Inequalities on Topological Indices

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PUBLISHED AND IN-PRESS CONTENT

Chapter 1 is composed entirely by the ideas and results contained in the papers.

- Edil D. Molina, José M. Rodríguez, José L. Sánchez and José M. Sigarreta. Some properties of the Arithmetic–Geometric Index. Symmetry (2021) 13, 857.
- E. Locia, A. Morales, José L. Sánchez and José M. Sigarreta. Epistemological study of mathematical Inequalities. Revista Brasileira de História da Matemática (2021). In Press.

Chapter 2 is composed entirely by the ideas and results contained in the paper.

- José M. Rodríguez, José L. Sánchez and José M. Sigarreta. On the inverse degree index. Journal of Mathematical Chemistry (2019) 57(5), 1524–1542.

Chapter 3 is composed entirely by the results contained in the paper.

- José M. Rodríguez, José L. Sánchez and José M. Sigarreta. On the first general Zagreb index. Journal of Mathematical Chemistry (2018) 7(56), 1849-1864.

Chapter 4 is composed entirely by the results contained in the papers.

- José M. Rodríguez, José L. Sánchez, José M. Sigarreta and E. Tourís. Bounds on the Arithmetic-Geometric Index. Symmetry (2021) 13, 689.
- Edil D. Molina, José M. Rodríguez, José L. Sánchez and José M. Sigarreta. Some properties of the Arithmetic–Geometric Index. Symmetry (2021) 13, 857.

Abstract

Topological indices have been widely used in different fields associated with scientific research. They are recognized as useful tools in applied research in Chemistry, Ecology, Biology, Physics, among others.

For many years, scientists have been trying to improve the predictive power of the famous Randi'c index. This led to the introduction and study of new topological descriptors that correlate or improve the level of prediction of the Randi'c index. Among the most commonly used descriptors are the *Inverse index*, the *first general Zagreb index* and the recently introduced *Arithmetic-Geometric index*. In this work we study the mathematical properties and relationships of the aforementioned topological indices.

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Chapter 1

Introduction

Mathematical inequalities have been present in the development and consolidation of Science. Nowadays, inequalities are essential tools in multiple applications to different problems, since they are involved in the basis of the processes of approximation, estimation, interpolation, extremals and, in general, they appear in the models used in the study of applied problems.

The formalization of mathematical inequalities begins in the 18th century, essentially, with the works of the so-called “Prince of Mathematics" Johann Carl Friedrich Gauss (1777 - 1855); passing through the investigations and applications of inequalities to Mathematical Analysis developed by Augustin-Louis Cauchy (1789-1857) and Pafnuti Lvóvich Chebyshov (1821-1894). It would be unfair not to mention among the formalizers of mathematical inequalities to Viktor Yakovlevich Bunyakovsky (1804-1889). This remarkable Russian mathematician received all possible mathematical influence from his thesis advisor Augustin-Louis Cauchy. This remarkable scientist is credited with having proved in 1859, many years before Hermann Schwarz, the well-known Cauchy-Schwarz Inequality for the infinite-dimensional case. It is worth noting that in many texts the famous inequality is known as: Cauchy-Bunyakovsky-Schwarz.

The proof of Hardy's famous inequality involved an important group of prominent mathematicians of his time such as: Edmund Hermann Landau (1887-1938), George Pólya (1887-1985), Issai Schur (1875-1941) and Marcel Riesz (1886-1969), among others. It is worth noting the coordinating role played by Godfrey Harold Hardy (1887-1947) in the study of inequalities; his work has been very significant, fundamentally, for the systematization and application of the Theory of Mathematical Inequalities. Hardy was the founder of the Journal of the London Mathematical Society, a suitable publication for many articles on inequalities. In addition, along with Littlewood and Polya, Hardy was the editor of the volume Inequalities (Hardy, Littlewood and Polya, 1934) see [30], which was the first monograph, on inequalities, immediately used as the basis for the later development of mathematical inequalities. For more information on the epistemological evolution of the Theory of Mathematical Inequalities see [36].

It is well known that mathematical inequalities have played a very important role in solving both theoretical and practical problems. In our case they will serve as a basis for the study of mathematical properties and relations between topological indices.

Harold Wiener can be considered the pioneer in the study of topological indices, his first investigations appeared in 1947, when he introduced the nowadays known Wiener index to analyze and correlate the physicochemical properties of alkenes. The topological indices, mathematically, are associated with a numerical value that characterizes the topology of a given discrete structure. Winner's work did not have an immediate repercussion; note that almost 30 years later, in 1971, the scientist Haruo Hosoya introduced the Hosoya index $Z(G)$, which has been successfully applied to structure-property relationships (QSPRs) and quantitative structure-activity relationships (QSARs) see [13].

As a basis for the development of topological indices, it is worth mentioning the efforts and contributions made by two important research groups, first of all the now defunct group of the Boškovic Institute in Zagreb, where the mathematical and computational properties of the now worldwide known Zagreb indices were studied for the first time. The first and second Zagreb indices appeared for the first time in 1972, only one year after the one published by Hosoya, in a paper published by the scientists Gutman and Trinajstíc. Secondly, the work developed by Milan Randić and his collaborators, whose first paper was published in 1975. Probably the most studied, with more than 500 papers, is the Randić index defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \, ,$$

where uv denotes the edge of the graph G joining the vertices u and v, and d_x is the degree of the vertex x.

For more information on the epistemological evolution of the Topological Indices see [35, 44].

Throughout this work, $G = (V(G), E(G))$ denotes a (non-oriented or undirected) finite simple graph (without multiple edges and loops) such that each connected connected component of G has at least an edge. 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. In many cases, we deal with connected graphs. Note that the connectivity of G is not an important constraint for the study of topological indices $IT(G)$, since: if G

has r-connected components $G_1, G_2, \ldots, G_r,$ then

$$IT(G) = IT(G_1) + IT(G_2) + \cdots + IT(G_r).$$

In this research we study the mathematical properties and relationships of the topological indices named *Inverse index*, *first general Zagreb index* and the recently introduced *Arithmetic-Geometric index*.

The *Inverse index* is defined as

$$ID(G) = \sum_{uv \in E(G)} \left(\frac{1}{d_u^2} + \frac{1}{d_v^2}\right) = \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u^2 d_v^2}\,.$$

The *first general Zagreb index* is defined as

$$M_1^{\alpha}(G) = \sum_{u \in V(G)} d_u^{\alpha},$$

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

The *Arithmetic-Geometric index* was introduced in 2016 as

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

Chapter 2

On the inverse degree index

The inverse degree index, also called inverse index, first attracted attention through numerous conjectures generated by the computer programme Graffiti. In this chapter, we obtain new inequalities involving the inverse degree index, and we characterize graphs which are extremal with respect to them.

The best known among the degree–based structure–descriptors are the two Zagreb indices; for recent surveys focusing on their mathematical properties, see [3, 25, 27, 37].

The *first and second Zagreb indices*, denoted by M_1 and M_2, are defined as

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

where uv denotes the edge of the graph G connecting the vertices u and v, and d_x denotes the degree of the vertex x.

The *inverse degree index* $ID(G)$ of a graph G is defined by

$$ID(G) = \sum_{u\in V(G)} \frac{1}{d_u} = \sum_{uv\in E(G)} \Big(\frac{1}{d_u^2} + \frac{1}{d_v^2}\Big) = \sum_{uv\in E(G)} \frac{d_u^2 + d_v^2}{d_u^2 d_v^2}\,.$$

The inverse degree index first attracted attention through numerous conjectures generated by the computer programme Graffiti [19]. Since then, its relationship with other graph invariants, such as diameter, edge-connectivity, matching number, Wiener index has been studied by several authors (see, e.g., [7], [11], [16], [17], [42], [63]).

Miličević and Nikolić defined in [39] the *first and second variable Zagreb indices* as

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

with $\alpha \in \mathbb{R}$. In [33] and [4] the *first and second general Zagreb indices* are introduced as

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

respectively. It is clear that these indices are equivalent to the previous ones, since ${}^{\alpha}M_1(G) = M_1^{2\alpha}(G)$ and ${}^{\alpha}M_2(G) = M_2^{\alpha}(G)$. We prefer to use $M_j^{\alpha}(G)$ instead of ${}^{\alpha}M_j(G)$, for $j = 1, 2$, since the inequalities obtained in this chapter become simpler with them.

Note that M_1^1 is $2m$, M_1^2 is the first Zagreb index M_1, M_1^{-1} is the inverse index $ID(G)$ [19], M_1^3 is the forgotten index $F(G)$ [22], 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 [44], etc. Note that it is interesting to study M_1^{α} for

$\alpha \neq 0, 1$, and M_2^α for $\alpha \neq 0$, since if G has n vertices and m vertices, then $M_1^0(G) = n$, $M_1^1(G) = 2m$ and $M_2^0(G) = m$.

The concept of the variable molecular descriptors was proposed as a new way of characterizing heteroatoms in molecules (see [46], [47]), but also to assess the structural differences (e.g., the relative role of carbon atoms of acyclic and cyclic parts in alkylcycloalkanes [48]). 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 studied property is as small as possible.

The second variable Zagreb index is used in the structure-boiling point modeling of benzenoid hydrocarbons [45]. Various properties and relations of these indices are discussed in several papers (see, e.g., [2], [34], [32], [54], [61], [62]).

In the paper of Gutman and Tosovic [28], 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 general 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 ($R = M_2^{-1/2}$).

2.1 Inequalities involving Zagreb and sum-connectivity indices

Let us start by recalling two well-known and useful inequalities for the inverse degree index of a graph G with n edges, maximum degree Δ and minimum degree δ:

$$\frac{n}{\Delta} \le ID(G) \le \frac{n}{\delta}\,. \tag{2.1}$$

Moreover, both equalities are attained if and only if G is regular.

In order to prove our first result, we need the following useful and well-known Polya-Szegö inequality (see [30, p.62]). See, e.g., [38, Lemma 3.4] for a proof of the statement of equality.

Lemma 1 *If $a_j, b_j \ge 0$ and $Mb_j \le a_j \le Nb_j$ for $1 \le j \le k$ and some positive constants M, N, then*

$$\Big(\sum_{j=1}^{k} a_j^2\Big)^{1/2}\Big(\sum_{j=1}^{k} b_j^2\Big)^{1/2} \le \frac{1}{2}\left(\sqrt{\frac{N}{M}}+\sqrt{\frac{M}{N}}\right)\sum_{j=1}^{k} a_j b_j.$$

If $a_j > 0$ for some $1 \le j \le k$, then the equality holds if and only if $M = N$ and $a_j = Mb_j$ for every $1 \le j \le k$.

Theorem 2 *If G is a non-trivial graph with n vertices, m edges, minimum degree δ and maximum degree Δ, then*

$$\frac{n^2}{2m} \le ID(G) \le \frac{(\Delta+\delta)^2 n^2}{8\Delta\delta m}\,.$$

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

Proof. Cauchy-Schwarz inequality gives

$$n^2 = \Big(\sum_{u\in V(G)} \sqrt{d_u}\,\frac{1}{\sqrt{d_u}}\Big)^2 \le \Big(\sum_{u\in V(G)} d_u\Big)\Big(\sum_{u\in V(G)} \frac{1}{d_u}\Big) = 2m\, ID(G).$$

On the other hand, since

$$\delta \le \frac{\sqrt{d_u}}{\frac{1}{\sqrt{d_u}}} = d_u \le \Delta,$$

Lemma 1 gives

$$\begin{aligned} n^2 &= \Big(\sum_{u\in V(G)} \sqrt{d_u}\,\frac{1}{\sqrt{d_u}} \Big)^2 \ge \frac{\Big(\sum_{u\in V(G)} d_u\Big)\Big(\sum_{u\in V(G)} \frac{1}{d_u}\Big)}{\frac{1}{4}\Big(\sqrt{\frac{\Delta}{\delta}}+\sqrt{\frac{\delta}{\Delta}}\,\Big)^2} \\ &= \frac{2m\,ID(G)}{\frac{1}{4}\frac{(\Delta+\delta)^2}{\Delta\delta}} = \frac{8m\Delta\delta\,ID(G)}{(\Delta+\delta)^2}\,. \end{aligned}$$

If the graph is regular, then the lower and upper bound are the same, and they are equal to $ID(G)$.

If the equality is attained in the lower bound, then Cauchy-Schwarz inequality gives that the vectors $\big(d_u^{1/2}\big)_{u\in V(G)}$ and $\big(d_u^{-1/2}\big)_{u\in V(G)}$ are parallel; this is equivalent to $d_u = d_v$ for every $u, v \in V(G)$, and G is regular. If the equality is attained in the upper bound, then Lemma 1 gives $\delta = \Delta$ and the graph is regular. ■

In order to prove Theorem 5 below we need a kind of converse of Hölder's inequality, which is interesting by itself.

