SPECTRAL PROPERTIES OF GEOMETRIC-ARITHMETIC INDEX

JOSÉ M. RODRÍGUEZ AND JOSÉ M. SIGARRETA

Abstract. The concept of geometric-arithmetic index was introduced in the chemical graph theory recently, but it has shown to be useful. One of the main aims of algebraic graph theory is to determine how, or whether, properties of graphs are reflected in the algebraic properties of some matrices. The aim of this paper is to study the geometric-arithmetic index GA_1 from an algebraic viewpoint. Since this index is related to the degree of the vertices of the graph, our main tool will be an appropriate matrix that is a modification of the classical adjacency matrix involving the degrees of the vertices. Moreover, using this matrix, we define a GA Laplacian matrix which determines the geometric-arithmetic index of a graph and satisfies properties similar to the ones of the classical Laplacian matrix.

Keywords: Geometric-arithmetic index; Spectral properties; Laplacian matrix; Laplacian eigenvalues; Topological index; Graph invariant.

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Telephone/fax number and email address of the corresponding author: +34 91 624 9098, +34 91 624 9151, jomaro@math.uc3m.es

1. Introduction

A single number, representing a chemical structure in graph-theoretical terms via the molecular graph, is called a topological descriptor and if it in addition correlates with a molecular property it is called topological index, which is used to understand physicochemical properties of chemical compounds. Topological indices are interesting since they capture some of the properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes (see [45]).

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best know such descriptor is the Randić connectivity index (R) [34]. There are more than thousand papers and a couple of books dealing with this molecular descriptor (see, e.g., [2], [15], [17], [20], [25], [27], [31], [36], [37], [40] and the references therein). During many years, scientists were trying to improve the predictive power of the Randić index. This led to the introduction of a large number of new topological descriptors resembling the original Randić index. The first geometric-arithmetic index GA_1, defined in [44] as

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

where uv denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u, is one of the successors of the Randić index. Although GA_1 was introduced just a few years ago, there are many papers dealing with this index (see, e.g., [9], [10], [38], [39], [41], [44] and the references therein). There are other geometric-arithmetic indices, like $Z_{p,q}$ ($Z_{0,1} = GA_1$), but the results in [9, p.598] show that the GA_1 index gathers the same information on observed molecule as other $Z_{p,q}$ indices.

The reason for introducing a new index is to gain prediction of some property of molecules somewhat better than obtained by already presented indices. Therefore, a test study of predictive power of a new

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index must be done. The GA_1 index gives better correlation coefficients than Randić index for many physico-chemical properties of octanes, but the differences between them are not significant. However, the predicting ability of the GA_1 index compared with Randić index is reasonably better (see [9, Table 1]). Furthermore, the improvement in prediction with GA_1 index comparing to Randić index in the case of standard enthalpy of vaporization is more than 9%. Hence, one can think that GA_1 index should be considered in the QSPR/QSAR researches.

Throughout this paper, $G = (V, E) = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) connected graph with $E \neq \emptyset$. Note that the connectivity of G is not an important restriction, since if G has connected components $G_1, \dots, G_r$, then $GA_1(G) = GA_1(G_1) + \cdots + GA_1(G_r)$; furthermore, every molecular graph is connected.

Spectral graph theory is a useful subject that studies the relation between graph properties and the spectrum of some important matrices in graph theory, as the adjacency matrix, the Laplacian matrix, and the incidence matrix, see e.g. [1], [6], [18]. Eigenvalues of graphs appear in a natural way in mathematics, physics, chemistry and computer science. One of the main aims of algebraic graph theory is to determine how, or whether, properties of graphs are reflected in the algebraic properties of such matrices [18]. Many papers study several topological indices from an algebraic viewpoint (for instance, [21], [36] and [37] study the Randić index, and [39] deals with the geometric-arithmetic index).

The aim of this paper is to obtain new results on the geometric-arithmetic index GA_1 from an algebraic viewpoint. Since this index is related to the degree of the vertices of the graph, our main tool will be an appropriate matrix, denoted by $\mathcal{D}$, that is a modification of the classical adjacency matrix involving the degrees of the vertices. Using $\mathcal{D}$, we will define a GA Laplacian matrix $\mathcal{L}$ and we will prove that it determines the geometric-arithmetic index of a graph; besides, we show that $\mathcal{L}$ satisfies many properties of the classical Laplacian matrix. It is usual to define energies associated to some topological indices (see, e.g., [21]). Along the paper we denote by n the order $n = |V(G)|$ of the graph G and by m its size $m = |E(G)|$. The minimum degree of a graph is denoted by δ and the maximum by Δ. We will denote by $tr(M)$ the trace of the matrix M.

2. Bounds for GA_1

In order to state some bounds for GA_1 we need some previous technical results.

Lemma 2.1. *Let f be the function $f(t) = \frac{2t}{1+t^2}$ on the interval $[0, \infty)$. Then f strictly increases in $[0, 1]$, strictly decreases in $[1, \infty)$, $f(t) = 1$ if and only if $t = 1$ and $f(t) = f(t_0)$ if and only if either $t = t_0$ or $t = t_0^{-1}$.*

Proof. The statements follow from $f'(t) = \frac{2(1-t^2)}{(1+t^2)^2}$. □

Corollary 2.2. *Let g be the function $g(x, y) = \frac{2\sqrt{xy}}{x+y}$ with $0 < a \le x, y \le b$. Then $\frac{2\sqrt{ab}}{a+b} \le g(x, y) \le 1$. The equality in the lower bound is attained if and only if either $x = a$ and $y = b$, or $x = b$ and $y = a$, and the equality in the upper bound is attained if and only if $x = y$. Besides, $g(x, y) = g(x', y')$ if and only if x/y is equal to either x'/y' or y'/x'. Finally, if $x' < x \le y$, then $g(x', y) < g(x, y)$.*

Proof. It suffices to apply Lemma 2.1, since $g(x, y) = f(t)$ with $t = \sqrt{\frac{x}{y}}$, and $\sqrt{\frac{a}{b}} \le t \le \sqrt{\frac{b}{a}}$. □

We will need the following result.

