1(G) = m$ and the equality in the first bound holds.

If G is a bipartite graph where vertices in each part have the same degree, then

$$\frac{4\sqrt{\Delta\delta}\, m^2}{(\Delta+\delta)^2 H(G)} = \frac{4\sqrt{\Delta\delta}\, m^2}{(\Delta+\delta)^2 2m/(\Delta+\delta)} = \frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\, m = GA_1(G). \qquad \blacksquare$$

Theorem 2.9. *Let G be a graph with m edges and maximum degree Δ. Then*

$$GA_1(G) \geq \frac{\sqrt{2}\, m^2}{\sqrt{\Delta M_1(G) M_2^{-1}(G)}},$$

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

Proof. Since $f(x) = 1/x$ is a convex function in $\mathbb{R}_+$, Lemma 2.7 gives

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

Using the Cauchy-Schwarz inequality, we obtain

$$\begin{aligned} \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}} &\leq \Big(\sum_{uv\in E(G)} \frac{(d_u + d_v)^2}{4} \Big)^{1/2} \Big(\sum_{uv\in E(G)} \frac{1}{d_u d_v} \Big)^{1/2} \\ &\leq \Big(\sum_{uv\in E(G)} \frac{\Delta(d_u + d_v)}{2} \Big)^{1/2} \Big(M_2^{-1}(G) \Big)^{1/2} \\ &= \sqrt{\frac{\Delta}{2} M_1(G) M_2^{-1}(G)}. \end{aligned}$$

Thus, we have

$$\frac{\sqrt{2}\, m^2}{\sqrt{\Delta M_1(G) M_2^{-1}(G)}} \leq GA_1(G).$$

Now if the graph is regular, then $M_1(G) = 2m\Delta$, $M_2^{-1}(G) = m/\Delta^2$ and $GA_1(G) = m$, so the equality holds. On the other hand if the equality holds, then $d_u + d_v = 2\Delta$ for every $uv \in E(G)$ which implies that $d_u = \Delta$ for every $u \in V(G)$, i.e., G is regular. ∎

Theorem 2.10. *Let G be a graph with m edges and maximum degree Δ. Then*

$$GA_1(G) \geq 2m - \frac{1}{2}\sqrt{2\Delta M_1(G) M_2^{-1}(G)}\,,$$

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

Proof. Since, for all $a, b > 0$,

$$\frac{a}{b} + \frac{b}{a} \geq 2,$$

and the equality is attained if and only if $a = b$, we have

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

Using the Cauchy-Schwarz inequality, we obtain

$$\begin{aligned}
\sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}} &\leq \Big(\sum_{uv \in E(G)} \frac{(d_u + d_v)^2}{4} \Big)^{1/2} \Big(\sum_{uv \in E(G)} \frac{1}{d_u d_v} \Big)^{1/2} \\
&\leq \Big(\sum_{uv \in E(G)} \frac{\Delta(d_u + d_v)}{2} \Big)^{1/2} \Big(M_2^{-1}(G) \Big)^{1/2} \\
&= \sqrt{\frac{\Delta}{2}\, M_1(G) M_2^{-1}(G)}\,.
\end{aligned}$$

Thus, we have

$$GA_1(G) \geq 2m - \frac{1}{2}\sqrt{2\Delta M_1(G) M_2^{-1}(G)}\,.$$

If the equality is attained, then $d_u + d_v = 2\Delta$ for every $uv \in E(G)$ which implies that G is regular.

If G is regular, then

$$2m - \frac{1}{2}\sqrt{2\Delta M_1(G) M_2^{-1}(G)} = 2m - \frac{1}{2}\sqrt{2\Delta 2\Delta m \Delta^{-2} m} = m = GA_1(G).$$ ∎

Estrada et al. [12] defined atom-bond connectivity index as

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

They showed that the ABC index correlates well with the heats of formation of alkanes and can therefore serve the purpose of predicting their thermodynamic properties. Furtula et al. [14] made a generalization of ABC index, defined as

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

Theorem 2.11. *Let G be a graph with maximum degree Δ and without isolated edges, and $\alpha > 0$. Then*

$$\left(\frac{2\Delta - 2}{\Delta^2}\right)^\alpha GA_1(G) \le ABC_\alpha(G) \le \frac{(\Delta-1)^\alpha(\Delta+1)}{2\Delta^{\alpha+\frac{1}{2}}}\, GA_1(G).$$

Furthermore, the lower bound is attained if and only if G is regular, and the upper bound is attained if and only if G is union of start graphs $S_{\Delta+1}$.