Theorem 3 *Let (X,μ) be a measure space and $f,g : X \to \mathbb{R}$ non-negative measurable functions, and $1 < p,q < \infty$ with $1/p+1/q = 1$. If $f \in L^p(X,\mu)$, $g \in L^q(X,\mu)$ and $\omega g^q \le f^p \le \Omega g^q$ μ-a.e. for some positive constants ω,Ω, then*

$$\Big(\int_X f^p\,d\mu\Big)^{1/p}\Big(\int_X g^q\,d\mu\Big)^{1/q} \le c_p(\omega,\Omega)\int_X fg\,d\mu, \tag{2.2}$$

where

$$c_p(\omega,\Omega) = \max\Big\{\frac{1}{p}\Big(\frac{\omega}{\Omega}\Big)^{1/q} + \frac{1}{q}\Big(\frac{\Omega}{\omega}\Big)^{1/p},\ \frac{1}{p}\Big(\frac{\Omega}{\omega}\Big)^{1/q} + \frac{1}{q}\Big(\frac{\omega}{\Omega}\Big)^{1/p}\Big\}.$$

The equality is attained if and only if we have $\omega = \Omega$ *and* $f^p = \omega g^q$ μ*-a.e. or* $f = g = 0$ μ*-a.e.*

Proof. Fix $\lambda \in (0,1)$ and $0 < m \le M$. Let us define $F_\lambda(t) := \lambda t^{1-\lambda} + (1-\lambda)t^{-\lambda}$ for $t > 0$. Since $F'_\lambda(t) = \lambda(1-\lambda)t^{-\lambda} - \lambda(1-\lambda)t^{-\lambda-1} = \lambda(1-\lambda)t^{-\lambda-1}(t-1)$, we have that F_λ is strictly decreasing on $(0,1)$ and strictly increasing on $(1,\infty)$. Hence, $F_\lambda(t) \le \max\{F_\lambda(m), F_\lambda(M)\} =: D$ for every $m \le t \le M$, and if $F_\lambda(t) = D$ for some $m \le t \le M$, then $t = m$ or $t = M$.

If $x, y > 0$ and $my \le x \le My$, then

$$\lambda\Big(\frac{x}{y}\Big)^{1-\lambda} + (1-\lambda)\Big(\frac{y}{x}\Big)^{\lambda} \le D,$$

$$\lambda x + (1-\lambda)y \le D x^\lambda y^{1-\lambda}.$$

Note that, by continuity, this last inequality holds for every $x, y \ge 0$ with $my \le x \le My$. If the equality is attained for some $x, y \ge 0$ with $my \le x \le My$, then $x = my$ or $x = My$ (the cases $x = 0$ and $y = 0$ are direct).

Consider $\lambda = 1/p$ (and so, $1 - \lambda = 1/q$), $a = x^\lambda = x^{1/p}$ and $b = y^{1-\lambda} = y^{1/q}$. Thus,

$$\frac{a^p}{p} + \frac{b^q}{q} \le Dab \tag{2.3}$$

for every $a, b \ge 0$ with $mb^q \le a^p \le Mb^q$. If the equality is attained for some $a, b \ge 0$ with $mb^q \le a^p \le Mb^q$, then $a^p = mb^q$ or $a^p = Mb^q$.

Since $\omega g^q \le f^p \le \Omega g^q$ μ-a.e., we have $\omega\|g\|_q^q \le \|f\|_p^p \le \Omega\|g\|_q^q$. If $\|f\|_p = 0$ or $\|g\|_q = 0$, then $\|f\|_p = \|g\|_q = 0$ and the equality in (2.2) holds.

Assume now that $\|f\|_p \neq 0 \neq \|g\|_q$. Thus,

$$\frac{\omega}{\Omega}\,\frac{g^q}{\|g\|_q^q} \leq \frac{f^p}{\|f\|_p^p} \leq \frac{\Omega}{\omega}\,\frac{g^q}{\|g\|_q^q} \quad \mu\text{-a.e.}$$

If we consider $a = f/\|f\|_p$ and $b = g/\|g\|_q$ in (2.3) and we integrate both sides with respect to μ, then we obtain

$$1 = \frac{1}{p}\,\frac{\|f\|_p^p}{\|f\|_p^p} + \frac{1}{q}\,\frac{\|g\|_q^q}{\|g\|_q^q} \leq c_p(\omega,\Omega)\frac{\|fg\|_1}{\|f\|_p\|g\|_q}\,,$$

$$\|f\|_p\|g\|_q \leq c_p(\omega,\Omega)\|fg\|_1.$$

If the equality is attained, then

$$\frac{f^p}{\|f\|_p^p} = \frac{\omega}{\Omega}\,\frac{g^q}{\|g\|_q^q} \quad \text{or} \quad \frac{f^p}{\|f\|_p^p} = \frac{\Omega}{\omega}\,\frac{g^q}{\|g\|_q^q} \quad \mu\text{-a.e.} \tag{2.4}$$

Assume that the first equality in (2.4) holds in a set A of positive μ-measure. Therefore, we have both $f^p = \omega g^q$ in A and $\|f\|_p^p = \Omega\|g\|_q^q$. Since $\|f\|_p \neq 0$, these facts imply $\omega = \Omega$ and $f^p = \omega g^q$ μ-a.e.

If the second equality in (2.4) holds in a set of positive μ-measure, then a similar argument gives $\omega = \Omega$ and $f^p = \omega g^q$ μ-a.e. ■

Theorem 3 has the following consequence.

Corollary 4 *If $1 < p, q < \infty$, $a_j, b_j \geq 0$ and $\omega b_j^q \leq a_j^p \leq \Omega b_j^q$ for $1 \leq j \leq k$ and some positive constants ω, Ω, then*

$$\Big(\sum_{j=1}^k a_j^p\Big)^{1/p}\Big(\sum_{j=1}^k b_j^q\Big)^{1/q} \leq c_p(\omega,\Omega)\sum_{j=1}^k a_j b_j,$$

where $c_p(\omega,\Omega)$ is the constant in Theorem 3. If $a_j > 0$ for some $1 \leq j \leq k$, then the equality holds if and only if $\omega = \Omega$ and $a_j^p = \omega b_j^q$ for every $1 \leq j \leq k$.

Next, we prove three theorems that state several inequalities involving the inverse and the first general Zagreb indices.

Theorem 5 *If $\alpha \in \mathbb{R}$ and G is a non-trivial graph with n vertices, m edges, minimum degree δ and maximum degree Δ, then*

$$
\begin{aligned}
2^\alpha m^\alpha n^{1-\alpha} \le M_1^\alpha(G) \le c_\alpha(\delta^\alpha, \Delta^\alpha)^\alpha 2^\alpha m^\alpha n^{1-\alpha}, &\quad \text{if } \alpha \ge 1,\\
c_{\frac{1}{\alpha}}(\delta, \Delta)^{-1} 2^\alpha m^\alpha n^{1-\alpha} \le M_1^\alpha(G) \le 2^\alpha m^\alpha n^{1-\alpha}, &\quad \text{if } 0 \le \alpha \le 1,\\
c_{-\frac{1}{\alpha}}(\Delta^{-1}, \delta^{-1})^{-1} n^{1+\alpha} \le M_1^\alpha(G)\, ID(G)^\alpha \le n^{1+\alpha}, &\quad \text{if } -1 \le \alpha \le 0,\\
c_{-\alpha}(\Delta^\alpha, \delta^\alpha)^{-1} M_1^\alpha(G)^{\frac{-1}{\alpha}} n^{\frac{\alpha+1}{\alpha}} \le ID(G) \le M_1^\alpha(G)^{\frac{-1}{\alpha}} n^{\frac{\alpha+1}{\alpha}}, &\quad \text{if } \alpha \le -1,
\end{aligned}
$$

where $c_p(\omega, \Omega)$ is the constant in Theorem 3 if $1 < p < \infty$, and $c_1(\omega, \Omega) = c_\infty(\omega, \Omega) = 1$. If $\alpha \ne -1, 0, 1$, then the equality is attained in each inequality if and only if G is regular. If $\alpha \in \{-1, 0, 1\}$, then the inequalities are equalities for every graph G.

Proof. If $\alpha = 1$, then $M_1^1(G) = 2m$ for every graph G. If $\alpha = 0$, then $M_1^0(G) = n$ for every graph G. If $\alpha = -1$, then $M_1^{-1}(G) = ID(G)$ for every graph G. Thus, in the three cases the inequalities are equalities for every graph G.

If $\alpha > 1$, then Hölder's inequality gives

$$
2m = \sum_{u \in V(G)} d_u \le \Big(\sum_{u \in V(G)} d_u^\alpha \Big)^{\frac{1}{\alpha}} \Big(\sum_{u \in V(G)} 1^{\frac{\alpha}{\alpha-1}} \Big)^{\frac{\alpha-1}{\alpha}} = M_1^\alpha(G)^{\frac{1}{\alpha}} n^{\frac{\alpha-1}{\alpha}},
$$

and so $M_1^\alpha(G) \ge 2^\alpha m^\alpha n^{1-\alpha}$. Since $\delta^\alpha \le d_u^\alpha = d_u^\alpha / 1^{\frac{\alpha}{\alpha-1}} \le \Delta^\alpha$, Corollary 4 gives

$$2m = \sum_{u\in V(G)} d_u \ge \frac{\Big(\sum_{u\in V(G)} d_u^\alpha\Big)^{\frac{1}{\alpha}}\Big(\sum_{u\in V(G)} 1^{\frac{\alpha}{\alpha-1}}\Big)^{\frac{\alpha-1}{\alpha}}}{c_\alpha(\delta^\alpha,\Delta^\alpha)} = \frac{M_1^\alpha(G)^{\frac{1}{\alpha}} n^{\frac{\alpha-1}{\alpha}}}{c_\alpha(\delta^\alpha,\Delta^\alpha)}\,,$$

If $\alpha < -1$, then

$$\begin{aligned} ID(G) &= \sum_{u\in V(G)} d_u^{-1} \le \Big(\sum_{u\in V(G)} (d_u^{-1})^{-\alpha}\Big)^{\frac{-1}{\alpha}}\Big(\sum_{u\in V(G)} 1^{\frac{\alpha}{\alpha+1}}\Big)^{\frac{\alpha+1}{\alpha}} \\ &= M_1^\alpha(G)^{\frac{-1}{\alpha}} n^{\frac{\alpha+1}{\alpha}}. \end{aligned}$$

Since $\Delta^\alpha \le d_u^\alpha = (d_u^{-1})^{-\alpha}/1^{\frac{\alpha}{\alpha+1}} \le \delta^\alpha$, Corollary 4 gives

$$\begin{aligned} ID(G) &= \sum_{u\in V(G)} d_u^{-1} \ge \frac{\Big(\sum_{u\in V(G)}(d_u^{-1})^{-\alpha}\Big)^{\frac{-1}{\alpha}}\Big(\sum_{u\in V(G)} 1^{\frac{\alpha}{\alpha+1}}\Big)^{\frac{\alpha+1}{\alpha}}}{c_{-\alpha}(\Delta^\alpha,\delta^\alpha)} \\ &= \frac{M_1^\alpha(G)^{\frac{-1}{\alpha}} n^{\frac{\alpha+1}{\alpha}}}{c_{-\alpha}(\Delta^\alpha,\delta^\alpha)}\,. \end{aligned}$$

If $0 < \alpha < 1$, then

$$M_1^\alpha(G) = \sum_{u\in V(G)} d_u^\alpha \le \Big(\sum_{u\in V(G)} (d_u^\alpha)^{\frac{1}{\alpha}}\Big)^\alpha \Big(\sum_{u\in V(G)} 1^{\frac{1}{1-\alpha}}\Big)^{1-\alpha} = 2^\alpha m^\alpha n^{1-\alpha}.$$

Since $\delta \le d_u = (d_u^\alpha)^{\frac{1}{\alpha}}/1^{\frac{1}{1-\alpha}} \le \Delta$, Corollary 4 gives

$$M_1^\alpha(G) \ge \frac{\Big(\sum_{u\in V(G)}(d_u^\alpha)^{\frac{1}{\alpha}}\Big)^\alpha\Big(\sum_{u\in V(G)} 1^{\frac{1}{1-\alpha}}\Big)^{1-\alpha}}{c_{\frac{1}{\alpha}}(\delta,\Delta)} = \frac{2^\alpha m^\alpha n^{1-\alpha}}{c_{\frac{1}{\alpha}}(\delta,\Delta)}\,.$$

If $-1 < \alpha < 0$, then $\Delta^{-1} \le d_u^{-1} = (d_u^\alpha)^{-\frac{1}{\alpha}}/1^{\frac{\alpha}{\alpha+1}} \le \delta^{-1}$, and Corollary 4 gives

$$M_1^\alpha(G) = \sum_{u\in V(G)} d_u^\alpha \geq \frac{\left(\sum_{u\in V(G)} (d_u^\alpha)^{-\frac{1}{\alpha}}\right)^{-\alpha} \left(\sum_{u\in V(G)} 1^{\frac{1}{1+\alpha}}\right)^{1+\alpha}}{c_{-\frac{1}{\alpha}}(\Delta^{-1},\delta^{-1})}$$
$$= \frac{ID(G)^{-\alpha} n^{1+\alpha}}{c_{-\frac{1}{\alpha}}(\Delta^{-1},\delta^{-1})}\,.$$

Assume that $\alpha \neq -1, 0, 1$, and consider any inequality proved by using Hölder's inequality. By Hölder's inequality, the equality is attained if and only if the vectors $(d_u^\beta)_{u\in V(G)}$ (for some constant $\beta \neq 0$ which depends on α) and $(1)_{u\in V(G)}$ are parallel; this is equivalent to $d_u = d_v$ for every $u, v \in V(G)$, i.e., G is regular.