Proposition 2.3. *Given an $n \times n$ symmetric matrix $B = (b_{ij})$ with $b_{ij} \ge 0$ for every $1 \le i, j \le n$ and the diagonal matrix D with entries $d_{ii} = \sum_{j=1}^{n} b_{ij}$, then $L := D - B$ is a positive semi-definite matrix.*

Proof. Let $\mathbf{x} := (x_1, \dots, x_n) \in \mathbb{R}^n$. Since $x_i^2 + x_j^2 \ge 2x_ix_j$ for every $1 \le i, j \le n$, we have

$$\sum_{i=1}^{n}\sum_{j=1}^{n} b_{ij}x_i^2 + \sum_{i=1}^{n}\sum_{j=1}^{n} b_{ij}x_j^2 \ge 2\sum_{i=1}^{n}\sum_{j=1}^{n} b_{ij}x_ix_j.$$

Since $b_{ij} = b_{ji}$ for every $1 \geq i, j \geq n$, we conclude

$$\mathbf{x}D\,\mathbf{x}^T = \left\{\sum_{i=1}^{n} x_i^2 \left\{\sum_{j=1}^{n} b_{ij} \infty \left\{\sum_{i=1}^{n} \left\{\sum_{j=1}^{n} b_{ij}x_i x_j = \mathbf{x}B\,\mathbf{x}^T,$$

and $\mathbf{x}L\,\mathbf{x}^T \infty 0$ for every $\mathbf{x} \,/\, \mathbb{R}^n$. □

Given a graph G, let us define the *GA-adjacency matrix* $\mathcal{D}$ with entries

$$a_{uv} := \begin{cases} \frac{2\sqrt{d_u d_v}}{d_u+d_v}, & \text{if } uv \,/\, E(G), \\ 0, & \text{otherwise.} \end{cases}$$

Note that $\mathcal{D}$ is a modification of the classical adjacency matrix involving the degrees of the vertices.

Let us define also $\mathcal{L}$ as the diagonal matrix with entries $d_{uu} := \sum_{v\sim u} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$, where $v \sim u$ means that v is a neighbor of u, i.e., $uv \,/\, E(G)$. Finally, define the *GA Laplace matrix* $\cup := \mathcal{L} \quad \mathcal{D}$. Note that $\cup$ is the classical Laplace matrix for every regular graph.

Denote by A the adjacency matrix of a graph. Since the adjacency matrix A, $\mathcal{D}$ and $\cup$ are real symmetric matrices, their eigenvalues are real numbers. Denote by $\lambda_1 \infty \times\times\times \infty \lambda_n$, $\mu_1 \infty \times\times\times \infty \mu_n$ and $\eta_1 \infty \times\times\times \infty \eta_n$ the ordered eigenvalues of A, $\mathcal{D}$ and $\cup$, respectively.

It is well known that the second smallest (classical) Laplacian eigenvalue of a graph (its *algebraic connectivity*) is the most important information about its spectrum. This eigenvalue is related to several important graph invariants and provides good bounds on the values of several parameters of graphs which are very hard to compute. In in the third item of Proposition 2.4 below we obtain an identity for $\eta_{n\ \ 1}$ which is similar to the one for the algebraic connectivity. Theorem 2.5 states that the geometric-arithmetic index is completely determined by the GA Laplacian spectrum, and provides bounds of GA_1 involving $\eta_{n\ \ 1}$ and η_1. Hence, Proposition 2.4 and Theorem 2.5 collect the main results about the spectrum of the GA Laplace matrix $\cup$, which are similar to the properties of the classical Laplace matrix and its generalizations, see [36, 37].

Proposition 2.4. *For any graph G with n vertices $\}v_1, \dots, v_n\langle$ and $a_{ij} := 2\sqrt{d_{v_i} d_{v_j}}/(d_{v_i} + d_{v_j})$ for every $1 \geq i, j \geq n$, the following statements hold.*

$\subseteq$ $\cup$ *is a positive semi-definite matrix.*

$\subseteq$ $\eta_n = 0$ *is an eigenvalue with multiplicity one and eigenvector* $\mathbf{j} = (1, 1, \dots, 1)^T \,/\, \mathbb{R}^n$.

$\subseteq$ $\eta_{n\ \ 1} = 2n \min \left\} \frac{\sum_{v_i\sim v_j} a_{ij}(w_i \quad w_j)^2}{\sum_{v_i,v_j\in V(G)}(w_i \quad w_j)^2} \right(\mathbf{w} := (w_1, \dots, w_n) \,/\, \mathbb{R}^n,\ \mathbf{w} \not\Leftarrow a\mathbf{j}$ *with* $a \,/\, \mathbb{R} \surd$.

$\subseteq$ $\eta_1 = 2n \max \left\} \frac{\sum_{v_i\sim v_j} a_{ij}(w_i \quad w_j)^2}{\sum_{v_i,v_j\in V(G)}(w_i \quad w_j)^2} \right(\mathbf{w} := (w_1, \dots, w_n) \,/\, \mathbb{R}^n,\ \mathbf{w} \not\Leftarrow a\mathbf{j}$ *with* $a \,/\, \mathbb{R} \surd$.

Proof. The first item is a direct consequence of Proposition 2.3.

Since $\cup$ is a positive semi-definite matrix, we have $\eta_1 \infty \times\times\times \infty \eta_n \infty 0$.

Since $\mathcal{L}\,\mathbf{j} = \mathcal{D}\,\mathbf{j}$, we have $\cup\,\mathbf{j} = 0 \times \mathbf{j}$, and so 0 is an eigenvalue with multiplicity one and eigenvector $\mathbf{j}$. This fact and $\eta_1 \infty \times\times\times \infty \eta_n \infty 0$ give $\eta_n = 0$. It is well known that the multiplicity of the eigenvalue 0 of the classical Laplacian matrix of a graph is equal to the cardinality of the connected components of the graph (see, e.g., [6]); the argument in [6] also gives the same result for the GA Laplacian. Since G is connected, 0 is an eigenvalue with multiplicity one of $\cup$.

The results of Fielder [16] and the Rayleigh quotient give third and fourth items, respectively. □

Theorem 2.5. *For any graph G with n vertices the following statements hold.*

$\subseteq$ *The geometric-arithmetic index of G is* $GA_1(G) = \frac{1}{2}\sum_{j=1}^{n} \eta_j$.

$\subseteq$ *The geometric-arithmetic index of G satisfies the inequalities* $\frac{1}{2}(n \quad 1)\eta_{n\ \ 1} \geq GA_1(G) \geq \frac{1}{2}(n \quad 1)\eta_1$.

$\subseteq$ *If G is a bipartite graph with parts X, Y, then* $\frac{\sqrt{X\ Y}}{\sqrt{n}}\eta_{n\ \ 1} \geq GA_1(G) \geq \frac{\sqrt{X\ Y}}{\sqrt{n}}\eta_1$.

