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Spectral study of the Geometric–Arithmetic Index

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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.

1 Introduction

The study of topological indices is a subject of increasing interest, both in pure and applied mathematics. Topological indices are interesting since they capture some of the properties of a molecule (or a graph) in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener [23] in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes.

Topological indices based on end-vertex degrees of edges have been used over 40 years. Probably, the best know such descriptor is the Randić connectivity index, denoted by R (see [18, 19]). There are more than thousand papers and a couple of books dealing with this index (see, e.g., [11, 14, 15] and the references therein). Trying to improve the predictive power of the Randić index, scientists have introduced a large number of topological indices. The first geometric–arithmetic index GA_1, defined in [22] as

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

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 five years ago, there are many papers dealing with this index (see, e.g., [4–7, 10, 17, 20–22, 25] and the references cited therein). There are other geometric–arithmetic indices, like $Z_{p,q}$ ($Z_{0,1} = GA_1$), but the results in [5, p.598] show empirically that the GA_1 index gathers the same information on observed molecules 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 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 [5, 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.

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, 2, 9]. 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 [9]. 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, denoted by $\mathcal{A}$, that is a modification of the classical adjacency matrix involving the degrees of the vertices. Besides, we will use the known sum–connectivity matrix in order to obtain more algebraic properties of GA_1 in Section 2.

We begin by stating some notation. Throughout this paper, $G = (V, E) = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) connected graph of order $n = |V(G)|$ and size $m = |E(G)|$ with $E(G) \neq \emptyset$. We denote two adjacent vertices u and v by $u \sim v$. For a vertex $u \in V$ we denote $N(v) = \{u \in V : u \sim v\}$. The degree of a vertex $v \in V$ will be denoted by $d_v = |N(v)|$. We denote by δ and Δ the minimum and maximum degree of the graph, respectively. We use the classical notation uv for the edge of a graph joining the vertices u and v. 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.

2 The Sum–Connectivity Matrix and GA_1

We will need the following classical result, which provides a converse of Cauchy–Schwarz inequality (see [13, p.62]).

Lemma 2.1. *If $0 < n_1 \leq a_j \leq N_1$ and $0 < n_2 \leq b_j \leq N_2$ for $1 \leq j \leq k$, then*

$$\Big(\sum_{j=1}^{k} a_j^2\Big)^{1/2}\Big(\sum_{j=1}^{k} b_j^2\Big)^{1/2} \leq \frac{1}{2}\left(\sqrt{\frac{N_1N_2}{n_1n_2}} + \sqrt{\frac{n_1n_2}{N_1N_2}}\right)\Big(\sum_{j=1}^{k} a_jb_j\Big).$$

We also need the following result (see [20]).

Lemma 2.2. *Let g be the function $g(x,y) = \frac{2\sqrt{xy}}{x+y}$ with $0 < a \leq x, y \leq b$. Then*

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

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 $x = y$.

The Sum-Connectivity Matrix $\mathcal{S} = \mathcal{S}(G)$ of the graph G is defined as the matrix with entries (see [29]):

$$S_{uv} := \begin{cases} \frac{1}{\sqrt{d_u+d_v}}, & \text{if } uv \in E(G), \\ 0, & \text{otherwise.} \end{cases}$$

We will denote by $tr(A)$ the trace of the matrix A.

Theorem 2.3. *We have for any graph G*

$$\delta\, tr(\mathcal{S}^2) \le GA_1(G) \le \Delta\, tr(\mathcal{S}^2),$$

and the equality in each inequality holds if and only if G is regular.