Proof. Note that $(d_u, d_v) \neq (1,1)$ since G does not have isolated edges and consequently $\Delta \ge 2$. We are going to compute the minimum and maximum values of $f(x,y) = \left(\frac{x+y-2}{xy}\right)^\alpha \frac{x+y}{2\sqrt{xy}} = \frac{y^{-\alpha-\frac{1}{2}}}{2}(x+y-2)^\alpha(x+y)x^{-\alpha-\frac{1}{2}}$ on $1 \le x \le y, 2 \le y \le \Delta$. We have

$$\begin{aligned}
\frac{\partial f}{\partial x} &= \frac{y^{-\alpha-\frac{1}{2}}}{2}\left[\alpha(x+y-2)^{\alpha-1}(x+y)x^{-\alpha-\frac{1}{2}} + (x+y-2)^\alpha x^{-\alpha-\frac{1}{2}}\right] \\
&\quad - \frac{y^{-\alpha-\frac{1}{2}}}{2}\left[(x+y-2)^\alpha(x+y)\Big(\alpha+\frac{1}{2}\Big)x^{-\alpha-\frac{3}{2}}\right] \\
&= \frac{y^{-\alpha-\frac{1}{2}}}{2}(x+y-2)^{\alpha-1}x^{-\alpha-\frac{3}{2}}\left[\alpha(x+y)x + (x+y-2)x\right] \\
&\quad - \frac{y^{-\alpha-\frac{1}{2}}}{2}(x+y-2)^{\alpha-1}x^{-\alpha-\frac{3}{2}}\left[\Big(\alpha+\frac{1}{2}\Big)(x+y-2)(x+y)\right] \\
&= \frac{y^{-\alpha-\frac{1}{2}}}{2}(x+y-2)^{\alpha-1}x^{-\alpha-\frac{3}{2}}\left[\alpha(x+y)\big(x-(x+y-2)\big)\right] \\
&\quad + \frac{y^{-\alpha-\frac{1}{2}}}{2}(x+y-2)^{\alpha-1}x^{-\alpha-\frac{3}{2}}\left[(x+y-2)\Big(x-\frac{1}{2}(x+y)\Big)\right] \\
&= \frac{y^{-\alpha-\frac{1}{2}}}{2}(x+y-2)^{\alpha-1}x^{-\alpha-\frac{3}{2}}\left[\alpha(x+y)(2-y) + \frac{1}{2}(x+y-2)(x-y)\right] \\
&\le 0.
\end{aligned}$$

So, $f(x,y) \ge f(y,y)$ for every $x \in [1,y]$ and $y \ge 2$. Indeed, $f(x,y)$ is strictly decreasing on $x \in [1,y]$ for every fixed $y \ge 2$. Now consider

$$g(y) = f(y,y) = \left(\frac{y+y-2}{yy}\right)^\alpha \frac{y+y}{2\sqrt{yy}} = 2^\alpha\left(\frac{y-1}{y^2}\right)^\alpha.$$

Note that $g'(y) = 2^\alpha \alpha \left(\frac{y-1}{y^2}\right)^{\alpha-1} \left(\frac{y-1}{y^2}\right)' = 2^\alpha \alpha \left(\frac{y-1}{y^2}\right)^{\alpha-1} \frac{2-y}{y^3} \le 0$ on $2 \le y \le \Delta$. Moreover, g is strictly decreasing on $y \in [2, \Delta]$. Thus, we have $f(x, y) \ge g(y) \ge g(\Delta)$ for every $1 \le x \le y$, $2 \le y \le \Delta$ and the equalities hold if and only if $x = y = \Delta$. Therefore,

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

and the equality is attained if and only if $d_u = d_v = \Delta$. Then we obtain the lower bound by summing up.