Proof. The first item follows from $2\,GA_1(G) = tr(\mathcal{U}) = \sum_{j=1}^{n} \eta_j$, and the second one is a consequence of this equality. Finally, if G is a bipartite graph with parts X, Y, then consider $\mathbf{w} := (w_1, \dots, w_n) \in \mathbb{R}^n$ defined as $w_j := 1$ if $v_j \in X$ and $w_j := -1$ if $v_j \in Y$. Thus,

$$\sum_{v_i, v_j \in V(G)} (w_i - w_j)^2 = |X|4|Y| + |Y|4|X| = 8|X||Y|.$$

The previous results give

$$\eta_{n-1} \geq \frac{n \sum_{v_i \sim v_j} a_{ij}(w_i - w_j)^2}{4|X||Y|} \geq \eta_1.$$

Since G is a bipartite graph,

$$a_{ij}(w_i - w_j)^2 = 4\,\frac{2\sqrt{d_{v_i} d_{v_j}}}{d_{v_i} + d_{v_j}}$$

if $v_i \sim v_j$, we have

$$\frac{|X||Y|}{n}\eta_{n-1} \geq GA_1(G) \geq \frac{|X||Y|}{n}\eta_1.$$

□

Since $GA_1(G) \geq m$, we have the following consequence.

Corollary 2.6. *We have for any graph G the inequalities* $\sum_{j=1}^{n} \eta_j \geq 2m, \qquad \eta_{n-1} \geq \frac{2m}{n-1}.$

The following result relates the eigenvalues λ_1 and μ_1.

Theorem 2.7. *We have for any graph G, $\lambda_1 \geq |\lambda_j|$, $\mu_1 \geq |\mu_j|$ for every j, $\lambda_1, \mu_1 > 0$, and*

$$\frac{2\sqrt{\Delta\delta}}{\Delta + \delta}\lambda_1 \geq \mu_1 \geq \lambda_1, \tag{2.1}$$

and the equalities in (2.1) *are attained simultaneously if and only if G is regular.*

Proof. Since A are $\mathcal{D}$ non-negative and irreducible (we just consider connected graphs) Perron-Frobenius Theorem gives $\lambda_1 \geq |\lambda_j|$ and $\mu_1 \geq |\mu_j|$ for every j and then $\lambda_1, \mu_1 > 0$.

Perron-Frobenius Theorem also gives that λ_1 (respectively, μ_1) is a simple eigenvalue and there exists an eigenvector v of A with eigenvalue λ_1 (respectively, v' of $\mathcal{D}$ with eigenvalue μ_1) such that all components of v (respectively, v') are non-negative. Note that if a_{ij} and α_{ij} denote the entry (i, j) of A and $\mathcal{D}$, respectively, then

$$\frac{2\sqrt{\Delta\delta}}{\Delta + \delta} a_{ij} \geq \alpha_{ij} \geq a_{ij}$$

for every i, j. Hence, using Rayleigh quotient, we obtain

$$\mu_1 = \max_{\mathbf{x} \neq 0} \frac{\langle \mathcal{D}\mathbf{x}, \mathbf{x}\rangle}{\|\mathbf{x}\|^2} = \frac{\langle \mathcal{D}v', v'\rangle}{\|v'\|^2} \geq \frac{\langle Av', v'\rangle}{\|v'\|^2} \geq \max_{\mathbf{x} \neq 0} \frac{\langle A\mathbf{x}, \mathbf{x}\rangle}{\|\mathbf{x}\|^2} = \lambda_1,$$

$$\frac{2\sqrt{\Delta\delta}}{\Delta + \delta}\lambda_1 = \frac{2\sqrt{\Delta\delta}}{\Delta + \delta}\max_{\mathbf{x} \neq 0} \frac{\langle A\mathbf{x}, \mathbf{x}\rangle}{\|\mathbf{x}\|^2} = \frac{2\sqrt{\Delta\delta}}{\Delta + \delta}\frac{\langle Av, v\rangle}{\|v\|^2} \geq \frac{\langle \mathcal{D}v, v\rangle}{\|v\|^2} \geq \max_{\mathbf{x} \neq 0} \frac{\langle \mathcal{D}\mathbf{x}, \mathbf{x}\rangle}{\|\mathbf{x}\|^2} = \mu_1.$$

If the equalities in (2.1) are attained simultaneously, then $\Delta = \delta$ by Corollary 2.2, and the graph G is regular.

Reciprocally, if G is regular, then the lower and upper bound are the same, and they are equal to μ_1. □

We deal in this part with some results related to the traces of powers of $\mathcal{D}$. We start with a basic result which can be obtained by a computation.

Lemma 2.8. *We have for any graph G*

$$
\begin{aligned}
tr(\mathcal{D}) &= 0,\\
tr(\mathcal{D}^2) &= 2\sum_{uv\in E(G)} \frac{4\,d_ud_v}{(d_u+d_v)^2}\,,\\
tr(\mathcal{D}^3) &= 2\sum_{uv\in E(G)} \frac{4\,d_ud_v}{d_u+d_v}\sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\,d_w}{(d_u+d_w)(d_v+d_w)}\,,\\
tr(\mathcal{D}^4) &= \sum_{u\in V(G)}\Bigg(\sum_{\substack{v\in V(G)\\ v\sim u}} \frac{4\,d_ud_v}{(d_u+d_v)^2}\Bigg)^2 + \sum_{\substack{u,v\in V(G)\\ u\neq v}} 4\,d_ud_v\Bigg(\sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\,d_w}{(d_u+d_w)(d_v+d_w)}\Bigg)^2.
\end{aligned}
$$

Remark 2.9. *As usual, we define the sum over the empty set as zero. Hence, since $u \nsim v$, we have $\sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\,d_w}{(d_u+d_w)(d_v+d_w)} = 0$ if $N(u)\cap N(v)=\emptyset$*

Theorem 2.10. *We have for any graph G, $\frac{1}{2}\,tr(\mathcal{D}^2) \geq GA_1(G) \geq \frac{n\,tr(\mathcal{D}^2)}{4\sqrt{n-1}}$. 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 a star graph.*