Proof. Since the i-th entry β_{ii} in the diagonal of $\mathcal{S}^2$ is

$$\beta_{ii} = \sum_{\substack{1\le j\le n \\ v_i v_j \in E(G)}} \frac{1}{d_{v_i} + d_{v_j}}\,,$$

we deduce

$$tr(\mathcal{S}^2) = \sum_{i=1}^{n} \beta_{ii} = \sum_{i=1}^{n} \sum_{\substack{1\le j\le n \\ v_i v_j \in E(G)}} \frac{1}{d_{v_i} + d_{v_j}} = \sum_{uv\in E(G)} \frac{2}{d_u + d_v}\,.$$

Then we have

$$GA_1(G) = \sum_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} \ge \delta \sum_{uv\in E(G)} \frac{2}{d_u + d_v} = \delta\, tr(\mathcal{S}^2),$$

$$GA_1(G) = \sum_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} \le \Delta \sum_{uv\in E(G)} \frac{2}{d_u + d_v} = \Delta\, tr(\mathcal{S}^2).$$

If $GA_1(G) = \delta\, tr(\mathcal{S}^2)$ (respectively, $GA_1(G) = \Delta\, tr(\mathcal{S}^2)$), then $\sqrt{d_u d_v} = \delta$ for every $uv \in E(G)$ and we conclude $d_u = \delta$ (respectively, $d_u = \Delta$) for every $u \in V(G)$. Reciprocally, if G is regular, then the lower and upper bound are the same, and they are equal to $GA_1(G)$. ∎

We deal now with an additional topological descriptor, called *harmonic* index, defined as

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

This index has attracted a great interest in the lasts years (see, e.g., [8, 24, 27, 28]).

Notice that

$$tr(\mathcal{S}^2) = \sum_{uv\in E(G)} \frac{2}{d_u + d_v} = H(G).$$

Thus, we have the following corollary (see [20]).

Corollary 2.4. *We have for any graph G*

$$\delta\, H(G) \le GA_1(G) \le \Delta\, H(G),$$

and the equality in each inequality holds if and only if G is regular.

We will denote by $M_1(G)$ and $M_2(G)$ the first and the second Zagreb indices of the graph G, respectively, defined in [12] as

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

These indices have attracted growing interest, see e.g., [3, 4, 12, 16] (in particular, they are included in a number of programs used for the routine computation of topological indices).

Theorem 2.5. *We have for any graph G*

$$\frac{2\delta\sqrt{\Delta M_2(G)\, tr(\mathcal{S}^2)}}{\Delta^2+\delta^2} \le GA_1(G) \le \sqrt{\frac{M_2(G)\, tr(\mathcal{S}^2)}{\delta}}\,,$$

and the equality in each inequality holds if and only if G is regular.

Proof. Cauchy-Schwarz inequality gives

$$\begin{aligned} GA_1(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \le \Big(\sum_{uv \in E(G)} d_u d_v\Big)^{1/2} \Big(\sum_{uv \in E(G)} \frac{4}{(d_u+d_v)^2}\Big)^{1/2} \\ &\le \big(M_2(G)\big)^{1/2} \Big(\frac{1}{\delta} \sum_{uv \in E(G)} \frac{2}{d_u+d_v}\Big)^{1/2} = \sqrt{\frac{M_2(G)\, tr(\mathcal{S}^2)}{\delta}}\,. \end{aligned}$$

If the equality holds, then $\frac{1}{2}(d_u+d_v)=\delta$ for every $uv \in E(G)$ and we conclude $d_u = \delta$ for every $u \in V(G)$.

Since

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

Lemma 2.1 gives

$$\begin{aligned} GA_1(G) &= \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \ge \frac{\Big(\sum_{uv \in E(G)} d_u d_v\Big)^{1/2} \Big(\sum_{uv \in E(G)} \frac{4}{(d_u+d_v)^2}\Big)^{1/2}}{\frac{1}{2}\Big(\frac{\Delta}{\delta}+\frac{\delta}{\Delta}\Big)} \\ &\ge \frac{2\Delta\delta\big(M_2(G)\big)^{1/2}\Big(\frac{1}{\Delta}\sum_{uv \in E(G)} \frac{2}{d_u+d_v}\Big)^{1/2}}{\Delta^2+\delta^2} = \frac{2\delta\sqrt{\Delta M_2(G)\, tr(\mathcal{S}^2)}}{\Delta^2+\delta^2}\,. \end{aligned}$$

If the equality holds, then $\frac{1}{2}(d_u+d_v)=\Delta$ for every $uv \in E(G)$ and we conclude $d_u = \Delta$ for every $u \in V(G)$.