Assume that $\alpha \neq -1, 0, 1$, and consider any inequality proved by using Corollary 4. By Corollary 4, the equality is attained if and only if $\delta^\beta = \Delta^\beta$ (for some constant $\beta \neq 0$ which depends on α), i.e., G is regular. ■

Remark 6 *Recall that the number α in $M_1^\alpha(G)$ is not an exponent, it is a parameter.*

Theorem 7 *If $\alpha \in \mathbb{R}$ and G is a non-trivial graph with n vertices, minimum degree δ and maximum degree Δ, then*

$$\delta^{\alpha-1} n^2 \leq M_1^\alpha(G)\, ID(G) \leq \frac{(\Delta^\alpha + \delta^\alpha)^2 n^2}{4\Delta\delta^\alpha}\,, \qquad \text{if } \alpha \geq 1,$$
$$\Delta^{\alpha-1} n^2 \leq M_1^\alpha(G)\, ID(G) \leq \frac{(\Delta^\alpha + \delta^\alpha)^2 n^2}{4\Delta^\alpha\delta}\,, \qquad \text{if } \alpha \leq 1.$$

Any equality is attained for some $\alpha \in \mathbb{R}$ if and only if G is regular.

Proof. If $\alpha \geq 1$, then Cauchy-Schwarz inequality gives

$$\begin{aligned} n^2 &= \Big(\sum_{u \in V(G)} d_u^{\alpha/2} d_u^{-\alpha/2} \Big)^2 \leq \Big(\sum_{u \in V(G)} d_u^{\alpha} \Big) \Big(\sum_{u \in V(G)} d_u^{-\alpha} \Big) \\ &= M_1^{\alpha}(G) \sum_{u \in V(G)} d_u^{-\alpha+1} d_u^{-1} \leq \delta^{-\alpha+1} M_1^{\alpha}(G) \, ID(G). \end{aligned}$$

The same argument gives $\Delta^{\alpha-1} n^2 \leq M_1^{\alpha}(G) \, ID(G)$ for $\alpha \leq 1$.

On the other hand, since we have for every $\alpha \in \mathbb{R}$,

$$\min \{\delta^{\alpha}, \Delta^{\alpha}\} \leq \frac{d_u^{\alpha/2}}{d_u^{-\alpha/2}} = d_u^{\alpha} \leq \max \{\delta^{\alpha}, \Delta^{\alpha}\},$$

and

$$\begin{aligned} \left(\sqrt{\frac{\max \{\delta^{\alpha}, \Delta^{\alpha}\}}{\min \{\delta^{\alpha}, \Delta^{\alpha}\}}} + \sqrt{\frac{\min \{\delta^{\alpha}, \Delta^{\alpha}\}}{\max \{\delta^{\alpha}, \Delta^{\alpha}\}}} \right)^2 &= \left(\frac{\Delta^{\alpha/2}}{\delta^{\alpha/2}} + \frac{\delta^{\alpha/2}}{\Delta^{\alpha/2}} \right)^2 \\ &= \frac{\left(\Delta^{\alpha} + \delta^{\alpha}\right)^2}{\Delta^{\alpha} \delta^{\alpha}} , \end{aligned}$$

Lemma 1 gives

$$\begin{aligned} n^2 &= \Big(\sum_{u \in V(G)} d_u^{\alpha/2} d_u^{-\alpha/2} \Big)^2 \geq \frac{\Big(\sum_{u \in V(G)} d_u^{\alpha} \Big) \Big(\sum_{u \in V(G)} d_u^{-\alpha} \Big)}{\frac{(\Delta^{\alpha}+\delta^{\alpha})^2}{4\Delta^{\alpha}\delta^{\alpha}}} \\ &= \frac{4\Delta^{\alpha}\delta^{\alpha} M_1^{\alpha}(G) \Big(\sum_{u \in V(G)} d_u^{-\alpha+1} d_u^{-1} \Big)}{\left(\Delta^{\alpha} + \delta^{\alpha}\right)^2} . \end{aligned}$$

If $\alpha \geq 1$, then $d_u^{-\alpha+1} \geq \Delta^{-\alpha+1}$ and

$$n^2 \geq \frac{4\Delta\delta^{\alpha} M_1^{\alpha}(G) \, ID(G)}{\left(\Delta^{\alpha} + \delta^{\alpha}\right)^2} .$$

If $\alpha \le 1$, then $d_u^{-\alpha+1} \ge \delta^{-\alpha+1}$ and

$$n^2 \ge \frac{4\Delta^\alpha \delta\, M_1^\alpha(G)\, ID(G)}{\left(\Delta^\alpha + \delta^\alpha\right)^2}\,.$$

If the graph is regular, then for each $\alpha \in \mathbb{R}$ both bounds are the same, and they are equal to $M_1^\alpha(G)\, ID(G)$.

If an equality is attained for some $\alpha \neq 1$, then we have either $d_u = \delta$ for every $u \in V(G)$ or $d_u = \Delta$ for every $u \in V(G)$, and G is regular in both cases. If the lower bound is attained for $\alpha = 1$, then Cauchy-Schwarz inequality gives that the vectors $(d_u^{1/2})_{u\in V(G)}$ and $(d_u^{-1/2})_{u\in V(G)}$ are parallel; this is equivalent to $d_u = d_v$ for every $u, v \in V(G)$, and G is regular. If the upper bound is attained for $\alpha = 1$, then Lemma 1 gives that $\delta = \Delta$, and G is regular. ■

Theorem 8 *If G is a non-trivial graph with n vertices, minimum degree δ and maximum degree Δ, then*

$$ID(G) \ge \frac{n}{\Delta+\delta} + \frac{\Delta\delta}{\Delta+\delta}\, M_1^{-2}(G).$$

The equality is attained if and only if each vertex has degree either δ or Δ.

Proof. We have

$$\Big(\frac{1}{\delta} - \frac{1}{d_u}\Big)\Big(\frac{1}{d_u} - \frac{1}{\Delta}\Big) \ge 0, \qquad \frac{1}{d_u\delta} - \frac{1}{\delta\Delta} - \frac{1}{d_u^2} + \frac{1}{d_u\Delta} \ge 0,$$
$$\frac{1}{d_u}\frac{\Delta+\delta}{\Delta\delta} \ge \frac{1}{\Delta\delta} + \frac{1}{d_u^2}\,, \qquad \frac{1}{d_u} \ge \frac{1}{\Delta+\delta} + \frac{\Delta\delta}{\Delta+\delta}\,\frac{1}{d_u^2}\,,$$
$$ID(G) \ge \frac{n}{\Delta+\delta} + \frac{\Delta\delta}{\Delta+\delta}\, M_1^{-2}(G).$$

The equality is attained if and only if $(\delta - d_u)(d_u - \Delta)$ for every $u \in V(G)$, i.e., each vertex has degree either δ or Δ. ■

With motivation from the first Zagreb and harmonic indices, *general sum-connectivity index* χ_α was defined by Zhou and Trinajstić in [66] as

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

with $\alpha \in \mathbb{R}$. 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, etc. Some mathematical properties of the general sum-connectivity index were given in [14], [51], [64], [66] and [67].

The following results relate the general first Zagreb and the general sum-connectivity indices.

Theorem 9 *If $\alpha \in \mathbb{R}$ and G is a non-trivial graph, then*

$$M_1^{\alpha+1}(G) \geq 2^{1-\alpha}\chi_\alpha(G), \qquad \text{if } \alpha \geq 1 \text{ or } \alpha \leq 0,$$
$$M_1^{\alpha+1}(G) \leq 2^{1-\alpha}\chi_\alpha(G), \qquad \text{if } 0 \leq \alpha \leq 1.$$

If $\alpha \neq 0, 1$, then the equality is attained in each inequality if and only if every connected component of G is regular. If $\alpha \in \{0, 1\}$, then the equality holds for every graph G.

Proof. If $\alpha = 0$, then $2\chi_0(G) = 2\sum_{uv \in E(G)} 1 = 2m = \sum_{u \in V(G)} d_u = M_1^1(G)$.

If $\alpha = 1$, then $\chi_1(G) = \sum_{uv \in E(G)}(d_u + d_v) = M_1(G) = M_1^2(G)$.

Let us consider the function $f(x) = x^\alpha$ for $x > 0$, with $\alpha \neq 0, 1$.

If $\alpha > 1$ or $\alpha < 0$, then f is convex and

$$\Big(\frac{d_u + d_v}{2}\Big)^\alpha \le \frac{d_u^\alpha + d_v^\alpha}{2}, \qquad 2^{1-\alpha}(d_u + d_v)^\alpha \le d_u^\alpha + d_v^\alpha,$$

$$2^{1-\alpha}\chi_\alpha(G) = 2^{1-\alpha} \sum_{uv\in E(G)} (d_u + d_v)^\alpha \le \sum_{uv\in E(G)} (d_u^\alpha + d_v^\alpha) = \sum_{u\in V(G)} d_u^{\alpha+1} = M_1^{\alpha+1}(G).$$

If $0 < \alpha < 1$, then $f(x) = x^\alpha$ is concave and the converse inequality holds.

If we fix $\alpha \neq 0, 1$, then f is either strictly convex or strictly concave. Thus, the equality is attained if and only if $d_u = d_v$ for every $uv \in E(G)$, i.e., each connected component of G is regular. If $\alpha \in \{0, 1\}$, then we have proved that the equality holds for every graph G. ■

Corollary 10 *If G is a non-trivial graph, then*

$$ID(G) \ge 8\chi_{-2}(G).$$

The equality is attained if and only if every connected component of G is regular.

In [50] appears the following result.

Lemma 11 *If $0 < a \le x, y \le b$, then*

$$\frac{2\sqrt{ab}}{a+b} \le \frac{2\sqrt{xy}}{x+y} \le 1.$$

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 $x = y$.

Corollary 12 *If $0 < \delta \le x, y \le \Delta$, then*

$$2 \le \frac{x^2 + y^2}{xy} \le \frac{\Delta^2 + \delta^2}{\Delta\delta}\,.$$

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

Recall that 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. We say that a graph is (Δ, δ)-*biregular* if we want to write explicitly the maximum and minimum degrees.

The following results relate the second general Zagreb and the inverse indices.

Theorem 13 *If G is a non-trivial graph with m edges, minimum degree δ and maximum degree Δ, then*

$$\frac{4\Delta\delta}{\Delta^2 + \delta^2}\, m^{\frac{1}{2}} M_2^{-2}(G)^{\frac{1}{2}} \le ID(G) \le \frac{\Delta^2 + \delta^2}{\Delta\delta}\, m^{\frac{1}{2}} M_2^{-2}(G)^{\frac{1}{2}}\,.$$

The equality in the upper bound is attained if and only if G is either regular or (Δ, δ)-biregular. The equality in the lower bound is attained if and only if G is regular.

Proof. Cauchy-Schwarz inequality and Corollary 12 give

$$\begin{aligned} ID(G)^2 &= \Big(\sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u^2 d_v^2} \Big)^2 \le \sum_{uv \in E(G)} \Big(\frac{d_u^2 + d_v^2}{d_u d_v} \Big)^2 \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^2} \\ &\le \sum_{uv \in E(G)} \Big(\frac{\Delta^2 + \delta^2}{\Delta\delta} \Big)^2 \sum_{uv \in E(G)} (d_u d_v)^{-2} = \Big(\frac{\Delta^2 + \delta^2}{\Delta\delta} \Big)^2 m\, M_2^{-2}(G). \end{aligned}$$

On the other hand, since

$$2\delta^2 \leq \frac{\frac{d_u^2+d_v^2}{d_u d_v}}{\frac{1}{d_u d_v}} = d_u^2 + d_v^2 \leq 2\Delta^2, \quad \text{with} \quad \sqrt{\frac{2\Delta^2}{2\delta^2}} = \frac{\Delta}{\delta}\,,$$

Lemma 11 and Corollary 12 give

$$\begin{aligned} ID(G)^2 = \Big(\sum_{uv\in E(G)} \frac{d_u^2+d_v^2}{d_u^2 d_v^2} \Big)^2 &\geq \frac{\sum_{uv\in E(G)} \left(\frac{d_u^2+d_v^2}{d_u d_v}\right)^2 \sum_{uv\in E(G)} (d_u d_v)^{-2}}{\frac{1}{4}\big(\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\big)^2} \\ &\geq \frac{\sum_{uv\in E(G)} 4\, M_2^{-2}(G)}{\frac{1}{4}\,\frac{(\Delta^2+\delta^2)^2}{\Delta^2\delta^2}} = \frac{16\Delta^2\delta^2 m\, M_2^{-2}(G)}{(\Delta^2+\delta^2)^2}\,. \end{aligned}$$

By Cauchy-Schwarz inequality and Corollary 12, the equality in the upper bound is attained if and only if every edge has a vertex with degree δ and the other vertex with degree Δ; and this happens if and only if G is either regular (if $\Delta = \delta$) or (Δ, δ)-biregular (if $\Delta \neq \delta$).