Proof. By Corollary 2.2, taking $a = 1$ and $b = n-1$, we have $\frac{2\sqrt{n-1}}{n} \geq \frac{2\sqrt{d_ud_v}}{d_u+d_v} \geq 1$, and Lemma 2.8 gives

$$tr(\mathcal{D}^2) = 2\sum_{uv\in E(G)} \frac{2\sqrt{d_ud_v}}{d_u+d_v}\,\frac{2\sqrt{d_ud_v}}{d_u+d_v} \leq 2\,\frac{2\sqrt{n-1}}{n}\sum_{uv\in E(G)} \frac{2\sqrt{d_ud_v}}{d_u+d_v} = \frac{4\sqrt{n-1}}{n}\,GA_1(G),$$

and

$$tr(\mathcal{D}^2) = 2\sum_{uv\in E(G)} \frac{2\sqrt{d_ud_v}}{d_u+d_v}\,\frac{2\sqrt{d_ud_v}}{d_u+d_v} \geq 2\sum_{uv\in E(G)} \frac{2\sqrt{d_ud_v}}{d_u+d_v} = 2\,GA_1(G).$$

By Corollary 2.2, the equality in the upper bound holds for G if and only if every edge joins a vertex of degree 1 with a vertex of degree $n-1$, and this holds if and only if G is a star graph.

The equality in the lower bound holds, by Corollary 2.2, if and only if $d_u = d_v$ for every edge $uv \in E(G)$. Since G is a connected graph, this happens if and only if G is regular. □

Theorems 2.5 and 2.10 allow to obtain bounds of η_1 and η_{n-1} involving $tr(\mathcal{D}^2)$.

Corollary 2.11. *We have for any graph $\eta_1 \leq \frac{tr(\mathcal{D}^2)}{\sqrt{n-1}}$, $\qquad \eta_{n-1} \geq \frac{n\,tr(\mathcal{D}^2)}{2(n-1)^{3/2}}$.*

Proposition 2.12. *For any graph $tr(\mathcal{D}^2) \geq 2m$. Furthermore, a graph is regular if and only if $tr(\mathcal{D}^2) = 2m$.*

Proof. Lemma 2.8 gives

$$tr(\mathcal{D}^2) = 2\sum_{uv\in E(G)} \frac{4\,d_ud_v}{(d_u+d_v)^2} \geq 2m,$$

and the equality is attained if and only if $2\sqrt{d_ud_v}/(d_u+d_v) = 1$ for every $uv \in E(G)$. By Corollary 2.2, this last condition holds if and only if $d_u = d_v$ for every $uv \in E(G)$. Since the graph G is connected, the equality is attained if and only if G is regular. □

Recall that a (Δ, δ)-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. The following result improves Theorem 2.10, although its inequalities are not so nice as the ones in Theorem 2.10.

Theorem 2.13. *We have for any graph G*

$$\sqrt{\frac{1}{2}\,tr(\mathcal{D}^2) + \frac{4\Delta\delta}{(\Delta+\delta)^2}\,m(m-1)} \ge GA_1(G) \ge \frac{(\Delta+\delta)\,tr(\mathcal{D}^2)}{4\sqrt{\Delta\delta}}\,,$$

and the equality in each inequality holds if and only if G is either regular or (Δ,δ)-biregular.

Proof. Let us prove first the lower bound of $GA_1(G)$.

Lemma 2.8 gives

$$\begin{aligned} GA_1(G)^2 &= \Big(\sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\Big)^2 \\ &= \sum_{uv\in E(G)} \frac{4 d_u d_v}{(d_u+d_v)^2} + \sum_{uv\neq xy} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\,\frac{2\sqrt{d_x d_y}}{d_x+d_y} \\ &= \frac{1}{2}\,tr(\mathcal{D}^2) + \sum_{uv\neq xy} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\,\frac{2\sqrt{d_x d_y}}{d_x+d_y}\,. \end{aligned}$$

By Corollary 2.2, taking $a=\delta$ and $b=\Delta$, we have

$$\frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \ge \frac{2\sqrt{d_u d_v}}{d_u+d_v}\,, \tag{2.2}$$

and we obtain

$$\begin{aligned} GA_1(G)^2 &= \frac{1}{2}\,tr(\mathcal{D}^2) + \sum_{uv\neq xy} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\,\frac{2\sqrt{d_x d_y}}{d_x+d_y} \le \frac{1}{2}\,tr(\mathcal{D}^2) + \sum_{uv\neq xy} \frac{4\Delta\delta}{(\Delta+\delta)^2} \\ &= \frac{1}{2}\,tr(\mathcal{D}^2) + \frac{4\Delta\delta}{(\Delta+\delta)^2}\,m(m-1). \end{aligned}$$

Let us prove now the upper bound of $GA_1(G)$. Lemma 2.8 and (2.2) give

$$tr(\mathcal{D}^2) = 2\sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\,\frac{2\sqrt{d_u d_v}}{d_u+d_v} \le 2\,\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} = \frac{4\sqrt{\Delta\delta}}{\Delta+\delta}\,GA_1(G).$$

The equality in each inequality holds if and only if the equality is attained in (2.2), and by Corollary 2.2, this happens if and only if either $d_u=\Delta$ and $d_v=\delta$, or viceversa, for each $uv\in E(G)$. Since G is connected, this happens if and only if G is a regular graph if $\Delta=\delta$ or a (Δ,δ)-biregular graph otherwise. □

Given a graph G, denote by $N(u)$ the set of neighbors of the vertex u, and by δ_0 and Δ_0 the integer numbers

$$\delta_0 := \min_{uv\in E(G)} |N(u)\setminus N(v)|, \qquad \Delta_0 := \max_{uv\in E(G)} |N(u)\setminus N(v)|.$$

It is clear that $0 \le \delta_0 \le \Delta_0 \le \Delta$.

Theorem 2.14. *We have for any graph G with $\Delta_0>0$,*

$$GA_1(G) \le \frac{\delta^2\,tr(\mathcal{D}^3)}{2\,\Delta^2\Delta_0}\,.$$

Furthermore, if $\delta_0>0$, then

$$GA_1(G) \ge \frac{\Delta^2\,tr(\mathcal{D}^3)}{2\,\delta^2\delta_0}\,.$$

The equality is attained in each inequality if and only if G is regular and $\delta_0=\Delta_0$.