Reciprocally, if G is regular, then both bounds have the same value, and they are equal to $GA_1(G)$. ∎

Corollary 2.6. *We have for any graph G*

$$\frac{2\delta\sqrt{\Delta M_2(G)\,H(G)}}{\Delta^2+\delta^2} \le GA_1(G) \le \sqrt{\frac{M_2(G)\,H(G)}{\delta}}\,,$$

and the equality in each inequality holds if and only if G is regular.

3 The Geometric–Arithmetic Matrix and GA_1

Given a graph G, let us define the geometric–arithmetic Matrix $\mathcal{A}$ with entries

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

We start with the following elementary result which allows to obtain new bounds for $GA_1(G)$.

Lemma 3.1. *We have for any graph*

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

Proof. Since every element in the main diagonal of $\mathcal{A}$ is 0, we obtain $tr(\mathcal{A}) = 0$.

Since the i-th entry α_{ii} in the diagonal of $\mathcal{A}^2$ is

$$\alpha_{ii} = \sum_{\substack{1\le j\le n\\ v_iv_j\in E(G)}} \frac{4\,d_{v_i}d_{v_j}}{(d_{v_i}+d_{v_j})^2}\,,$$

we have

$$tr(\mathcal{A}^2) = \sum_{i=1}^n \alpha_{ii} = \sum_{i=1}^n \sum_{\substack{1\le j\le n\\ v_iv_j\in E(G)}} \frac{4\,d_{v_i}d_{v_j}}{(d_{v_i}+d_{v_j})^2} = 2\sum_{uv\in E(G)} \frac{4\,d_u d_v}{(d_u+d_v)^2}\,.$$

One can check in a similar way the last equality. ■

Proposition 3.2. *We have for any graph G*

$$\frac{\delta^2 tr(\mathcal{A}^2)}{2} \le M_2(G) \le \frac{\Delta^2 tr(\mathcal{A}^2)}{2}.$$

Furthermore, the equality in each inequality is attained if and only if G is a regular graph.

Proof. We deduce the inequalities

$$\frac{1}{\Delta^2}\, M_2(G) = \frac{1}{\Delta^2} \sum_{uv\in E(G)} d_u d_v \le \sum_{uv\in E(G)} \frac{4 d_u d_v}{(d_u+d_v)^2} \le \frac{1}{\delta^2} \sum_{uv\in E(G)} d_u d_v = \frac{1}{\delta^2}\, M_2(G).$$

If G is a regular graph, then both bounds have the same value, and they are equal to

$$\frac{tr(\mathcal{A}^2)}{2} = m.$$

If the first inequality is attained, then $\frac{1}{2}(d_u+d_v) = \delta$ for every $uv \in E(G)$ and thus $d_u = \delta$ for every $u \in V(G)$. If the second inequality is attained, then $\frac{1}{2}(d_u + d_v) = \Delta$ for every $uv \in E(G)$ and $d_u = \Delta$ for every $u \in V(G)$. ■

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.

Theorem 3.3. *We have for any graph G*

$$\frac{1}{2}\, tr(\mathcal{A}^2) \le GA_1(G) \le \frac{(\Delta+\delta)\, tr(\mathcal{A}^2)}{4\sqrt{\Delta\delta}}\,.$$

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 either regular or (Δ, δ)-biregular.

Proof. By Lemma 2.2, taking $a = \delta$ and $b = \Delta$, we have

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

Thus Lemma 3.1 gives

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

and

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

By Lemma 2.2, the equality in the upper bound is attained 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.

The equality in the lower bound holds, by Lemma 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.

■

Denote by A the adjacency matrix of a graph. Since the adjacency matrix A and $\mathcal{A}$ are real symmetric matrices, their eigenvalues are real numbers. Denote by $\lambda_1 \geq \cdots \geq \lambda_n$ and $\mu_1 \geq \cdots \geq \mu_n$ the ordered eigenvalues of A and $\mathcal{A}$, respectively.