By Lemma 11 and Corollary 12, the equality is attained in the lower bound if and only if $2\delta^2 = 2\Delta^2$, i.e., G is regular. ■

Theorem 14 *Let G be a non-trivial graph with minimum degree δ and max-*

imum degree Δ. Then

$$2\delta^{-2\alpha-2}M_2^{\alpha}(G) \le ID(G) \le 2\Delta^{-2\alpha-2}M_2^{\alpha}(G), \quad \text{if } \alpha \le -2\Delta^2/(\Delta^2+\delta^2),$$

$$\min\Big\{2\delta^{-2\alpha-2},\, \frac{2}{-\alpha}\Big(\frac{\alpha+2}{-\alpha}\Big)^{-\alpha/2-1}\Delta^{-2\alpha-2}\Big\}M_2^{\alpha}(G) \le ID(G)$$
$$\le \max\{2\Delta^{-2\alpha-2},\, (\Delta^2+\delta^2)(\Delta\delta)^{-\alpha-2}\}M_2^{\alpha}(G),$$
$$\text{if } -2\Delta^2/(\Delta^2+\delta^2) < \alpha < -1,$$

$$2M_2^{-1}(G) \le ID(G) \le \frac{\Delta^2+\delta^2}{\Delta\delta}M_2^{-1}(G), \qquad \text{if } \alpha = -1,$$

$$\min\Big\{2\Delta^{-2\alpha-2},\, \frac{2}{-\alpha}\Big(\frac{\alpha+2}{-\alpha}\Big)^{-\alpha/2-1}\delta^{-2\alpha-2}\Big\}M_2^{\alpha}(G) \le ID(G)$$
$$\le \max\{2\delta^{-2\alpha-2},\, (\Delta^2+\delta^2)(\Delta\delta)^{-\alpha-2}\}M_2^{\alpha}(G),$$
$$\text{if } -1 < \alpha < -2\delta^2/(\Delta^2+\delta^2),$$

$$2\Delta^{-2\alpha-2}M_2^{\alpha}(G) \le ID(G) \le 2\delta^{-2\alpha-2}M_2^{\alpha}(G), \quad \text{if } \alpha \ge -2\delta^2/(\Delta^2+\delta^2).$$

Every bound is attained for every regular graph G. Furthermore, in the first and last cases, each inequality is attained if and only if G is regular.

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

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

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

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

If $\alpha \le -2$, then $\partial f/\partial x, \partial f/\partial y > 0$ and so, f is an increasing function in both variables. Hence,

$$
\begin{aligned}
2\delta^{-2\alpha-2} &\le f(x,y) \le 2\Delta^{-2\alpha-2}, \\
2\delta^{-2\alpha-2}(d_u d_v)^{\alpha} &\le \frac{1}{d_u^2} + \frac{1}{d_v^2} \le 2\Delta^{-2\alpha-2}(d_u d_v)^{\alpha}, \\
2\delta^{-2\alpha-2} M_2^{\alpha}(G) &\le ID(G) \le 2\Delta^{-2\alpha-2} M_2^{\alpha}(G).
\end{aligned}
\tag{2.5}
$$

If $\alpha \ge 0$, then $\partial f/\partial x, \partial f/\partial y < 0$ and

$$
\begin{aligned}
2\Delta^{-2\alpha-2} &\le f(x,y) \le 2\delta^{-2\alpha-2}, \\
2\Delta^{-2\alpha-2}(d_u d_v)^{\alpha} &\le \frac{1}{d_u^2} + \frac{1}{d_v^2} \le 2\delta^{-2\alpha-2}(d_u d_v)^{\alpha}, \\
2\Delta^{-2\alpha-2} M_2^{\alpha}(G) &\le ID(G) \le 2\delta^{-2\alpha-2} M_2^{\alpha}(G).
\end{aligned}
\tag{2.6}
$$

We deal now with the case $-2 < \alpha < 0$. If $\nabla f(x,y) = 0$, then

$$
\begin{aligned}
0 &= \alpha x^2 + 2y^2 + \alpha y^2, \\
0 &= -\alpha x^2 - 2x^2 - \alpha y^2,
\end{aligned}
$$

and we conclude $x = y$. Therefore, the maximum and the minimum values of f are attained on the boundary $\{x = \delta,\ \delta \le y \le \Delta\} \cup \{y = \Delta,\ \delta \le x \le \Delta\} \cup \{\delta \le x = y \le \Delta\}$.

On the set $\{\delta \le x = y \le \Delta\}$ we have $f(x,x) = 2x^{-2\alpha-2}$. If $-2 < \alpha \le -1$, then $2\delta^{-2\alpha-2} \le f(x,x) \le 2\Delta^{-2\alpha-2}$. If $-1 \le \alpha < 0$, then $2\Delta^{-2\alpha-2} \le f(x,x) \le 2\delta^{-2\alpha-2}$.

We have $\partial f/\partial y(\delta, y) = 0$ for some $y > 0$ if and only if

$$
-\alpha y^2 - (\alpha+2)\delta^2 = 0 \qquad \Leftrightarrow \qquad y = y_0 := \sqrt{\frac{\alpha+2}{-\alpha}}\,\delta\,.
$$

Thus, $\delta < y_0 < \Delta$ if and only if

$$-1 < \alpha < \frac{-2\delta^2}{\Delta^2 + \delta^2}\,. \tag{2.7}$$

If $-2 < \alpha \le -1$, then $\partial f/\partial y(\delta, y) > 0$ for $\delta < y < \Delta$, and

$$2\delta^{-2\alpha-2} = f(\delta,\delta) \le f(\delta, y) \le f(\delta,\Delta) = (\Delta^2 + \delta^2)(\Delta\delta)^{-\alpha-2}.$$

If $-2\delta^2/(\Delta^2 + \delta^2) \le \alpha < 0$, then $\partial f/\partial y(\delta, y) < 0$ for $\delta < y < \Delta$, and

$$(\Delta^2 + \delta^2)(\Delta\delta)^{-\alpha-2} \le f(\delta, y) \le 2\delta^{-2\alpha-2}.$$

If (2.7) holds, then $\partial f/\partial y(\delta,\delta) = -2\delta^{-2\alpha-3}(\alpha+1) < 0$, and $\partial f/\partial y(\delta,\Delta) = \Delta^{-\alpha-3}\delta^{-\alpha-2}\big(-\alpha\Delta^2 - (\alpha+2)\delta^2\big) > 0$, and we conclude

$$\begin{aligned}&\frac{2}{-\alpha}\Big(\frac{\alpha+2}{-\alpha}\Big)^{-\alpha/2-1}\delta^{-2\alpha-2} = f(\delta, y_0) \le f(\delta, y)\\ &\quad\le \max\big\{f(\delta,\delta),\ f(\delta,\Delta)\big\} = \max\big\{2\delta^{-2\alpha-2},\ (\Delta^2+\delta^2)(\Delta\delta)^{-\alpha-2}\big\}.\end{aligned}$$

We have $\partial f/\partial x(x,\Delta) = 0$ for some $x > 0$ if and only if

$$-\alpha x^2 - (\alpha+2)\Delta^2 = 0 \qquad \Leftrightarrow \qquad x = x_0 := \sqrt{\frac{\alpha+2}{-\alpha}}\,\Delta\,.$$

Thus, $\delta < x_0 < \Delta$ if and only if

$$\frac{-2\Delta^2}{\Delta^2+\delta^2} < \alpha < -1. \tag{2.8}$$

If $-1 \le \alpha < 0$, then $\partial f/\partial x(x,\Delta) < 0$ for $\delta < x < \Delta$, and

$$2\Delta^{-2\alpha-2} = f(\Delta,\Delta) \le f(x,\Delta) \le f(\delta,\Delta) = (\Delta^2+\delta^2)(\Delta\delta)^{-\alpha-2}.$$

If $-2 < \alpha \le -2\Delta^2/(\Delta^2+\delta^2)$, then $\partial f/\partial x(x,\Delta) > 0$ for $\delta < x < \Delta$, and

$$(\Delta^2+\delta^2)(\Delta\delta)^{-\alpha-2} \le f(x,\Delta) \le 2\Delta^{-2\alpha-2}.$$

If (2.8) holds, then $\partial f/\partial x(\delta,\Delta) = \delta^{-\alpha-3}\Delta^{-\alpha-2}\big(-\alpha\delta^2-(\alpha+2)\Delta^2\big) < 0$, and $\partial f/\partial x(\Delta,\Delta) = -2\Delta^{-2\alpha-3}(\alpha+1) > 0$, and we conclude

$$\begin{aligned}\frac{2}{-\alpha}\Big(\frac{\alpha+2}{-\alpha}\Big)^{-\alpha/2-1}\Delta^{-2\alpha-2} &= f(x_0,\Delta) \le f(x,\Delta)\\ \le \max\big\{f(\delta,\Delta),\, f(\Delta,\Delta)\big\} &= \max\big\{(\Delta^2+\delta^2)(\Delta\delta)^{-\alpha-2},\, 2\Delta^{-2\alpha-2}\big\}.\end{aligned}$$

Hence, if $-2 < \alpha \le -2\Delta^2/(\Delta^2+\delta^2)$ or $-2\delta^2/(\Delta^2+\delta^2) \le \alpha < 0$, then (2.5) or (2.6) holds, respectively.

If $-2\Delta^2/(\Delta^2+\delta^2) < \alpha < -1$, then

$$\begin{aligned}\min\Big\{2\delta^{-2\alpha-2},\, \frac{2}{-\alpha}\Big(\frac{\alpha+2}{-\alpha}\Big)^{-\alpha/2-1}\Delta^{-2\alpha-2}\Big\} &\le f(x,y)\\ &\le \max\big\{2\Delta^{-2\alpha-2},\, (\Delta^2+\delta^2)(\Delta\delta)^{-\alpha-2}\big\}.\end{aligned}$$

If $-1 < \alpha < -2\delta^2/(\Delta^2+\delta^2)$, then

$$\begin{aligned}\min\Big\{2\Delta^{-2\alpha-2},\, \frac{2}{-\alpha}\Big(\frac{\alpha+2}{-\alpha}\Big)^{-\alpha/2-1}\delta^{-2\alpha-2}\Big\} &\le f(x,y)\\ &\le \max\big\{2\delta^{-2\alpha-2},\, (\Delta^2+\delta^2)(\Delta\delta)^{-\alpha-2}\big\}.\end{aligned}$$

These inequalities finish the proofs of the bounds if $\alpha \neq -1$. If $\alpha = -1$, then we can obtain the bounds by taking limits on the inequalities when $\alpha > -1$.

In the first and last cases, the properties of the function f give that each inequality 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 this happens if and only if G is regular.

If the graph is regular, then the lower and upper bounds are the same in each case, and they are equal to $ID(G)$ (note that we do not have the second and fourth cases if $\delta = \Delta$). ■

2.2 Inequalities involving the geometric-arithmetic index

The geometric-arithmetic index GA was introduced in [59] as

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

Although GA was introduced in 2009, there are many papers dealing with this index (see, e.g., [8], [9], [10], [49], [50], [55], [59] and the references therein).

The following results provide inequalities relating inverse degree and geometric-arithmetic indices.

Theorem 15 *If G is a non-trivial graph with m edges and maximum degree Δ, then*

$$2GA(G) + \Delta^2 ID(G) \geq 4m,$$

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

Proof. The inequality $2xy \leq x^2 + y^2$ for every $x, y \in \mathbb{R}$, and the geometric-arithmetic inequality give

$$
\begin{aligned}
&\frac{2d_ud_v}{(d_u+d_v)^2}+\frac{d_u^2+d_v^2}{(d_u+d_v)^2}=1, \quad \frac{1}{2}\,\frac{2\sqrt{d_ud_v}}{d_u+d_v}\,\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\frac{d_u^2+d_v^2}{4d_ud_v}\geq 1,\\
&\quad \frac{1}{2}\,\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\frac{d_u^2+d_v^2}{4\frac{d_u^2d_v^2}{\Delta^2}}\geq 1, \quad 2\,\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\Delta^2\frac{d_u^2+d_v^2}{d_u^2d_v^2}\geq 4,\\
&\qquad\qquad 2GA(G)+\Delta^2 ID(G)\geq 4m.
\end{aligned}
$$

If the graph is regular, then $2GA(G)+\Delta^2 ID(G)=4m$.

If the equality is attained, then $d_ud_v=\Delta^2$ for every $uv\in E(G)$, and so $d_u=\Delta$ for every $u\in V(G)$ and G is regular. ■

Theorem 16 *Let G be a non-trivial graph with minimum degree δ and maximum degree Δ. Then*

$$
ID(G)\leq \max\Big\{\frac{2}{\delta^2}\,,\,\frac{(\Delta+\delta)(\Delta^2+\delta^2)}{2(\Delta\delta)^{5/2}}\Big\}GA(G),
$$

and the equality is attained for every regular graph G.

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

$$
f(x,y)=\Big(\frac{1}{x^2}+\frac{1}{y^2}\Big)\frac{x+y}{2\sqrt{xy}}=\frac{1}{2}(x+y)(x^2+y^2)x^{-5/2}y^{-5/2}.
$$

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

$$
\begin{aligned}
\frac{\partial f}{\partial x}(x,y) &= \frac{1}{2}(x^2+y^2)x^{-5/2}y^{-5/2} + (x+y)x \cdot x^{-5/2}y^{-5/2} \\
&\quad - \frac{5}{4}(x+y)(x^2+y^2)x^{-7/2}y^{-5/2} \\
&= \frac{1}{4}\,x^{-7/2}y^{-5/2}\big(2x(x^2+y^2) + 4x^2(x+y) - 5(x+y)(x^2+y^2)\big) \\
&= \frac{1}{4}\,x^{-7/2}y^{-5/2}\big(x^3 - x^2y - 3xy^2 - 5y^3\big), \\
\frac{\partial f}{\partial y}(x,y) &= \frac{1}{4}\,y^{-7/2}x^{-5/2}\big(y^3 - y^2x - 3yx^2 - 5x^3\big).
\end{aligned}
$$

If we define $g(t) := t^3 - t^2 - 3t - 5$, then

$$
\frac{\partial f}{\partial x}(x,y) = \frac{1}{4}\,x^{-7/2}y^{1/2}g\Big(\frac{x}{y}\Big).
$$

Since $g'(t) = 3t^2 - 2t - 3 = 0$ if and only if $t = (1 \pm \sqrt{10}\,)/3$, g is a decreasing function on $[0,1]$. Since $g(0) = -5$, we have $g(t) < 0$ for every $t \in [0,1]$, and

$$
\frac{\partial f}{\partial x}(x,y) < 0, \qquad \text{if } \delta \le x \le y \le \Delta.
$$

Thus, $f(\delta, y) > f(x,y) > f(y,y)$ for every $x \in (\delta, y)$ and so, the maximum value of f is attained on the set $\{x = \delta,\, \delta \le y \le \Delta\}$, and the minimum value of f is attained on the set $\{\delta \le x = y \le \Delta\}$.