On the other hand, we have $f(x, y) \le f(1, y)$ for every $x \in [1, y]$ and $y \ge 2$. Consider

$$h(y) = f(1, y) = \left(\frac{1 + y - 2}{y}\right)^\alpha \frac{1 + y}{2\sqrt{y}} = \frac{1}{2}(y-1)^\alpha (y+1) y^{-\alpha - \frac{1}{2}}.$$

Then

$$\begin{aligned} h'(y) = &\frac{1}{2}\left[\alpha(y-1)^{\alpha-1}(y+1)y^{-\alpha-\frac{1}{2}} + (y-1)^\alpha y^{-\alpha-\frac{1}{2}}\right] \\ &- \frac{1}{2}\left[\left(\alpha + \frac{1}{2}\right)(y-1)^\alpha (y+1) y^{-\alpha-\frac{3}{2}}\right] \\ =& \frac{1}{2}(y-1)^{\alpha-1} y^{-\alpha-\frac{3}{2}} \left[\alpha(y+1)y + (y-1)y - \left(\alpha + \frac{1}{2}\right)(y-1)(y+1)\right] \\ =& \frac{1}{2}(y-1)^{\alpha-1} y^{-\alpha-\frac{3}{2}} \left[\alpha(y+1)\big(y - (y-1)\big) + (y-1)\left(y - \frac{1}{2}(y+1)\right)\right] \\ =& \frac{1}{2}(y-1)^{\alpha-1} y^{-\alpha-\frac{3}{2}} \left[\alpha(y+1) + \frac{1}{2}(y-1)^2\right] > 0. \end{aligned}$$

Thus, we have $f(x, y) \le h(y) \le h(\Delta)$ for every $1 \le x \le y$, $2 \le y \le \Delta$ and the equalities hold if and only if $x = 1$ and $y = \Delta$. Therefore,

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

and the equality is attained if and only if $\{d_u, d_v\} = \{1, \Delta\}$ for every $uv \in E(G)$, *i.e.*, every connected component of G is a star graph $S_{\Delta+1}$. Then we obtain the upper bound by summing up. ∎

References

[1] M.O. Albertson, The irregularity of a graph, *Ars Comb.* **46** (1997) 219–225.

[2] A. Ali, I. Gutman, E. Milovanović, I. Milovanović, Sum of powers of the degrees of graphs: extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **80** (2018) 5–84.

[3] V. Andova, M. Petrusevski, Variable Zagreb indices and Karamatas inequality, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 685–690.

[4] W. Carballosa, A. Granados, D. Pestana, A. Portilla, J.M. Sigarreta, Relations between some topological indices and the line graph, *J. Math. Chem.* **58** (3) (2020) 632–646.

[5] W. Carballosa, D. Pestana, J.M. Sigarreta, E. Tourís, Relations between the general sum connectivity index and the line graph, *J. Math. Chem.* **58** (10) (2020) 2273–2290.

[6] K.C. Das, On geometric-arithmetic index of graphs, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 619–630.

[7] K.C. Das, I. Gutman, B. Furtula, Survey on geometric-arithmetic indices of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 595–644.

[8] K.C. Das, I. Gutman, B. Furtula, On first geometric-arithmetic index of graphs, *Discrete Appl. Math.* **159** (2011) 2030–2037.

[9] K.C. Das, J.M. Rodríguez, J.M. Sigarreta, On the maximal general ABC index of graphs with given maximum degree, *Appl. Math. Comput.* **386** (2020), #125531, 12 pp.

[10] M. Drmota, *Random Trees: An Interplay Between Combinatorics and Probability,* Springer, Wien-New York, 2009.

[11] M. Eliasi, A. Iranmanesh, I. Gutman, Multiplicative versions of first Zagreb index, *MATCH Commun. Math. Comput. Chem.* **68** (1) (2012) 217–230.

[12] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom-bond connectivity index. Modelling the enthalpy of formation of alkanes, *Indian J. Chem.* **37** A (1998) 849–855.

[13] G.H. Fath-Tabar, Old and new Zagreb indices of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 79–84.

[14] B. Furtula, A. Graovac, D. Vukičević, Augmented Zagreb index, *J. Math. Chem.* **48** (2010) 370–380.

[15] A. Granados, A. Portilla, J.M. Rodriguez, J.M. Sigarreta, Inequalities on the geometric-arithmetic index, *Hacet. J. Math. Stat.* **50** (3) (2021) 778–794.

[16] I. Gutman, Degree–based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361.

[17] I. Gutman, K.C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

[18] I. Gutman, T. Réti, Zagreb group indices and beyond, *Int. J. Chem. Model.* **6** (2-3) (2014) 191–200.

[19] I. Gutman, J. Tošović, Testing the quality of molecular structure descriptors. Vertex–degreebased topological indices, *J. Serb. Chem. Soc.* **78** (6) (2013) 805–810.

[20] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[21] J.C. Hernández, JM. Rodríguez, J.M. Sigarreta, On the geometric-arithmetic index by decompositions, *J. Math. Chem.* **55** (2017) 1376–1391.