Theorem 3.4. *For any graph G the inequalities*

$$\frac{\mu_1^2 n}{2(n-1)} \leq GA_1(G) \leq \frac{1}{2}\,\mu_1 n$$

hold. Furthermore, the equality in the lower bound is attained for every complete graph and the equality in the upper bound is attained for every regular graph.

Proof. Denote by $\mathbf{j}$ the vector $\mathbf{j} = (1, 1, \ldots, 1) \in \mathbb{R}^n$. Since $\mathcal{A}$ is non–negative and irreducible (we just consider connected graphs) Perron–Frobenius Theorem gives $\mu_1 \geq |\mu_j|$ for every j and then $\mu_1 > 0$. Hence, using Rayleigh quotient, we obtain

$$\mu_1 = \max_{\mathbf{x}\neq 0} \frac{\langle \mathcal{A}\mathbf{x}, \mathbf{x}\rangle}{\|\mathbf{x}\|^2} \geq \frac{\langle \mathcal{A}\mathbf{j}, \mathbf{j}\rangle}{\|\mathbf{j}\|^2} = \frac{2\,GA_1(G)}{n}\,.$$

Since $\sum_{i=1}^n \mu_i = tr(\mathcal{A}) = 0$, we have $\mu_1 = -\sum_{i=2}^n \mu_i$ and Cauchy-Schwarz inequality gives

$$\mu_1^2 = \Big(\sum_{i=2}^n \mu_i\Big)^2 \leq \Big(\sum_{i=2}^n \mu_i^2\Big)(n-1), \qquad \sum_{i=1}^n \mu_i^2 = \mu_1^2 + \sum_{i=2}^n \mu_i^2 \geq \mu_1^2 + \frac{\mu_1^2}{n-1} = \frac{n\mu_1^2}{n-1}\,.$$

We have by Theorem 3.3

$$\frac{n\mu_1^2}{n-1} \leq \sum_{i=1}^n \mu_i^2 = tr(\mathcal{A}^2) \leq 2\,GA_1(G).$$

Assume now that G is a Δ-regular graph. Then $\mathcal{A}$ is equal to the adjacency matrix. It is well known that the greatest eigenvalue λ_1 of the adjacency matrix of a Δ-regular graph is equal to Δ. Hence, $\mu_1 = \Delta$ and $GA_1(G) = m = \frac{1}{2}\,\Delta n = \frac{1}{2}\,\lambda_1 n = \frac{1}{2}\,\mu_1 n$.

Assume now that G is a complete graph K_n, thus G is a $(n-1)$-regular graph and $\lambda_1 = \mu_1 = n-1$. Hence,

$$\frac{\mu_1^2 n}{2(n-1)} = \frac{n(n-1)}{2} = m = GA_1(G).$$

∎

The argument in the proof of Theorem 3.4 gives, in fact, the following result.

Corollary 3.5. *We have for any graph G*

$$\mu_1 \leq \sqrt{\frac{(n-1)tr(\mathcal{A}^2)}{n}}\,.$$

We also have the following consequence.

Corollary 3.6. *We have for any graph G the inequality $\mu_1 \leq n-1$.*

We will need the following lemma (see [20]).

Lemma 3.7. *We have for any graph G*

$$\sum_{uv \in E(G)} \frac{1}{d_u + d_v} \geq \frac{m^2}{M_1(G)}\,.$$

Proposition 3.8. *We have for any graph G*

$$\frac{8m^2\sqrt{\Delta\delta^3}}{(\Delta+\delta)tr(\mathcal{A}^2)} \leq M_1(G),$$

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

Proof. By Lemma 3.1,

$$tr(\mathcal{A}^2) = \sum_{uv \in E(G)} \frac{8d_ud_v}{(d_u+d_v)^2}\,.$$

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

$$\frac{2\sqrt{d_ud_v}}{d_u+d_v} \geq \frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\,,$$

and we obtain by Lemma 3.7

$$tr(\mathcal{A}^2) \geq \frac{8\sqrt{\Delta\delta}}{\Delta+\delta} \sum_{uv \in E(G)} \frac{\sqrt{d_ud_v}}{d_u+d_v} \geq \frac{8\sqrt{\Delta\delta^3}}{\Delta+\delta} \sum_{uv \in E(G)} \frac{1}{d_u+d_v} \geq \frac{8m^2\sqrt{\Delta\delta^3}}{(\Delta+\delta)M_1(G)}\,.$$