If we define $h(t) := t^3 - \delta t^2 - 3\delta^2 t - 5\delta^3$, then

$$
\frac{\partial f}{\partial y}(\delta, y) = \frac{1}{4}\,y^{-7/2}\delta^{-5/2}h(y).
$$

Since $h'(t) = 3t^2 - 2\delta t - 3\delta^2 = 0$ if and only if $t = (1 \pm \sqrt{10}\,)\delta/3$, h is a decreasing function on $[\delta, (1+\sqrt{10}\,)\delta/3)$ and increasing on $((1+\sqrt{10}\,)\delta/3, \infty)$. Since $h(\delta) = -8\delta^3$, we have $h < 0$ on $[\delta, t_1)$ and $h > 0$ on (t_1, ∞) for some

$t_1 > \delta$. Thus,

$$\begin{aligned}
f(x,y) &\leq \max_{\delta \leq y \leq \Delta} f(\delta, y) = \max\left\{f(\delta,\delta),\ f(\delta,\Delta)\right\} \\
&= \max\left\{\frac{2}{\delta^2}\,,\ \frac{(\delta+\Delta)(\delta^2+\Delta^2)}{2(\delta\Delta)^{5/2}}\right\}, \\
\frac{1}{d_u^2} + \frac{1}{d_v^2} &\leq \max\left\{\frac{2}{\delta^2}\,,\ \frac{(\Delta+\delta)(\Delta^2+\delta^2)}{2(\Delta\delta)^{5/2}}\right\}\frac{2\sqrt{d_u d_v}}{d_u + d_v}\,, \\
ID(G) &\leq \max\left\{\frac{2}{\delta^2}\,,\ \frac{(\Delta+\delta)(\Delta^2+\delta^2)}{2(\Delta\delta)^{5/2}}\right\}GA(G).
\end{aligned}$$

If the graph is regular, then

$$\begin{aligned}
\max\left\{\frac{2}{\delta^2}\,,\ \frac{(\Delta+\delta)(\Delta^2+\delta^2)}{2(\Delta\delta)^{5/2}}\right\}GA(G) &= \max\left\{\frac{2}{\delta^2}\,,\ \frac{(2\delta)(2\delta^2)}{2\delta^5}\right\}m \\
&= \frac{2m}{\delta^2} = ID(G).
\end{aligned}$$

■

Chapter 3

On the first general Zagreb index

The aim of this chapter is to obtain new inequalities involving the first general Zagreb index, and characterize graphs which are extremal with respect to them. We also obtain inequalities involving the forgotten and second general Zagreb indices.

3.1 Bounds for M_1^α

We start by proving some bounds for M_1^α involving different parameters.

Theorem 17 *Let G be a nontrivial graph with m edges, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$2\Delta^{\alpha-1}m \leq M_1^\alpha(G) \leq 2\delta^{\alpha-1}m, \qquad \text{if } \alpha < 1,$$
$$2\delta^{\alpha-1}m \leq M_1^\alpha(G) \leq 2\Delta^{\alpha-1}m, \qquad \text{if } \alpha \geq 1,$$

and the equality holds in each inequality for some $\alpha \neq 1$ if and only if G is *regular.*

Proof. If $\alpha \geq 1$, then

$$M_1^\alpha(G) = \sum_{u \in V(G)} d_u^{\alpha-1} d_u \leq \Delta^{\alpha-1} 2m,$$
$$M_1^\alpha(G) = \sum_{u \in V(G)} d_u^{\alpha-1} d_u \geq \delta^{\alpha-1} 2m.$$

If $\alpha < 1$, then the same argument gives

$$\Delta^{\alpha-1} 2m \leq \sum_{u \in V(G)} d_u^{\alpha-1} d_u \leq \delta^{\alpha-1} 2m.$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $M_1^\alpha(G)$. If an equality holds for some $\alpha \neq 1$, then $d_u^{\alpha-1}$ has the same value ($\delta^{\alpha-1}$ or $\Delta^{\alpha-1}$) for every $u \in V(G)$; since $\alpha \neq 1$, $d_u = \delta$ (or $d_u = \Delta$) for every $u \in V(G)$ and G is regular. Note that if $\alpha = 1$, then each inequality is an equality for every G. ■

Lemma 18 *Let $f(x) = x^\alpha - 1 - \alpha(x-1)$.*

(1) If $\alpha \leq 0$ or $\alpha \geq 1$, then $f(x) \geq 0$ for every $x > 0$. If $\alpha \neq 0, 1$, then $f(x) = 0$ if and only if $x = 1$.

(2) If $0 < \alpha < 1$, then $f(x) \leq 0$ for every $x > 0$, and $f(x) = 0$ if and only if $x = 1$.

Theorem 19 *Let G be a nontrivial graph with n vertices and m edges, and $\alpha \in \mathbb{R}$. Then*

$$M_1^\alpha(G) \geq 2m\alpha + n(1-\alpha), \qquad \text{if } \alpha \leq 0 \text{ or } \alpha \geq 1,$$
$$M_1^\alpha(G) \leq 2m\alpha + n(1-\alpha), \qquad \text{if } 0 < \alpha < 1.$$

The equality holds in the inequality for some $\alpha \neq 0, 1$ if and only if G is a union of pairwise disjoint edges.

Proof. Assume that $\alpha \leq 0$ or $\alpha \geq 1$. By Lemma 18,

$$d_u^\alpha \geq \alpha\, d_u + 1 - \alpha,$$
$$M_1^\alpha(G) \geq 2m\alpha + n(1 - \alpha).$$

A similar argument gives the second inequality.

If $\alpha \neq 0, 1$, then Lemma 18 gives that the equality holds if and only if $d_u = 1$ for every $u \in V(G)$, i.e., G is a union of pairwise disjoint edges. Note that if $\alpha = 0$ or $\alpha = 1$, then the equality is attained for every graph. ■

Next, we prove some inequalities relating two indices M_1^α and M_1^β.

Theorem 20 *Let G be a nontrivial graph with n vertices, maximum degree Δ and minimum degree δ, and $\alpha, \beta \in \mathbb{R}$. Then*

$$\begin{aligned}
M_1^\alpha(G) &\leq \delta^{\alpha-\beta} M_1^\beta(G), && \text{if } \alpha \leq \beta, \\
M_1^\alpha(G) &\leq \Delta^{\alpha-\beta} M_1^\beta(G), && \text{if } \alpha \geq \beta, \\
M_1^\alpha(G) &\geq \frac{\Delta^{\alpha+\beta} n^2}{M_1^\beta(G)}\,, && \text{if } \alpha \leq -\beta, \\
M_1^\alpha(G) &\geq \frac{\delta^{\alpha+\beta} n^2}{M_1^\beta(G)}\,, && \text{if } \alpha \geq -\beta.
\end{aligned}$$

The equality is attained in the lower bound with $(\alpha, \beta) \neq (0, 0)$ if and only if G is regular; if $\alpha = \beta = 0$, then the lower bound is attained for every graph. The equality holds in the upper bound for some $\alpha \neq \beta$ if and only if G is regular; if $\alpha = \beta$, then the upper bound is attained for every graph.

Proof. If $\alpha \geq \beta$, then

$$M_1^{\alpha}(G) = \sum_{u \in V(G)} d_u^{\alpha-\beta} d_u^{\beta} \leq \Delta^{\alpha-\beta} M_1^{\beta}(G).$$

If $\alpha \leq \beta$, then the same argument gives

$$M_1^{\alpha}(G) \leq \delta^{\alpha-\beta} M_1^{\beta}(G).$$

Cauchy-Schwarz inequality gives

$$\begin{aligned} n &= \sum_{u \in V(G)} d_u^{\alpha/2} d_u^{-\alpha/2} \leq \Big(\sum_{u \in V(G)} d_u^{\alpha} \Big)^{1/2} \Big(\sum_{u \in V(G)} d_u^{-\alpha} \Big)^{1/2}, \\ n^2 &\leq M_1^{\alpha}(G) M_1^{-\alpha}(G). \end{aligned}$$

Since we have proved

$$\begin{aligned} M_1^{-\alpha}(G) &\leq \delta^{-\alpha-\beta} M_1^{\beta}(G), \qquad \text{if } \alpha \geq -\beta, \\ M_1^{-\alpha}(G) &\leq \Delta^{-\alpha-\beta} M_1^{\beta}(G), \qquad \text{if } \alpha \leq -\beta, \end{aligned}$$

we obtain

$$\begin{aligned} M_1^{\alpha}(G) &\geq \frac{\delta^{\alpha+\beta} n^2}{M_1^{\beta}(G)}, \qquad \text{if } \alpha \geq -\beta, \\ M_1^{\alpha}(G) &\geq \frac{\Delta^{\alpha+\beta} n^2}{M_1^{\beta}(G)}, \qquad \text{if } \alpha \leq -\beta. \end{aligned}$$

If the graph is regular, then $M_1^{\beta}(G) = \Delta^{\beta} n$, the lower and upper bounds are the same, and they are equal to $M_1^{\alpha}(G) = \Delta^{\alpha} n$.

If $\alpha = \beta$, then the upper bound is an identity. If the equality is attained in the upper bound for some $\alpha \neq \beta$, then d_u has the same value (δ or Δ) for every $u \in V(G)$; hence, G is regular.

If $\alpha = \beta = 0$, then $M_1^0(G) = n$ and the lower bound is an identity. If the equality is attained in the lower bound for some $\alpha \neq -\beta$, then d_u has the same value (δ or Δ) for every $u \in V(G)$, and G is regular. If $\alpha = -\beta$, $(\alpha, \beta) \neq (0,0)$ and the lower bound is attained, then $\alpha \neq 0$ and Cauchy-Schwarz inequality gives that there exists a positive constant λ such that $d_u^{-1} = \lambda d_u$ for every $u \in V(G)$; thus, G is regular. ■

Proposition 21 *Let G be a nontrivial graph with n vertices, $s > 0$ and $\alpha \in \mathbb{R}$. Then*

$$2sn \leq s^2\, M_1^{\alpha}(G) + \, M_1^{-\alpha}(G),$$

Proof. Cauchy-Schwarz inequality gives

$$\begin{aligned} n &\leq \Big(\sum_{u \in V(G)} d_u^{\alpha} \Big)^{1/2} \Big(\sum_{u \in V(G)} d_u^{-\alpha} \Big)^{1/2}, \\ n &\leq \sqrt{M_1^{\alpha}(G) M_1^{-\alpha}(G)}\,. \end{aligned}$$

The inequality $\sqrt{ab} \leq \frac{s}{2} a + \frac{1}{2s} b$ (for $a, b \geq 0$ and $s > 0$) gives,

$$n \leq \frac{s}{2}\, M_1^{\alpha}(G) + \frac{1}{2s}\, M_1^{-\alpha}(G).$$

■

We will use the following particular case of Jensen inequality.

Lemma 22 *If f is a convex function in an interval I and $x_1, \ldots, x_k \in I$, then*

$$f\Big(\frac{x_1 + \cdots + x_k}{k}\Big) \leq \frac{1}{k}\, \big(f(x_1) + \cdots + f(x_k)\big).$$

Theorem 23 *Let G be a nontrivial graph with n vertices, $\alpha \in \mathbb{R}$ and $\beta > 0$. Then*

$$n^{\beta+1} \leq M_1^{-\alpha\beta}(G) M_1^{\alpha}(G)^{\beta},$$

and the equality is attained for some values $\alpha \neq 0$ and β if and only if G is regular.

Proof. Since $f(x) = x^{-\beta}$ is a convex function in $\mathbb{R}_+$ for each $\beta > 0$, Lemma 22 gives

$$\left(\frac{\sum_{u\in V(G)} d_u^\alpha}{n}\right)^{-\beta} \leq \frac{1}{n} \sum_{u\in V(G)} (d_u^\alpha)^{-\beta},$$

$$n^{\beta+1} \leq M_1^{-\alpha\beta}(G) M_1^\alpha(G)^\beta.$$

Assume that $\alpha \neq 0$. Since $f(x) = x^{-\beta}$ is a strictly convex function, the equality is attained if and only if d_u^α is constant for every $u \in V(G)$. Since $\alpha \neq 0$, this holds if and only if G is regular. Note that if $\alpha = 0$, then the inequality is an equality for every G. ■

The following result appears in [56].

Lemma 24 *If $\alpha \geq 1$ is an integer and $0 \leq x_1, \ldots, x_n \leq n-1$, then*

$$\Big(\sum_{j=1}^n x_j^\alpha\Big)^{1/\alpha} \leq (n-1)^{1-1/\alpha} \sum_{j=1}^n x_j^{1/\alpha}.$$

We prove now a generalization of this lemma which is interesting by itself.