Proof. For each $uv \in E(G)$, we have $w \sim u$, $w \sim v$ if and only if $w \in N(u) \cap N(v)$. Hence,

$$\begin{aligned}\sum_{uv\in E(G)} \frac{4\,d_u d_v}{d_u+d_v} \sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\,d_w}{(d_u+d_w)(d_v+d_w)} &\ge \sum_{uv\in E(G)} \frac{4\,d_u d_v}{d_u+d_v} \sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\Delta}{4\delta^2} \\ &\ge \sum_{uv\in E(G)} \frac{2\,d_u d_v}{d_u+d_v}\, \frac{\Delta}{\delta^2}\, \Delta_0,\end{aligned} \tag{2.3}$$

$$\begin{aligned}\sum_{uv\in E(G)} \frac{4\,d_u d_v}{d_u+d_v} \sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\,d_w}{(d_u+d_w)(d_v+d_w)} &\le \sum_{uv\in E(G)} \frac{4\,d_u d_v}{d_u+d_v} \sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\delta}{4\Delta^2} \\ &\le \sum_{uv\in E(G)} \frac{2\,d_u d_v}{d_u+d_v}\, \frac{\delta}{\Delta^2}\, \delta_0.\end{aligned} \tag{2.4}$$

Thus, Lemma 2.8 and (2.3) give

$$\begin{aligned} tr(\mathcal{D}^3) &= 2 \sum_{uv\in E(G)} \frac{4\,d_u d_v}{d_u+d_v} \sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\,d_w}{(d_u+d_w)(d_v+d_w)} \\ &\ge 2 \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \sqrt{d_u d_v}\, \frac{\Delta}{\delta^2}\, \Delta_0 \\ &\ge 2 \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\, \Delta\, \frac{\Delta}{\delta^2}\, \Delta_0 \\ &= \frac{2\,\Delta^2 \Delta_0}{\delta^2}\, GA_1(G).\end{aligned}$$

Using (2.4) instead of (2.3), we obtain

$$\begin{aligned} tr(\mathcal{D}^3) &= 2 \sum_{uv\in E(G)} \frac{4\,d_u d_v}{d_u+d_v} \sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\,d_w}{(d_u+d_w)(d_v+d_w)} \\ &\le 2 \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \sqrt{d_u d_v}\, \frac{\delta}{\Delta^2}\, \delta_0 \\ &\le 2 \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\, \delta\, \frac{\delta}{\Delta^2}\, \delta_0 \\ &= \frac{2\,\delta^2 \delta_0}{\Delta^2}\, GA_1(G).\end{aligned}$$

If the graph is regular and $\delta_0 = \Delta_0$, then the lower and upper bounds are the same, and they are equal to $GA_1(G)$.

If we have the equality in the lower bound of $GA_1(G)$, then $\sqrt{d_u d_v} = \Delta$ for every $uv \in E(G)$; hence, $d_u = \Delta$ for every $u \in V(G)$ and the graph is regular. Besides, we have the equality in (2.3) and so $|N(u) \cap N(v)| = \Delta_0$ for every $uv \in E(G)$; therefore, $\delta_0 = \Delta_0$.

If we have the equality in the upper bound, then $\sqrt{d_u d_v} = \delta$ for every $uv \in E(G)$; hence, $d_u = \delta$ for every $u \in V(G)$ and G is regular. Furthermore, we have the equality in (2.4) and so $|N(u) \cap N(v)| = \delta_0$ for every $uv \in E(G)$; thus, $\delta_0 = \Delta_0$. □

As usual, we denote by $M_1(G)$ the first Zagreb index of the graph G, defined in [23] as

$$M_1(G) = \sum_{u \in V(G)} d_u^2 .$$

This index has attracted growing interest, see e.g., [3], [11], [22], [23], [24], [32], [46] (in particular, it is included in a number of programs used for the routine computation of topological indices).

Theorem 2.15. *We have for any graph G*

$$\frac{1}{2\Delta}\, tr(\mathcal{D}^4) - \frac{1}{2}\big(M_1(G) - 2m\big) \ge GA_1(G) \ge \frac{(\Delta+\delta)^3}{16\Delta^{3/2}\delta^{5/2}}\, tr(\mathcal{D}^4) - \frac{\Delta^{1/2}}{\delta^{1/2}(\Delta+\delta)}\big(M_1(G) - 2m\big).$$

The equality is attained in the lower bound if and only if G is isomorphic to the complete bipartite graph $K_{\Delta,\Delta}$ with $\Delta \ge 1$. The equality is attained in the upper bound if and only if G is a regular graph without cycles of length 4.

Proof. Denote by CP_3 the cardinality of the set of paths of length 2 in G that are not cycles. For any fixed $w \in V(G)$, the set of paths of length 2 that are not cycles and have w as central vertex has cardinality $\frac{1}{2}\, d_w(d_w - 1)$. Hence,

$$CP_3 = \frac{1}{2} \sum_{w \in V(G)} d_w(d_w - 1) = \frac{1}{2}\, M_1(G) - m,$$

$$\sum_{\substack{u,v \in V(G) \\ u \neq v}} \; \sum_{\substack{w \in V(G) \\ w\sim u,\, w\sim v}} 1 = 2\, CP_3 = M_1(G) - 2m,$$

and we obtain by Corollary 2.2

$$\begin{aligned}
\sum_{\substack{u,v \in V(G) \\ u \neq v}} 4\, d_u d_v \Big(\sum_{\substack{w \in V(G) \\ w\sim u,\, w\sim v}} \frac{2\, d_w}{(d_u+d_w)(d_v+d_w)} \Big)^2 &= \sum_{\substack{u,v \in V(G) \\ u \neq v}} \Big(\sum_{\substack{w \in V(G) \\ w\sim u,\, w\sim v}} \frac{2\sqrt{d_u d_w}}{d_u+d_w}\, \frac{2\sqrt{d_v d_w}}{d_v+d_w} \Big)^2 \\
&\ge \sum_{\substack{u,v \in V(G) \\ u \neq v}} \Big(\sum_{\substack{w \in V(G) \\ w\sim u,\, w\sim v}} 1 \Big) \Big(\sum_{\substack{w \in V(G) \\ w\sim u,\, w\sim v}} 1 \Big) \\
&= \sum_{\substack{u,v \in V(G) \\ u \neq v}} \Big(\sum_{\substack{w \in V(G) \\ w\sim u,\, w\sim v}} 1 \Big) \big|N(u) \cap N(v)\big| \qquad (2.5) \\
&\ge \Delta \sum_{\substack{u,v \in V(G) \\ u \neq v}} \; \sum_{\substack{w \in V(G) \\ w\sim u,\, w\sim v}} 1 \\
&= \Delta \big(M_1(G) - 2m \big).
\end{aligned}$$