If the equality is attained, then $\sqrt{d_ud_v} = \delta$ for every $uv \in E(G)$ and thus $d_u = \delta$ for every $u \in V(G)$. If G is regular, then $M_1(G) = n\Delta^2 = 2m\Delta$, $tr(\mathcal{A}^2) = 2m$ and we have the equality. ∎

Denote by σ^2 the variance of the sequence of the terms $\left\{\frac{2\sqrt{d_ud_v}}{d_u+d_v}\right\}$ appearing in the definition of $GA_1(G)$.

Theorem 3.9. *We have for any graph G*

$$GA_1(G) = \sqrt{\frac{1}{2}\,m\,tr(\mathcal{A}^2) - m^2\sigma^2}\,.$$

Proof. Lemma 3.1 gives

$$\frac{1}{2}\,tr(\mathcal{A}^2) = \sum_{uv\in E(G)} \frac{4d_ud_v}{(d_u+d_v)^2}\,.$$

By the definition of σ^2, we have

$$\sigma^2 = \frac{1}{m}\sum_{uv\in E(G)}\Big(\frac{2\sqrt{d_ud_v}}{d_u+d_v}\Big)^2 - \Big(\frac{1}{m}\sum_{uv\in E(G)}\frac{2\sqrt{d_ud_v}}{d_u+d_v}\Big)^2 = \frac{1}{2m}\,tr(\mathcal{A}^2) - \frac{1}{m^2}\,GA_1(G)^2,$$

and this equality implies the result. ■

Theorem 3.10. *We have for any graph G*

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

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

Proof. Lemma 3.1 gives

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

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

$$\frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \le \frac{2\sqrt{d_ud_v}}{d_u+d_v} \le 1,$$

and we obtain

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

If G is a regular graph, then $tr(\mathcal{A}^2) = 2m$. Thus,

$$\frac{1}{2}\,tr(\mathcal{A}^2) + \frac{4\Delta\delta}{(\Delta+\delta)^2}\,m(m-1) = \frac{1}{2}\,tr(\mathcal{A}^2) + m(m-1) = m + m(m-1) = m^2 = GA_1(G)^2.$$

Assume now that the equality in the second inequality is attained. If G has just an edge, then G is 1-regular. Assume now that G has at least two edges. Hence,

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v}\,\frac{2\sqrt{d_x d_y}}{d_x + d_y} = 1$$

for every $uv \neq xy$. Since G has at least two edges, $\frac{1}{2}(d_u+d_v) = \sqrt{d_u d_v}$ for every $uv \in E(G)$, thus $d_u = d_v$ for every $uv \in E(G)$ and G is regular, since it is connected. ■

The well–known inequality

$$GA_1(G) \leq \frac{\sqrt{mM_2(G)}}{\delta}$$

was proved in [6] (see also [5, p.611]). Using a similar argument to the one in the proof of Theorem 3.10, we obtain a lower bound of GA_1 involving the second Zagreb index $M_2(G)$.

Proposition 3.11. *We have for any graph G*

$$GA_1(G) \geq \frac{\sqrt{n^2 M_2(G) + 4\Delta^2(n-1)m(m-1)}}{n\Delta}\,.$$

Proof. By Lemma 2.2, taking $a = 1$ and $b = n-1$, we have

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

Lemma 3.1 gives

$$\begin{aligned}
GA_1(G)^2 &= \Big(\sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}\Big)^2 \\
&= \sum_{uv\in E(G)} \frac{4 d_u d_v}{(d_u+d_v)^2} + \sum_{uv\neq xy} \frac{2\sqrt{d_u d_v}}{d_u + d_v}\,\frac{2\sqrt{d_x d_y}}{d_x + d_y} \\
&\geq \frac{1}{\Delta^2}\sum_{uv\in E(G)} d_u d_v + \sum_{uv\neq xy} \frac{4(n-1)}{n^2} \\
&= \frac{M_2(G)}{\Delta^2} + \frac{4(n-1)}{n^2}\,m(m-1) \\
&= \frac{n^2 M_2(G) + 4\Delta^2(n-1)m(m-1)}{n^2\Delta^2}\,.
\end{aligned}$$