Lemma 25 *Consider real numbers $0 < \beta \leq 1 \leq \alpha$, $\Delta > 0$ and $0 \leq x_1, \ldots, x_n \leq \Delta$. Then*

$$\Big(\sum_{j=1}^n x_j^\alpha\Big)^{1/\alpha} \leq \Delta^{1-\beta} \sum_{j=1}^n x_j^\beta.$$

Proof. It suffices to prove the result for $\beta < 1$, since the case $\beta = 1$ can be obtained as a limit. Let us consider the function

$$H(x_1,\dots,x_n) := \frac{\sum_{j=1}^n x_j^\beta}{\left(\sum_{j=1}^n x_j^\alpha\right)^{1/\alpha}},$$

on the domain

$$\big\{(x_1,\dots,x_n)\in\mathbb{R}^n\setminus\{0\} \mid 0\le x_1,\dots,x_n\le\Delta\big\}.$$

For any fixed $1\le k\le n$, consider the values of $x_1,\dots,x_{k-1},x_{k+1},\dots,x_n$ as constants and define the functions

$$\begin{aligned}
f(x_k) &:= H(x_1,\dots,x_n),\\
g(x_k) &:= \beta\sum_{j=1}^n x_j^\alpha - x_k^{\alpha-\beta}\sum_{j=1}^n x_j^\beta\\
&= \beta\Big(x_k^\alpha+\sum_{j\neq k}x_j^\alpha\Big) - x_k^{\alpha-\beta}\Big(x_k^\beta+\sum_{j\neq k}x_j^\beta\Big)\\
&= \beta\sum_{j\neq k}x_j^\alpha - (1-\beta)x_k^\alpha - x_k^{\alpha-\beta}\sum_{j\neq k}x_j^\beta.
\end{aligned}$$

We have

$$\begin{aligned}
f'(x_k) &= \frac{\beta x_k^{\beta-1}\left(\sum_{j=1}^n x_j^\alpha\right)^{1/\alpha} - \left(\sum_{j=1}^n x_j^\alpha\right)^{-1+1/\alpha} x_k^{\alpha-1}\sum_{j=1}^n x_j^\beta}{\left(\sum_{j=1}^n x_j^\alpha\right)^{2/\alpha}}\\
&= x_k^{\beta-1}\,\frac{\beta\sum_{j=1}^n x_j^\alpha - x_k^{\alpha-\beta}\sum_{j=1}^n x_j^\beta}{\left(\sum_{j=1}^n x_j^\alpha\right)^{1+1/\alpha}} = \frac{x_k^{\beta-1}g(x_k)}{\left(\sum_{j=1}^n x_j^\alpha\right)^{1+1/\alpha}}.
\end{aligned}$$

Hence, $f'(x_k)$ and $g(x_k)$ have the same sign. Since $0<\beta<1$, we have

$$g'(x_k) = -(1-\beta)\alpha\, x_k^{\alpha-1} - (\alpha-\beta)x_k^{\alpha-\beta-1}\sum_{j\neq k}x_j^\beta < 0$$

for every $x_k \in (0, \Delta]$, and g has at most a change of sign in $[0, \Delta]$. Since $g(0) \geq 0$, we have

$$\min_{x_k \in [0,\Delta]} f(x_k) = \min \{f(0), f(\Delta)\}.$$

Furthermore, if $\sum_{j \neq k} x_j^\alpha = 0$, then $x_1 = \cdots = x_{k-1} = x_{k+1} = \cdots = x_n = 0$, $\sum_{j \neq k} x_j^\beta = 0$, $g(x_k) = -(1-\beta)x_k^\alpha$ and $f'(x_k) \leq 0$. Thus,

$$\min_{x_k \in (0,\Delta]} f(x_k) = f(\Delta).$$

Consequently, the minimum value of H is attained at the vertices of the n-dimensional cube $[0, \Delta]^n$ minus the origin.

If a vertex x of $[0, \Delta]^n$ has r coordinates equal to Δ and $n-r$ coordinates equal to 0 for some $1 \leq r \leq n$, then

$$H(x) = \frac{r\Delta^\beta}{\big(r\Delta^\alpha\big)^{1/\alpha}} = \frac{r^{1-1/\alpha}}{\Delta^{1-\beta}} \geq \frac{1}{\Delta^{1-\beta}}\,.$$

Hence,

$$\frac{\sum_{j=1}^n x_j^\beta}{\Big(\sum_{j=1}^n x_j^\alpha\Big)^{1/\alpha}} \geq \frac{1}{\Delta^{1-\beta}}\,.$$

■

Proposition 26 *Let G be a nontrivial graph with maximum degree Δ, and consider real numbers $0 < \beta \leq 1 \leq \alpha$. Then*

$$M_1^\alpha(G)^{1/\alpha} \leq \Delta^{1-\beta} M_1^\beta(G).$$

Proof. We have $0 \le d_u \le \Delta$ for every $u \in V(G)$. Hence, Lemma 25 gives

$$\Big(\sum_{u \in V(G)} d_u^{\alpha} \Big)^{1/\alpha} \le \Delta^{1-\beta} \sum_{u \in V(G)} d_u^{\beta}.$$

Thus,

$$M_1^{\alpha}(G)^{1/\alpha} \le \Delta^{1-\beta} M_1^{\beta}(G).$$

■

Theorem 27 *Let G be a nontrivial graph with n vertices, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$\frac{2(\Delta\delta)^{\alpha/2}}{\Delta^{\alpha} + \delta^{\alpha}} \sqrt{n M_1^{2\alpha}(G)} \le M_1^{\alpha}(G) \le \sqrt{n M_1^{2\alpha}(G)}\,.$$

The lower bound is attained for every value of α if G is regular. The upper bound is attained for some $\alpha \neq 0$ if and only if G is regular.

Proof. Cauchy-Schwarz inequality gives

$$M_1^{\alpha}(G) = \sum_{u \in V(G)} d_u^{\alpha} \le \Big(\sum_{u \in V(G)} d_u^{2\alpha} \Big)^{1/2} \Big(\sum_{u \in V(G)} 1 \Big)^{1/2} = \sqrt{n M_1^{2\alpha}(G)}\,.$$

Since

$$\delta^{\alpha} \le d_u^{\alpha} \le \Delta^{\alpha} \qquad \text{if } \alpha \ge 0,$$
$$\Delta^{\alpha} \le d_u^{\alpha} \le \delta^{\alpha} \qquad \text{if } \alpha \le 0,$$

Lemma 1 gives

$$\begin{aligned} M_1^{\alpha}(G) = \sum_{u \in V(G)} d_u^{\alpha} &\ge \frac{\Big(\sum_{u \in V(G)} d_u^{2\alpha} \Big)^{1/2} \Big(\sum_{u \in V(G)} 1 \Big)^{1/2}}{\frac{1}{2}\Big(\big(\frac{\Delta}{\delta}\big)^{\alpha/2} + \big(\frac{\delta}{\Delta}\big)^{\alpha/2} \Big)} \\ &= \frac{2(\Delta\delta)^{\alpha/2}}{\Delta^{\alpha} + \delta^{\alpha}} \sqrt{n M_1^{2\alpha}(G)}\,. \end{aligned}$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $M_1^\alpha(G)$. If the upper bound is attained for some value of α, then Cauchy-Schwarz inequality gives that d_u^α is constant for every $u \in V(G)$; if $\alpha \neq 0$, then d_u is constant for every $u \in V(G)$, and G is regular. ■

Proposition 28 *Let G be a nontrivial graph with n edges, maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$M_1^\alpha(G) + (\Delta\delta)^\alpha M_1^{-\alpha}(G) \le n(\Delta^\alpha + \delta^\alpha),$$

and the equality holds for some $\alpha \neq 0$ if and only if $d_u \in \{\Delta, \delta\}$ for every $u \in V(G)$.

Proof. We have

$$\begin{aligned}
(\Delta^\alpha - d_u^\alpha)(d_u^\alpha - \delta^\alpha) &\ge 0,\\
d_u^\alpha(\Delta^\alpha + \delta^\alpha) &\ge (\Delta\delta)^\alpha + d_u^{2\alpha},\\
\Delta^\alpha + \delta^\alpha &\ge (\Delta\delta)^\alpha d_u^{-\alpha} + d_u^\alpha,\\
n(\Delta^\alpha + \delta^\alpha) &\ge (\Delta\delta)^\alpha M_1^{-\alpha}(G) + M_1^\alpha(G).
\end{aligned}$$

The equality holds for some $\alpha \neq 0$ if and only if $d_u^\alpha = \Delta^\alpha$ or $d_u^\alpha = \delta^\alpha$ for each $u \in V(G)$, i.e., if $d_u \in \{\Delta, \delta\}$ for every $u \in V(G)$. ■

Theorem 29 *Let G be a nontrivial graph with n vertices, and $\alpha, \beta \in \mathbb{R}$ with $\alpha > 0$. Then*

$$\begin{aligned}
n + \alpha M_1^\beta(G) &\le \left(M_1^{\alpha\beta}(G)^{1/\alpha} + n^{1/\alpha}\right)^\alpha, && \text{if } \alpha \ge 1,\\
n + \alpha M_1^\beta(G) &\ge \left(M_1^{\alpha\beta}(G)^{1/\alpha} + n^{1/\alpha}\right)^\alpha, && \text{if } 0 < \alpha < 1.
\end{aligned}$$

Proof. Assume first $\alpha \ge 1$. Minkowski inequality gives

$$\Big(\sum_{u \in V(G)} (d_u^\beta + 1)^\alpha \Big)^{1/\alpha} \le \Big(\sum_{u \in V(G)} d_u^{\alpha\beta} \Big)^{1/\alpha} + \Big(\sum_{u \in V(G)} 1 \Big)^{1/\alpha}.$$

Therefore, Bernoulli inequality $(1+x)^\alpha \ge 1 + \alpha x$, for $\alpha \ge 1$ and $x \ge -1$, gives

$$\sum_{u \in V(G)} (1 + \alpha d_u^\beta) \le \big(M_1^{\alpha\beta}(G)^{1/\alpha} + n^{1/\alpha} \big)^\alpha.$$

Thus,

$$n + \alpha M_1^\beta(G) \le \big(M_1^{\alpha\beta}(G)^{1/\alpha} + n^{1/\alpha} \big)^\alpha.$$

If $0 < \alpha < 1$, then the previous argument, reverse Minkowski inequality

$$\Big(\sum_{u \in V(G)} (d_u^\beta + 1)^\alpha \Big)^{1/\alpha} \ge \Big(\sum_{u \in V(G)} d_u^{\alpha\beta} \Big)^{1/\alpha} + \Big(\sum_{u \in V(G)} 1 \Big)^{1/\alpha}.$$

and Bernoulli inequality $(1+x)^\alpha \le 1 + \alpha x$, for $0 < \alpha < 1$ and $x \ge -1$, give the second bound. ■

We need the following Chebyshev inequalities (see, e.g., [1, Theorem 2.1, p.21]).

Lemma 30 *Consider* $0 < a_1 \le a_2 \le \cdots \le a_n$.

(1) *For every* $0 < b_1 \le b_2 \le \cdots \le b_n$, *we have*

$$\sum_{j=1}^n a_j b_j \ge \frac{1}{n} \sum_{j=1}^n a_j \sum_{j=1}^n b_j.$$

(2) *For every* $b_1 \ge b_2 \ge \cdots \ge b_n > 0$, *we have*

$$\sum_{j=1}^n a_j b_j \le \frac{1}{n} \sum_{j=1}^n a_j \sum_{j=1}^n b_j.$$

The bound is attained in each case if and only if $a_1 = a_2 = \cdots = a_n$ *or* $b_1 = b_2 = \cdots = b_n$.

Theorem 31 *Let* G *be a nontrivial graph with* n *vertices, and* $\alpha, \beta \in \mathbb{R}$ *with* $\beta > 0$. *Then*

$$M_1^{\alpha+\beta}(G) \geq \frac{1}{n} M_1^{\alpha}(G) M_1^{\beta}(G), \qquad \text{if } \alpha \geq 0,$$
$$M_1^{\alpha+\beta}(G) \leq \frac{1}{n} M_1^{\alpha}(G) M_1^{\beta}(G), \qquad \text{if } \alpha \leq 0,$$

and the equality holds in the inequality for some $\alpha \neq 0$ *if and only if* G *is regular.*

Proof. If $\alpha \geq 0$, then Lemma 30 gives

$$M_1^{\alpha+\beta}(G) = \sum_{u \in V(G)} d_u^{\alpha+\beta} \geq \frac{1}{n} \sum_{u \in V(G)} d_u^{\alpha} \sum_{u \in V(G)} d_u^{\beta} = \frac{1}{n} M_1^{\alpha}(G) M_1^{\beta}(G).$$

In a similar way, if $\alpha \leq 0$, then we obtain

$$M_1^{\alpha+\beta}(G) = \sum_{u \in V(G)} d_u^{\alpha+\beta} \leq \frac{1}{n} \sum_{u \in V(G)} d_u^{\alpha} \sum_{u \in V(G)} d_u^{\beta} = \frac{1}{n} M_1^{\alpha}(G) M_1^{\beta}(G).$$

Lemma 30 gives that the equality holds for some $\alpha \neq 0$ if and only if d_u has the same value for every $u \in V(G)$, i.e., G is regular. Note that if $\alpha = 0$, then $M_1^0(G) = n$ and the equality holds for every G. ■

Since $M_1^1(G) = 2m$, Theorem 31 has the following consequence.

Corollary 32 *Let* G *be a nontrivial graph with* n *vertices and* m *edges, and* $\alpha \in \mathbb{R}$. *Then*

$$M_1^{\alpha+1}(G) \geq \frac{2m}{n} M_1^{\alpha}(G), \qquad \text{if } \alpha \geq 0,$$
$$M_1^{\alpha+1}(G) \leq \frac{2m}{n} M_1^{\alpha}(G), \qquad \text{if } \alpha \leq 0,$$

and the equality holds in the inequality for some $\alpha \neq 0$ if and only if G is regular.