Note that if $N(u) \cap N(v) = \emptyset$ then $0 = \big(\sum_{w \in V(G),\, w\sim u,\, w\sim v} 1\big)\big(\sum_{w \in V(G),\, w\sim u,\, w\sim v} 1\big) = \sum_{w \in V(G),\, w\sim u,\, w\sim v} 1 = 0$, and otherwise $\big(\sum_{w \in V(G),\, w\sim u,\, w\sim v} 1\big)\big(\sum_{w \in V(G),\, w\sim u,\, w\sim v} 1\big) = \big(\sum_{w \in V(G),\, w\sim u,\, w\sim v} 1\big)\,\|N(u) \cap N(v)\| \ge \sum_{w \in V(G),\, w\sim u,\, w\sim v} 1$. Hence, we have in both cases $\big(\sum_{w \in V(G),\, w\sim u,\, w\sim v} 1\big)\big(\sum_{w \in V(G),\, w\sim u,\, w\sim v} 1\big) \ge \sum_{w \in V(G),\, w\sim u,\, w\sim v} 1$. This fact and Corollary 2.2 (taking $a = \delta$ and $b = \Delta$)

give

$$\begin{aligned}
\sum_{\substack{u,v\in V(G)\\ u\nsim v}} 4\, d_u d_v \Big(\sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\, d_w}{(d_u+d_w)(d_v+d_w)} \Big)^2 &= \sum_{\substack{u,v\in V(G)\\ u\nsim v}} \Big(\sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\sqrt{d_u d_w}}{d_u+d_w}\,\frac{2\sqrt{d_v d_w}}{d_v+d_w} \Big)^2 \\
&\ge \frac{16\Delta^2\delta^2}{(\Delta+\delta)^4} \sum_{\substack{u,v\in V(G)\\ u\nsim v}} \Big(\sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} 1 \Big) \Big(\sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} 1 \Big) \\
&\ge \frac{16\Delta^2\delta^2}{(\Delta+\delta)^4} \sum_{\substack{u,v\in V(G)\\ u\nsim v}} \sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} 1 \\
&= \frac{16\Delta^2\delta^2}{(\Delta+\delta)^4} \big(M_1(G) - 2m \big).
\end{aligned} \tag{2.6}$$

Lemma 2.8 and (2.5) give

$$\begin{aligned}
tr(\mathcal{D}^4) &= \sum_{u\in V(G)} \Big(\sum_{\substack{v\in V(G)\\ v\sim u}} \frac{4\, d_u d_v}{(d_u+d_v)^2} \Big)^2 + \sum_{\substack{u,v\in V(G)\\ u\nsim v}} 4\, d_u d_v \Big(\sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\, d_w}{(d_u+d_w)(d_v+d_w)} \Big)^2 \\
&\ge \sum_{u\in V(G)} \Big(\sum_{\substack{v\in V(G)\\ v\sim u}} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \Big)^2 + \Delta \big(M_1(G) - 2m \big) \\
&\ge \sum_{u\in V(G)} \Big(\sum_{\substack{v\in V(G)\\ v\sim u}} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \Big) \Big(\sum_{\substack{v\in V(G)\\ v\sim u}} 1 \Big) + \Delta \big(M_1(G) - 2m \big) \\
&= \sum_{u\in V(G)} \sum_{\substack{v\in V(G)\\ v\sim u}} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\, d_u + \Delta \big(M_1(G) - 2m \big) \\
&\ge 2 \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\, \Delta + \Delta \big(M_1(G) - 2m \big) \\
&= 2\Delta\, GA_1(G) + \Delta \big(M_1(G) - 2m \big).
\end{aligned}$$

Using (2.6) instead of (2.5) and Corollary 2.2 (taking $a=\delta$ and $b=\Delta$), we obtain

$$
\begin{aligned}
tr(\mathcal{D}^4) &= \sum_{u\in V(G)} \Big(\sum_{\substack{v\in V(G)\\ v\sim u}} \frac{4\, d_u d_v}{(d_u+d_v)^2} \Big)^2 + \sum_{\substack{u,v\in V(G)\\ u\neq v}} 4\, d_u d_v \Big(\sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\, d_w}{(d_u+d_w)(d_v+d_w)} \Big)^2 \\
&\ge \sum_{u\in V(G)} \Big(\frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \sum_{\substack{v\in V(G)\\ v\sim u}} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \Big)^2 + \frac{16\Delta^2\delta^2}{(\Delta+\delta)^4} \big(M_1(G) - 2m \big) \\
&\ge \frac{4\Delta\delta}{(\Delta+\delta)^2} \sum_{u\in V(G)} \Big(\sum_{\substack{v\in V(G)\\ v\sim u}} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \Big) \Big(\sum_{\substack{v\in V(G)\\ v\sim u}} \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \Big) + \frac{16\Delta^2\delta^2}{(\Delta+\delta)^4} \big(M_1(G) - 2m \big) \\
&= \frac{8\Delta^{3/2}\delta^{3/2}}{(\Delta+\delta)^3} \sum_{u\in V(G)} \sum_{\substack{v\in V(G)\\ v\sim u}} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\, d_u + \frac{16\Delta^2\delta^2}{(\Delta+\delta)^4} \big(M_1(G) - 2m \big) \\
&\ge \frac{8\Delta^{3/2}\delta^{3/2}}{(\Delta+\delta)^3} \cdot 2 \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\, \delta + \frac{16\Delta^2\delta^2}{(\Delta+\delta)^4} \big(M_1(G) - 2m \big) \\
&= \frac{16\Delta^{3/2}\delta^{5/2}}{(\Delta+\delta)^3}\, GA_1(G) + \frac{16\Delta^2\delta^2}{(\Delta+\delta)^4} \big(M_1(G) - 2m \big).
\end{aligned}
$$

If the equality is attained in the lower bound, then $d_u=\Delta$ for every $u\in V(G)$, and so G is regular. Furthermore, we have either $G=P_2$ or $|N(u)\cap N(v)|=\Delta$ for every $u,v,w\in V(G)$ with $w\sim u$ and $w\sim v$, by (2.5). Hence, in both cases we have either $N(u)\cap N(v)=\emptyset$ or $N(u)=N(v)$ for each $u,v\in V(G)$. If G is not $P_2=K_{1,1}$, then fix $u,v,w\in V(G)$ with $w\sim u$, $w\sim v$; hence, $N(u)=N(v)$. Let $N(u)=N(v)=\{w_1,w_2,\dots,w_\Delta\}$ with $w_1=w$. Fix $2\le j\le\Delta$. Since $\emptyset\neq\{u,v\}\subseteq N(w_1)\cap N(w_2)$, we have $N(w_1)=N(w_j)=\{u,v,z_3,\dots,z_\Delta\}$. Since $N(w_1)$ does not depend on j, we have $N(w_1)=N(w_2)=\cdots=N(w_\Delta)=\{u,v,z_3,\dots,z_\Delta\}$. Since $\{w_1,w_2,\dots,w_\Delta\}\subseteq N(z_3)\cap\cdots\cap N(z_\Delta)$, we obtain $N(z_3)=\cdots=N(z_\Delta)=\{w_1,w_2,\dots,w_\Delta\}$, and so G is a Δ-regular bipartite graph with parts $\{w_1,w_2,\dots,w_\Delta\}$ and $\{u,v,z_3,\dots,z_\Delta\}$. Hence, G is isomorphic to the complete bipartite graph $K_{\Delta,\Delta}$.