■

Theorem 3.12. *We have for any graph G*

$$\frac{1}{2}\sum_{j=1}^{n} \lambda_j \mu_{n-j+1} \leq GA_1(G) \leq \frac{1}{2}\sum_{j=1}^{n} \lambda_j \mu_j.$$

Furthermore, the equality in the second inequality is attained for every regular graph.

Proof. We have $2\,GA_1(G) = tr(A\,\mathcal{A})$, by using a similar argument to the one in the proof of Lemma 3.1, and we obtain both inequalities by using the results in [26] about the trace of a product of matrices.

Assume now that G is a regular graph. Then $\mathcal{A} = A$ and we have

$$\frac{1}{2}\sum_{j=1}^{n}\lambda_j\mu_j = \frac{1}{2}\sum_{j=1}^{n}\mu_j^2 = \frac{1}{2}\,tr(\mathcal{A}^2) = m = GA_1(G),$$

and the equality in the second inequality is attained. ■

Theorem 3.13. *We have for any graph G*

$$GA_1(G) \le \frac{n\,tr(\mathcal{A}^2)}{4\sqrt{n-1}}\,.$$

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

Proof. By Lemma 2.2, taking $a = 1$ and $b = n-1$, we have

$$\frac{2\sqrt{n-1}}{n} \le \frac{2\sqrt{d_u d_v}}{d_u + d_v} \le 1,$$

and Lemma 3.1 gives

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

By Lemma 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. ■

Theorem 3.14. *We have for any graph G*

$$\frac{\delta^2\,tr(\mathcal{A}^3)}{\Delta^2\big(M_1(G) - 2m\big)} \le GA_1(G) \le \frac{\Delta^2\,tr(\mathcal{A}^3)}{\delta^2\big(M_1(G) - 2m\big)}\,,$$

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

Proof. Denote by CP_3 the cardinality of the set of paths of length 2 in G. For any fixed $w \in E(G)$, the set of paths of length 2 which have w as central vertex has cardinality $\frac{1}{2}\,d_w(d_w - 1)$. Hence,

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

$$\sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}}\frac{2\,d_w}{(d_u + d_w)(d_v + d_w)} \le \sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}}\frac{2\Delta}{4\delta^2} = \frac{\Delta}{4\delta^2}\,2\,CP_3 = \frac{\Delta}{4\delta^2}\big(M_1(G) - 2m\big), \qquad (3.1)$$

$$\sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\,d_w}{(d_u+d_w)(d_v+d_w)} \ge \sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\delta}{4\Delta^2} = \frac{\delta}{4\Delta^2}\,2\,CP_3 = \frac{\delta}{4\Delta^2}\big(M_1(G)-2m\big). \quad (3.2)$$

Thus, Lemma 3.1 and (3.1) give

$$\begin{aligned} tr(\mathcal{A}^3) &= 2\sum_{uv\in E(G)} \frac{4\,d_u d_v}{d_u+d_v} \sum_{\substack{w\in V(G)\\ w\sim u,\, w\sim v}} \frac{2\,d_w}{(d_u+d_w)(d_v+d_w)} \\ &\le 2\sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\, 2\sqrt{d_u d_v}\,\frac{\Delta}{4\delta^2}\big(M_1(G)-2m\big) \\ &\le \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}\,\Delta\,\frac{\Delta}{\delta^2}\big(M_1(G)-2m\big) \\ &= \frac{\Delta^2}{\delta^2}\big(M_1(G)-2m\big)\,GA_1(G). \end{aligned}$$

Using (3.2) instead of (3.1), we obtain

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

If the graph is regular, then the lower and upper bound are the same, and they are equal to $GA_1(G)$.

If we have the equality in the lower 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 the graph is regular.

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. ■

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