3.2 Inequalities for M_1^α involving other topological indices

The following lemma will be an important tool to deduce some results.

Lemma 33 [55, Lemma 3] *Let h be the function $h(x,y) = \frac{2xy}{x+y}$ with $\delta \leq x, y \leq \Delta$. Then*

$$\delta \leq h(x,y) \leq \Delta.$$

Furthermore, the lower (respectively, upper) bound is attained if and only if $x = y = \delta$ (respectively, $x = y = \Delta$).

In the same paper, where Zagreb indices were introduced (see [29]), the *forgotten topological index* (or *F-index*) is defined as

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

Both the forgotten topological index and the first Zagreb index were employed in the formulas for total π-electron energy in [29], as a measure of branching extent of the carbon-atom skeleton of the underlying molecule. However, this index never got attention except recently, when Furtula and Gutman in [22] established some basic properties of the F-index and showed that its predictive ability is almost similar to that of the first Zagreb index for the entropy and acetic factor, both of them yield correlation coefficients greater than 0.95. Besides, [22] pointed out the importance of the F-index:

it can be used to obtain a high accuracy of the prediction of logarithm of the octanol-water partition coefficient. Recently, this index has been studied for different graph operations [12]. Furthermore, [5] contains more lower and upper bounds for the forgotten index.

The previous results for the first general Zagreb index hold, in particular, for the forgotten index. Next, we obtain particular bounds for the forgotten index.

Theorem 34 *Let G be a nontrivial graph with maximum degree Δ and minimum degree δ. Then*

$$\frac{4M_2^2(G)}{\Delta^2} - 2M_2(G) \le F(G) \le \frac{4M_2^2(G)}{\delta^2} - 2M_2(G),$$

and each inequality is attained if and only if G is regular.

Proof. Since

$$\sum_{uv\in E(G)} \big(f(d_u) + f(d_v)\big) = \sum_{u\in V(G)} d_u f(d_u),$$

for every function f defined on the positive integers, we have

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

Hence,

$$\sum_{uv\in E(G)} (d_u + d_v)^2 = \sum_{uv\in E(G)} (d_u^2 + d_v^2) + \sum_{uv\in E(G)} 2d_u d_v = F(G) + 2M_2(G).$$

Lemma 33 gives

$$\delta \le \frac{2d_u d_v}{d_u + d_v} \le \Delta.$$

Thus,

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

$$\frac{4M_2^2(G)}{\Delta^2} \le \sum_{uv \in E(G)} (d_u + d_v)^2 \le \frac{4M_2^2(G)}{\delta^2}.$$

Hence,

$$\frac{4M_2^2(G)}{\Delta^2} \le F(G) + 2M_2(G) \le \frac{4M_2^2(G)}{\delta^2}.$$

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $F(G)$. If a bound is attained, then Lemma 33 gives that d_u has the same value (δ or Δ) for every $u \in V(G)$, and G is regular.

■

We also have some inequalities relating the first and second general Zagreb indices.

Theorem 35 *Let G be a nontrivial graph with maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$. Then*

$$\begin{aligned} 2\Delta^{1-\alpha} M_2^{\alpha-1}(G) \le M_1^{\alpha}(G) \le 2\delta^{1-\alpha} M_2^{\alpha-1}(G), \qquad & \textit{if } \alpha \ge 1, \\ 2\delta^{1-\alpha} M_2^{\alpha-1}(G) \le M_1^{\alpha}(G) \le 2\Delta^{1-\alpha} M_2^{\alpha-1}(G), \qquad & \textit{if } \alpha \le 1, \end{aligned}$$

and the equality holds in each inequality for some $\alpha \neq 1$ if and only if G is regular.

Proof. If $\alpha \ge 1$, then

$$\begin{aligned} 2M_2^{\alpha-1}(G) &= 2 \sum_{uv \in E(G)} d_u^{\alpha-1} d_v^{\alpha-1} = \sum_{u \in V(G)} d_u^{\alpha-1} \sum_{v \in N(u)} d_v^{\alpha-1} \\ &\le \sum_{u \in V(G)} d_u^{\alpha-1} \sum_{v \in N(u)} \Delta^{\alpha-1} = \sum_{u \in V(G)} d_u^{\alpha-1} d_u \Delta^{\alpha-1} = \Delta^{\alpha-1} M_1^{\alpha}(G). \end{aligned}$$

We obtain the other inequalities in a similar way.

If the graph is regular, then the lower and upper bounds are the same, and they are equal to $M_1^\alpha(G)$. If an equality holds for some $\alpha \neq 1$, then $d_u^{\alpha-1}$ has the same value ($\delta^{\alpha-1}$ or $\Delta^{\alpha-1}$) for every $u \in V(G)$; since $\alpha \neq 1$, d_u has the same value (δ or Δ) for every $u \in V(G)$ and G is regular. Note that if $\alpha = 1$, then both inequalities are equalities for every G. ∎

The *modified Narumi-Katayama index*

$$NK^*(G) = \prod_{u \in V(G)} d_u^{d_u} = \prod_{uv \in E(G)} d_u d_v$$

is introduced in [23], inspired in the Narumi-Katayama index defined in [43]. Finally, we present an inequality relating the modified Narumi-Katayama and the first general Zagreb indices.

Theorem 36 *Let G be a nontrivial graph with m edges, and $\alpha \in \mathbb{R}$. Then*

$$M_1^\alpha(G) \geq 2m\, NK^*(G)^{(\alpha-1)/(2m)},$$

and the equality holds for some $\alpha \neq 1$ if and only if G is regular.

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

$$\begin{aligned}\frac{1}{2m}\, M_1^\alpha(G) &= \frac{1}{m} \sum_{uv \in E(G)} \frac{d_u^{\alpha-1} + d_v^{\alpha-1}}{2} \geq \frac{1}{m} \sum_{uv \in E(G)} \big(d_u d_v\big)^{(\alpha-1)/2} \\ &\geq \Big(\prod_{uv \in E(G)} \big(d_u d_v\big)^{(\alpha-1)/2} \Big)^{1/m} = NK^*(G)^{(\alpha-1)/(2m)}.\end{aligned}$$

Thus,

$$M_1^\alpha(G) \geq 2m\, NK^*(G)^{(\alpha-1)/(2m)}.$$

If the graph is regular, then $M_1^{\alpha}(G) = 2\delta^{\alpha-1}m$, $NK^*(G) = \delta^{2m}$ and we have the equality. If the equality holds for some α, then $d_u^{\alpha-1} = d_v^{\alpha-1}$ and $(d_u d_v)^{(\alpha-1)/2}$ is constant for every $uv \in E(G)$; if $\alpha \neq 1$, then these conditions give that $d_u = d_v$ for every $u, v \in V(G)$, and G is regular. Note that if $\alpha = 1$, then $M_1^1(G) = 2m$ and the inequality is an equality for every G. $\blacksquare$

Chapter 4

On the arithmetic-geometric index

The concept of arithmetic-geometric index was introduced in chemical graph theory recently, but it has proven to be useful from both a theoretical and practical point of view. The aim of this chapter is to obtain new bounds of the arithmetic-geometric index and characterize the extremal graphs with respect to them.

Several bounds are based on other indices such as the second variable Zagreb index or the general atom-bond connectivity index), and some of them involve some parameters as the number of edges, the maximum degree or the minimum degree of the graph. In most bounds, the graphs for which equality is attained are regular or biregular, or star graphs.

In 2015, Shegehall and Kanabur [52] introduced the *arithmetic-geometric index* as

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

The AG index of path graphs with pendant vertices attached to the middle vertices was discussed in the papers [52], [53]. The paper [65] studied spectrum and energy of the arithmetic-geometric matrix, in which the sum of all elements is equal to $2AG$. Other bounds of the arithmetic-geometric energy of graphs appeared in [24]. The paper [58] studies extremal AG-graphs for various classes of simple graphs, and it includes inequalities involving $AG+GA$, $AG-GA$, $AG \cdot GA$, and AG/GA. In [6] and [40] there are more bounds on the AG index and a discussion on the effect of deleting an edge from a graph on the arithmetic-geometric index.

4.1 Bounds involving other topological indices

Recall that 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. Note that a regular graph is biregular if and only if it is bipartite.

The following inequalities for graphs G with m edges, maximum degree Δ and minimum degree δ, follow from Lemma 11:

$$m \leq AG(G) \leq \frac{\Delta+\delta}{2\sqrt{\Delta\delta}}\, m. \tag{4.1}$$

The equality in the lower bound is attained if and only if G is regular, the equality in the upper bound is attained if and only if G is regular or biregular. The lower bound in (4.1) also follows from the inequalities $GA(G) \cdot AG(G) \geq m^2$ and $GA(G) \leq m$, see [8] and [9]. The upper bound in (4.1) appears in [40]. A study on the relationship between the $AG(G)$ and $GA(G)$ indices is presented in [26].

The following result improves the lower bound in (4.1), see Remark 38.

Theorem 37 *If G is a graph with m edges, maximum degree Δ and minimum degree δ, then*

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

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

Proof. We have

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

Since

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

we conclude

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

Since

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

$$= \frac{1}{2\delta}\Big(\sum_{uv\in E(G)} (d_u+d_v) - 2\sum_{uv\in E(G)} \sqrt{d_u d_v}\Big)$$

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

we conclude

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

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

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

Remark 38 *Since Cauchy–Schwarz inequality gives*

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

$$= \sum_{uv\in E(G)} \left(\sqrt{d_u}-\sqrt{d_v}\,\right)^2 \,\frac{1}{m} \sum_{uv\in E(G)} 1^2$$

$$\ge \frac{1}{m}\Big(\sum_{uv\in E(G)} \left|\sqrt{d_u}-\sqrt{d_v}\,\right|\Big)^2,$$

we have $M_1(G)-2M_2^{1/2}(G) \ge 0$ *and so, Theorem 39 improves the lower bound in* (4.1)*.*

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

Theorem 39 *If G is a graph with m edges, minimum degree δ and maximum degree Δ, then:*

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

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

Proof. Note that:

$$\frac{d_u + d_v}{2\sqrt{d_u d_v}} = 1 + \frac{\left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2}{2\sqrt{d_u d_v}},$$
$$AG(G) = m + \sum_{uv \in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\,\right)^2}{2\sqrt{d_u d_v}}\,.$$

Since:

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

we have:

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

The bound is tight if and only if:

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

for every $uv \in E(G)$, and this happens if and only if $d_u = \Delta$ and $d_v = \delta$, or vice versa, for every $uv \in E(G)$, so G is regular if $\Delta = \delta$ or is otherwise biregular. ■

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

Theorem 40 *If G is a graph with minimum degree δ and maximum degree Δ, and $a \in \mathbb{R}$, then:*

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

with:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

and thus, $\partial g/\partial x \leq 0$. Therefore, the maximum value of g is attained on

$\{x = \delta,\, \delta \le y \le \Delta\}$. Since:

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

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

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

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

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

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

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

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

The *misbalance rodeg index* is defined as

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

This is a significant predictor of enthalpy of vaporization and of standard enthalpy of vaporization for octane isomers (see [60]).

Theorem 39 and Remark 38 have the following consequence.

Corollary 41 *If G is a graph with m edges, maximum degree Δ and minimum degree δ, then*

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

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

The following fact is elementary.

Lemma 42 *Let us consider the function $f(x,y) = (xy)^\alpha$ with $\delta \le x, y \le \Delta$. Then*

$$f(x,y) \le \delta^{2\alpha}\,, \qquad \text{if } \alpha \le 0,$$
$$f(x,y) \le \Delta^{2\alpha}\,, \qquad \text{if } \alpha \ge 0.$$

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

Theorem 43 *If G is a graph with maximum degree Δ and minimum degree δ, and $\alpha \in \mathbb{R}$, then*

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

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

Proof. We have

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

If $\alpha \le 1/2$, then Lemma 42 gives

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

If $\alpha \ge 1/2$, then we have by Lemma 42

$$AG(G) \le \Delta^{2\alpha} \sum_{uv\in E(G)} (d_u d_v)^{-\alpha}.$$

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

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

The *symmetric division deg index* is another Adriatic index defined in [60] as

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

It was claimed in [60] that SDD correlates well with the total surface area of polychlorobiphenyls. The paper [20] tested the physico-chemical applicability of SDD on a much wider empirical basis, and compared it with other extensively used vertex-degree-based topological indices.

The following result relates the arithmetic-geometric and the symmetric division deg indices.

Theorem 44 *Let G be a graph with m edges, maximum degree Δ and minimum degree δ. Then*

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

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

Proof. Let us consider

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

We have, by Corollary 12,

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

Thus, Lemma 1 gives

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

Since

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

we conclude

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

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

If the equality in this bound is attained, then Lemma 1 gives

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

Thus, Corollary 12 gives $\Delta=\delta$, and so, G is a regular graph.

If G is a regular graph, then

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

On the other hand, the Cauchy–Schwarz inequality gives

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

Since

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

we conclude

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

If G is a regular or biregular graph, then

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

■

Estrada et al. [18] 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. [21] made a generalization of ABC index, defined as

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

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

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

Theorem 45 *Let G be a graph with maximum degree Δ and without isolated edges, and $\alpha>0$. Then*

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

and the equality in the bound is attained if and only if G is union of star graphs $S_{\Delta+1}$.