Conversely, if G is isomorphic to the complete bipartite graph $K_{\Delta,\Delta}$ with $\Delta\ge 1$, then G is regular and $N(u)\cap N(v)=\emptyset$ or $N(u)=N(v)$ for each $u,v\in V(G)$, and so every inequality in the proof of the lower bound is an equality.

If the equality is attained in the upper bound, then we have $d_u=\delta$ for every $u\in V(G)$, and so G is regular. Furthermore, we have either $G=P_2$ or for every $u,v,w\in V(G)$ with $w\sim u$ and $w\sim v$ we have $|N(u)\cap N(v)|=1$, by (2.6). Hence, in both cases we have $|N(u)\cap N(v)|\in\{0,1\}$ for any $u,v\in V(G)$, and so G does not have cycles of length 4.

Conversely, if G is a regular graph without cycles of length 4, then G is regular and $|N(u)\cap N(v)|\in\{0,1\}$ for any $u,v\in V(G)$, and so every inequality in the proof of the upper bound is an equality. □

3. Geometric-arithmetic energy

Recall that we denote by $\lambda_1\ge\cdots\ge\lambda_n$ and $\mu_1\ge\cdots\ge\mu_n$ the ordered eigenvalues of A and $\mathcal{D}$, respectively. It is well known (see, e.g., [6]) that $\sum_{j=1}^n \lambda_j^k$ is equal to the number of closed walks of length k in the graph G.

The energy of the graph G is defined in [19] as $E(G)=\sum_{j=1}^n |\lambda_j|$.

The *geometric-arithmetic energy* (GA energy) of the graph G is defined in an analogue way as

$$GAE(G)=\sum_{j=1}^n |\mu_j|.$$

It is usual and useful to define modified energies as matching energy, Randić energy, Laplacian energy, Laplacian-energy-like, incidence energy, skew energy, etc. (see, e.g., [4], [5], [7], [8], [12], [13], [14], [21], [28], [29], [30] and [47]). These modified energies have applications in theoretical organic chemistry [35], image processing [42] and information theory [26].

The following result appears in [39, Corollary 3.6].

Lemma 3.1. *We have for any graph G the inequality $\mu_1 \geq n - 1$.*

Theorem 2.7 and Lemma 3.1 have the following consequence.

Corollary 3.2. *We have for any graph G the inequality $GAE(G) \geq n(n-1)$.*

The following result is well known.

Lemma 3.3. *We have for any complete graph $\lambda_1 = n - 1$ and $\lambda_j = -1$ for every $2 \geq j \geq n$.*

Since for any regular graph we have $\lambda_j = \mu_j$ for every $1 \geq j \geq n$, we obtain the following consequences.

Corollary 3.4. *We have for any complete graph $\mu_1 = n - 1$ and $\mu_j = -1$ for every $2 \geq j \geq n$.*

Corollary 3.5. *For any complete graph G we have $GAE(G) = 2(n-1)$.*

We will use the following Ozeki's inequality [33].

Lemma 3.6. *If $0 \geq N_1 \geq x_1, \dots, x_n \geq N_2$, then $\frac{1}{n}\left(x_1^2 + \cdots + x_n^2\right) - \left(\frac{x_1+\cdots+x_n}{n}\right)^2 \geq \frac{1}{4}(N_2 - N_1)^2$.*

Theorem 3.7. *We have for any graph G*

$$\sqrt{n\, tr\left(\mathcal{D}^2\right) - \frac{1}{4}n^2(\mu_1 - \mu^{\leq})^2} \geq GAE(G) \geq \sqrt{n\, tr\left(\mathcal{D}^2\right)},$$

where $\mu^{\leq} = \min_{1 \leq j \leq n} |\mu_j|$.

Proof. Since $\mu_1^2, \dots, \mu_n^2$ are the eigenvalues of $\mathcal{D}^2$, Cauchy-Schwarz inequality gives

$$GAE(G) = \sum_{j=1}^{n} |\mu_j| \geq \left(\sum_{j=1}^{n} 1\right)^{1/2} \left(\sum_{j=1}^{n} \mu_j^2\right)^{1/2} = \sqrt{n\, tr\left(\mathcal{D}^2\right)}.$$

Since $\mu^{\leq} \geq |\mu_j| \geq \mu_1$ for every $1 \geq j \geq n$, Lemma 3.6 gives

$$\frac{1}{n}\, tr\left(\mathcal{D}^2\right) - \frac{1}{n^2}\, GAE(G)^2 = \frac{1}{n}\left(\mu_1^2 + \cdots + \mu_n^2\right) - \left(\frac{|\mu_1| + \cdots + |\mu_n|}{n}\right)^2 \geq \frac{1}{4}(\mu_1 - \mu^{\leq})^2,$$

and this implies the first inequality. □

We need the following lemma in order to obtain a lower bound of the GA energy involving $tr\left(\mathcal{D}^2\right)$ and $tr\left(\mathcal{D}^4\right)$.