[22] H. Kober, On the arithmetic and geometric means and on Hölders inequality, *Proc. Amer. Math. Soc.* **9** (1958) 452–459.

[23] X. Li, J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 195–208.

[24] X. Li, H. Zhao, Trees with the first smallest and largest generalized topological indices, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 57–62.

[25] M. Liu, B. Liu, Some properties of the first general Zagreb index, *Australas. J. Combin.* **47** (2010) 285–294.

[26] A. Martínez-Pérez, J.M. Rodríguez, New lower bounds for the geometric-arithmetic index, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 451–466.

[27] A. Martínez-Pérez, J.M. Rodríguez, New lower bounds for the first variable Zagreb index, *Discrete Appl. Math.* **306** (2022) 166–173.

[28] A. Martínez-Pérez, J.M. Rodríguez, J.M. Sigarreta, A new approximation to the geometric-arithmetic index, *J. Math. Chemistry* **56** (7) (2018) 1865–1883.

[29] A. Miličević, S. Nikolić, On variable Zagreb indices, *Croat. Chem. Acta* **77** (2004) 97–101.

[30] M. Mogharrab, G.H. Fath-Tabar, Some bounds on GA_1 index of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2010) 33–38.

[31] S. Nikolić, A. Miličević, N. Trinajstić, A. Jurić, On use of the variable Zagreb ${}^{\nu}M_2$ index in QSPR: boiling points of Benzenoid hydrocarbons, *Molecules* **9** (2004) 1208–1221.

[32] D. Pestana, J.M. Sigarreta, E. Tourís, Geometric-arithmetic index and line graph, *J. Math. Chem.* **57** (5) (2019) 1427–1447.

[33] M. Randić, Novel graph theoretical approach to heteroatoms in QSAR, *Chemometrics Intel. Lab. Syst.* **10** (1991) 213–227.

[34] M. Randić, On computation of optimal parameters for multivariate analysis of structure-property relationship, *J. Chem. Inf. Comput. Sci.* **31** (1991) 970–980.

[35] M. Randić, D. Plavšić, N. Lerš, Variable connectivity index for cycle-containing structures, *J. Chem. Inf. Comput. Sci.* **41** (2001) 657–662.

[36] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[37] J.M. Rodríguez, J.A. Rodríguez-Velázquez, J.M. Sigarreta, New inequalities involving the geometric-arithmetic index, *MATCH Commun. Math. Comput. Chem.* **78** (2) (2017) 361–374.

[38] J.M. Rodríguez, J.M. Sigarreta, On the geometric-arithmetic index, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 103–120.

[39] J.M. Rodríguez, J.M. Sigarreta, Spectral properties of geometric-arithmetic index, *Appl. Math. Comput.* **277** (2016) 142–153.

[40] J.M. Sigarreta, Bounds for the geometric-arithmetic index of a graph, *Miskolc Math. Notes* **16** (2) (2015) 1199–1212.

[41] *TRC Thermodynamic Tables. Hydrocarbons*, Thermodynamic Research Center, The Texas A & M University System: College Station, TX, 1987.

[42] R. Todeschini, V. Consonni, New local vertex invariants and molecular descriptors based on functions of the vertex degrees, *MATCH Commun. Math. Comput. Chem.* **64** (2) (2010) 359–372.

[43] M. Vöge, A.J. Guttmann, I. Jensen, On the number of benzenoid hydrocarbons, *J. Chem. Inf. Comput. Sci.* **42** (2002) 456–466.

[44] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.* **46** (2009) 1369–1376.

[45] D. Vukičević, M. Gašperov, Bond additive modeling 1. Adriatic indices, *Croat. Chem. Acta* **83** (3) (2010) 243–260.

[46] D. Vukičević, Bond additive modeling 2. Mathematical properties of maxmin rodeg index, *Croat. Chem. Acta* **83** (2010) 261–273.

[47] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[48] S. Zhang, W. Wang, T.C.E. Cheng, Bicyclic graphs with the first three smallest and largest values of the first general Zagreb index, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 579–592.

[49] H. Zhang, S. Zhang, Unicyclic graphs with the first three smallest and largest values of the first general Zagreb index, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 427–438.

[50] B. Zhou, I. Gutman, T. Aleksić, A note on Laplacian energy of graphs, *MATCH*

Commun. Math. Comput. Chem. **60** (2008) 441–446.

[51] B. Zhou, N. Trinajstić, On general sum-connectivity index, *J. Math. Chem.* **47** (2010) 210–218.