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

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

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

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

so $W(x,y)$ is strictly increasing on $x \in [1,y]$ for every fixed $y \geq 2$, and so $W(1,y) \leq W(x,y)$. Let us consider

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

Then

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

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

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

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. ■

Remark 46 *The argument in the proof of Theorem 45 (with the same hypotheses) allows to obtain the following lower bound of AG, but it is elementary:*

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

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

We can improve Theorem 45 when $\delta \ge 2$.

Theorem 47 *Let G be a graph with maximum degree Δ and minimum de-*

gree $\delta \geq 2$, and $\alpha > 0$. Then

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

The equality in the bound is attained if G is a regular graph.

Proof. Consider the notation in the proof of Theorem 45, and the function

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

with $2 \leq \delta \leq y \leq \Delta$. The argument in the proof of Theorem 45 gives that $c(y) = W(\delta, y) \leq W(x, y)$ for every $\delta \leq x \leq y \leq \Delta$.

We have

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

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

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

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

Assume now that $\delta \ge 3$. Let us consider the second degree polynomial

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

Since

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

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

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

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

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

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

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

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

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

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

If G is a regular graph, then $\Delta = \delta$ and

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

and the equality in the bound is attained. ■

We relate now the arithmetic-geometric and the general atom-bond connectivity indices with parameter greater than or equal to 1/2.

Theorem 48 *Let G be a graph with maximum degree Δ and minimum degree $\delta \geq 2$, and $\beta \geq 1/2$. Then*

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

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

Proof. Define $\alpha = -\beta \leq -1/2$. As in the proof of Theorem 45, let us consider the function

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

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

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

on $\{\delta \leq x \leq y \leq \Delta\}$. Hence, $W(y,y) \leq W(x,y)$ when $\delta \leq x \leq y \leq \Delta$. Let us consider

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

Then,

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

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

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

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

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

for every $\delta \leq x, y \leq \Delta$, and

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

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

■

Remark 49 *The argument in the proof of Theorem 48 (with the same hypotheses) allows to obtain the following lower bound of AG, but it is elementary:*

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

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

4.2 General bounds on the AG index and correlation

We obtain in this section additional lower bounds of AG improving the lower bound in (4.1), which do not involve other topological indices. The two following bounds involve m and the minimum degree.

Theorem 50 *Let G be a graph with m edges, minimum degree δ, maximum degree $\delta+1$, and α the cardinality of the set of edges $uv \in E(G)$ with $d_u \neq d_v$. Then α is an even integer and*

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

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

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

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

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

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

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

Assume for contradiction that α is an odd integer.

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

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

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

Theorem 51 *Let G be a connected graph with m edges, minimum degree δ and maximum degree $\delta + 1$. Then*

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

and the equality is attained for each δ.

Proof. Denote by α the cardinality of the set of edges $uv \in E(G)$ with $d_u \neq d_v$. Theorem 50 gives that α is an even integer. Since G is a connected graph, we have $\alpha \neq 0$ and so, $\alpha \geq 2$. Since

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

and $\alpha \geq 2$, Theorem 50 gives

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

Given a fixed δ, let us consider the complete graphs $K_{\delta+1}$ and $K_{\delta+2}$ with $\delta+1$ and $\delta+2$ vertices, respectively. Fix $u_1, u_2 \in V(K_{\delta+1})$ and $v_1, v_2 \in V(K_{\delta+2})$, and denote by $K'_{\delta+1}$ and $K'_{\delta+2}$ the graphs obtained from $K_{\delta+1}$ and $K_{\delta+2}$ by deleting the edges u_1u_2 and v_1v_2, respectively. Let Γ_δ be the graph with $V(\Gamma_\delta) = V(K'_{\delta+1}) \cup V(K'_{\delta+2})$ and $E(\Gamma_\delta) = E(K'_{\delta+1}) \cup E(K'_{\delta+2}) \cup \{u_1v_1\} \cup \{u_2v_2\}$. Thus, Γ_δ has $\delta^2+2\delta+1$ edges, minimum degree δ, maximum degree $\delta+1$, and Theorem 50 gives

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

Hence, the equality is attained for each δ. ■

Recall that a graph is said *chemical* if the degree of each vertex is at most 4. We have the following consequence for chemical graphs.

Corollary 52 *Let G be a connected chemical graph with m edges, minimum* *degree δ and maximum degree $\delta+1$. Then*

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

Furthermore, the equality in the bound is attained.

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

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

Theorem 51 gives the desired inequality.

The graph Γ_3 in the proof of Theorem 51 provides that the equality is attained. ■

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

$$A_0 = \{uv \in E(G) : \, d_u = \delta, d_v = \Delta\},$$

$$A_1 = \{uv \in E(G) : \, d_u = \delta, \delta < d_v < \Delta\},$$

$$A_2 = \{uv \in E(G) : \, d_u = \Delta, \delta < d_v < \Delta\},$$

respectively.

Theorem 53 *Let G be a graph with m edges, maximum degree Δ and minimum degree $\delta < \Delta - 1$. Then*

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

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

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

From the above argument, it follows that the function:

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

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

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

for every $uv \in A_1$.

In a similar way, the function:

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

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

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

for every $uv \in A_2$.

Since:

$$1 \leq \frac{d_u+d_v}{2\sqrt{d_u d_v}} \leq \frac{\Delta+\delta}{2\sqrt{\Delta\delta}}$$

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

$$\begin{aligned}
AG(G) &= \sum_{uv\in E(G)\setminus A_0\cup A_1\cup A_2} \frac{d_u+d_v}{2\sqrt{d_u d_v}} + \sum_{uv\in A_0} \frac{d_u+d_v}{2\sqrt{d_u d_v}} + \sum_{uv\in A_1} \frac{d_u+d_v}{2\sqrt{d_u d_v}} + \sum_{uv\in A_2} \frac{d_u+d_v}{2\sqrt{d_u d_v}} \\
&= \sum_{uv\in E(G)\setminus A_0\cup A_1\cup A_2} \frac{d_u+d_v}{2\sqrt{d_u d_v}} + \sum_{uv\in A_0} \frac{\Delta+\delta}{2\sqrt{\Delta\delta}} + \sum_{uv\in A_1} \frac{\delta+d_v}{2\sqrt{\delta d_v}} + \sum_{uv\in A_2} \frac{\Delta+d_v}{2\sqrt{\Delta d_v}},
\end{aligned}$$

therefore:

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

and:

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

■

We are going to use Theorem 53 in order to obtain the following lower bound of AG involving m and the minimum and maximum degree.

Theorem 54 *Let G be a connected graph with m edges, maximum degree Δ and minimum degree $\delta < \Delta - 1$. Then*

$$AG(G) \geq m + \min\Big\{ \frac{2\delta+1}{2\sqrt{\delta(\delta+1)}} + \frac{2\Delta-1}{2\sqrt{\Delta(\Delta-1)}} - 2\,,\; \frac{\Delta+\delta}{2\sqrt{\Delta\delta}} - 1 \Big\}.$$

The equality in the bound is attained.

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

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

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

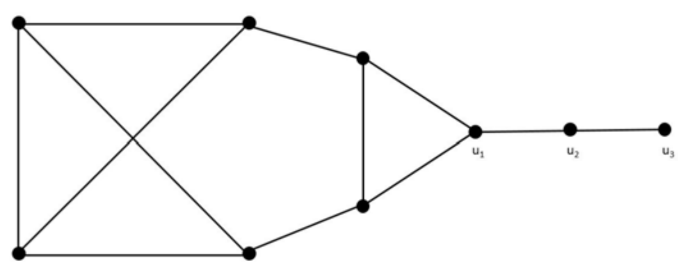
Theorem 53 gives

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

In the second case, $\alpha_1, \alpha_2 \geq 1$ and Lemma 53 gives

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

Let G be the graph in the figure.



We have $m = 12$, $\Delta = 3$, $\delta = 1$, $A_0 = \emptyset$, $\alpha_0 = 0$, $A_1 = \{u_2u_3\}$, $\alpha_1 = 1$, $A_2 = \{u_1u_2\}$ and $\alpha_2 = 1$. Also, if $uv \notin A_0 \cup A_1 \cup A_2$, then $d_u = d_v$. Thus,

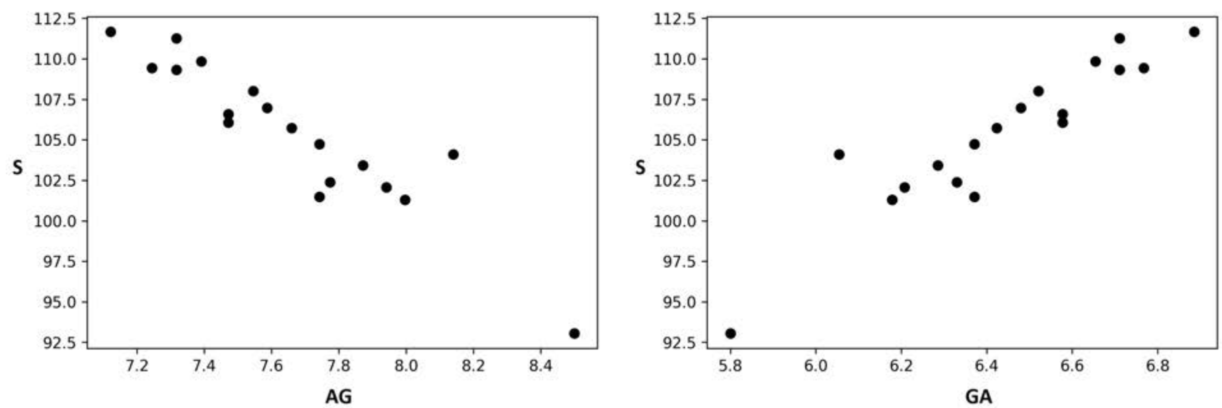
$$\begin{aligned} AG(G) &= \sum_{uv \in E(G) \setminus A_0 \cup A_1 \cup A_2} \frac{d_u + d_v}{2\sqrt{d_u d_v}} + \sum_{uv \in A_0} \frac{\Delta + \delta}{2\sqrt{\Delta\delta}} + \sum_{uv \in A_1} \frac{\delta + d_v}{2\sqrt{\delta d_v}} + \sum_{uv \in A_2} \frac{\Delta + d_v}{2\sqrt{\Delta d_v}} \\ &=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

The lower bound is

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

and so, the equality in the bound is attained. ■

Note that, although the arithmetic–geometric index AG and the geometric–arithmetic index GA are mathematically represented by an inverse relationship, their scope and results from both theoretical and practical points of view are different. In some cases, the reciprocal topological indices have shown better correlation with some physico–chemical properties than their related indices. In the case of the AG index, in order to investigate its predictive power, we used a datum for entropy (S) of octane isomers, and the results are compared with those obtained for the GA index, see the following figure. The correlation coefficient obtained for the AG index is $\mathbf{r}_{AG}=-0.927$, while for the GA index, it is $\mathbf{r}_{GA}=0.912$, so the AG index, in this case, shows better predictive power than the GA index. However, when we used a datum for the boiling point of octane isomers, it turned out that the GA index showed better predictive power than the AG index.


112.5
110.0
107.5
105.0
102.5
100.0
97.5
95.0
92.5
S
7.2
7.4
7.6
7.8
8.0
8.2
8.4
AG
5.8
6.0
6.2
6.4
6.6
6.8
GA

Chapter 5

Conclusions

Topological indices have become a useful tool for the study of theoretical and practical problems in different areas of science. With this thesis, an important line of research associated with topological indices is strengthened, which is to determine the optimal bounds and relations between known topological indices.

The present research begins with a brief overview of the Theory of Mathematical Inequalities and Topological Indices from its beginnings to the present. In the same direction we study the mathematical properties and fundamental relationships between important topological indices, such as: the *Inverse index*, the *first general Zagreb index* and the recently introduced *Arithmetic-Geometric index*. Moreover, in this work we find and show optimal inequalities, which do not involve other topological indices, in particular, for the topological index AG as a function of graph invariants such as the number of edges and the minimum and maximum degree.

Open problems

1. Study the mathematical and computational properties of other topological indices.

2. To apply topological indices to the study of topological and structural properties of complex systems.

3. To propose new topological indices for the study of problems associated with Environmental Sciences.

Contributions of this work

This doctoral research generated the following scientific papers:

- José M. Rodríguez, José L. Sánchez and José M. Sigarreta. On the first general Zagreb index. Journal of Mathematical Chemistry (2018) 7(56), 1849-1864.
- José M. Rodríguez, José L. Sánchez and José M. Sigarreta. On the inverse degree index. Journal of Mathematical Chemistry (2019) 57(5), 1524–1542.
- José M. Rodríguez, José L. Sánchez, José M. Sigarreta and E. Tourís. Bounds on the Arithmetic-Geometric Index. Symmetry (2021) 13, 689.
- Edil D. Molina, José M. Rodríguez, José L. Sánchez and José M. Sigarreta. Some properties of the Arithmetic–Geometric Index. Symmetry (2021) 13, 857.

- E. Locia, A. Morales, José L. Sánchez and José M. Sigarreta. Epistemological study of mathematical Inequalities. Revista Brasileira de História da Matemática (2021). In Press.

These results were presented in the following international and national conferences and Seminars:

- 18th International Conference Computational and Mathematical Methods in Science and Engineering, June-July 2018, Cadiz, Spain.
- 19th International Conference Computational and Mathematical Methods in Science and Engineering, June-July 2019, Cadiz, Spain.
- Seminario de la Matemática, Octubre 2020, Acapulco, México.
- XI Simposio de Matemática y Educación Matemática, febrero 2021, Bogotá, Colombia.
- II Simposio de Matemática Virtual, Mayo 2021, Luján, Argentina.

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