Lemma 3.8. *For every $a_1, \dots, a_n \infty 0$, we have $\left(\sum_{j=1}^n a_j^2\right)^{3/2} \geq \left(\sum_{j=1}^n a_j\right)\left(\sum_{j=1}^n a_j^4\right)^{1/2}$.*

Proof. Fix $a_1, \dots, a_n \infty 0$. Applying Hölder's inequality with exponents $p = 3/2$ and $q = 3$, we obtain

$$\sum_{j=1}^{n} a_j^2 = \sum_{j=1}^{n} a_j^{2/3} a_j^{4/3} \geq \left(\sum_{j=1}^{n} \left(a_j^{2/3}\right)^{3/2}\right)^{2/3} \left(\sum_{j=1}^{n} \left(a_j^{4/3}\right)^{3}\right)^{1/3} = \left(\sum_{j=1}^{n} a_j\right)^{2/3} \left(\sum_{j=1}^{n} a_j^4\right)^{1/3}$$

and the inequality holds. □

Theorem 3.9. *We have for any graph G, $GAE(G) \infty \sqrt{\frac{tr\left(\mathcal{D}^2\right)^3}{tr\left(\mathcal{D}^4\right)}}$.*

Proof. Since $\mu_1^2, \dots, \mu_n^2$ and $\mu_1^4, \dots, \mu_n^4$ are the eigenvalues of $\mathcal{D}^2$ and $\mathcal{D}^4$, respectively, Lemma 3.8 gives

$$\Big(\sum_{j=1}^{n} \mu_j^2 \Big)^{3/2} \le \Big(\sum_{j=1}^{n} |\mu_j| \Big) \Big(\sum_{j=1}^{n} \mu_j^4 \Big)^{1/2},$$

$$tr\big(\mathcal{D}^2\big)^{3/2} \le GAE(G)\; tr\big(\mathcal{D}^4\big)^{1/2}.$$

□

The following result appears in [43, Theorem 2].

Theorem 3.10. *If $p \ge 1$ is an integer and $0 \le x_1, \dots, x_n \le n-1$, then*

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

We will use also the following particular case of Jensen's inequality.

Lemma 3.11. *If f is a convex function in $\mathbb{R}_+$ and $x_1, \dots, x_m > 0$, then*

$$f\Big(\frac{x_1 + \cdots + x_n}{n} \Big) \le \frac{1}{n} \big(f(x_1) + \cdots + f(x_n) \big).$$

Next, we obtain several lower bounds of $GAE(G)$ involving $tr(\mathcal{D}^2)$ and $\det \mathcal{D}$.

Theorem 3.12. *We have for any graph G, $GAE(G) \ge \frac{tr(\mathcal{D}^2)}{n(n-1)}$.*

Proof. Applying Lemma 3.11 to the convex function $f(x) = x^2$, we obtain

$$\Big(\frac{1}{n} \sum_{j=1}^{n} |\mu_j|^{1/2} \Big)^2 \le \frac{1}{n} \sum_{j=1}^{n} |\mu_j|,$$

$$GAE(G) \ge \frac{1}{n} \Big(\sum_{j=1}^{n} |\mu_j|^{1/2} \Big)^2.$$

Since $|\mu_j| \le \mu_1 \le n-1$ by Lemma 3.1, Theorem 3.10 (with $p = 2$) gives

$$\Big(\sum_{j=1}^{n} |\mu_j|^{1/2} \Big)^2 \ge (n-1)^{-1} \sum_{j=1}^{n} \mu_j^2 = \frac{tr(\mathcal{D}^2)}{n-1},$$

and we obtain the result. □

Theorem 3.13. *We have for any graph G, $GAE(G) \ge \sqrt{tr(\mathcal{D}^2)}$.*

Proof. Since the inequality

$$\sum_{j=1}^{n} x_j^2 \le \Big(\sum_{j=1}^{n} x_j \Big)^2$$

holds for every $x_1, \dots, x_n \ge 0$, we obtain

$$GAE(G)^2 = \Big(\sum_{j=1}^{n} |\mu_j| \Big)^2 \ge \sum_{j=1}^{n} |\mu_j|^2 = tr(\mathcal{D}^2).$$

□

Theorems 2.10, 2.13, 3.7 and 3.13 have the following consequence.

Proposition 3.14. *We have for any graph G*

- $2\sqrt{\frac{n-1}{n}\, GA_1(G)} \le GAE(G) \le \sqrt{2n\, GA_1(G)}$,

$$\subseteq \tfrac{1}{2n}\, GAE(G)^2 + \tfrac{4\Delta\delta}{(\Delta+\delta)^2}\, m(m \quad 1) \geq GA_1(G)^2\,,$$
$$\subseteq GAE(G) \infty 2\sqrt{\tfrac{\Delta\delta}{\Delta+\delta}\, GA_1(G)}\,.$$

Theorem 3.15. *We have for any graph G, $GAE(G) \infty n \big(\det \mathcal{D}\big(^{1/n}$.*

Proof. Since the arithmetic mean is greater than the geometric mean, we deduce

$$\frac{1}{n}\, GAE(G) = \frac{1}{n} \sum_{j=1}^{n} \|\mu_j\| \infty \quad \|\mu_1\| \times\!\times\!\times \|\mu_n\|^{\,1/n} = \big(\det \mathcal{D}\big(^{1/n}.$$

□

Theorem 3.16. *We have for any graph G*

$$GAE(G) \infty \sqrt{tr(\mathcal{D}^2) + n(n \quad 1)\|\det \mathcal{D}\|^{2/n}}\,.$$

Proof. We have

$$GAE(G)^2 = \Big) \sum_{j=1}^{n} \|\mu_j\| \Big\{^2 = \sum_{j=1}^{n} \mu_j^2 + 2 \sum_{1\prime\ i<j\prime\ n} \|\mu_i\mu_j\| = tr(\mathcal{D}^2) + 2 \sum_{1\prime\ i<j\prime\ n} \|\mu_i\mu_j\|.$$

Since the arithmetic mean is greater than the geometric mean, we deduce

$$\frac{2}{n(n \quad 1)} \sum_{1\prime\ i<j\prime\ n} \|\mu_i\mu_j\| \infty \quad \|\mu_1\|^{n \quad 1} \times\!\times\!\times \|\mu_n\|^{n \quad 1\,|\,2/(n(n \quad 1))} = \|\det \mathcal{D}\|^{2/n},$$

and

$$GAE(G)^2 = tr(\mathcal{D}^2) + 2 \sum_{1\prime\ i<j\prime\ n} \|\mu_i\mu_j\| \infty tr(\mathcal{D}^2) + n(n \quad 1)\|\det \mathcal{D}\|^{2/n}.$$

□

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Departamento de Matemáticas, Universidad Carlos III de Madrid, Avenida de la Universidad 30, 28911 Leganés, Madrid, Spain
E-mail address jomaro@math.uc3m.es

Facultad de Matemáticas, Universidad Autónoma de Guerrero, Carlos E. Adame No.54 Col. Garita, 39650 Acalpulco Gro., Mexico
E-mail address jsmathguerrero@gmail.com