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Comparing the Geometric–Arithmetic Index and the Spectral Radius of Graphs

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Abstract

The geometric-arithmetic index GA of a graph G is the sum of ratios, over all edges of G, of the geometric mean to the arithmetic mean of the end vertices degrees of an edge. The spectral radius λ_1 of G is the largest eigenvalue of its adjacency matrix. These two parameters are known to be used as molecular descriptors in chemical graph theory. In the present paper, we compare GA and λ_1 of a connected graph with given order. We prove, among other results, upper and lower bounds on the ratio GA/λ_1 as well as a lower bound on the ratio GA/λ_1^2. In addition, we characterize all extremal graphs corresponding to each of these bounds.

1 Introduction and definitions

We begin by recalling some definitions. In this paper, we consider only simple, undirected and finite graphs, *i.e*, undirected graphs on a finite number of vertices without multiple edges or loops. A graph is denoted by $G = G(V, E)$, where V is its vertex set and E its edge set. The *order* of G is the number $n = |V|$, its *size* is the number $m = |E|$. For two vertices u and v ($u, v \in V$), if $uv \in E$, we say u and v are *adjacent* in G. The *degree* of a vertex u, denoted d_u, is the number of vertices adjacent to it in G. A graph G is said to be *regular* of degree d, or *d-regular* if $d_u = d$ for every vertex u in G. The minimum,

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average and maximum degrees in a graph G are denoted δ, $\overline{d}$ and Δ, respectively. As usual, P_n, S_n and K_n denote path, cycle and complete graph on n vertices, respectively.

Molecular descriptors play a very important role in mathematical chemistry especially in QSAR (quantitative structure-activity relationship) and/or in QSPR (quantitative structure-property relationship) related studies. Among those descriptors, a special interest is devoted to so-called topological indices. They are used to understand physicochemical properties of chemical compounds in a simple way, since they sum up some of the properties of a molecule in a single number. During the last decades, a large number of topological indices were introduced and found some applications in chemistry, see *e.g.*, [19, 20, 37]. The study of topological indices goes back to the seminal work by Wiener [39] in which he used the sum of all shortest-path distances, nowadays known as the *Wiener index*, of a (molecular) graph for modeling physical properties of alkanes.

Another very important molecular descriptor, was introduced by Randić [29]. It is called the *Randić (connectivity) index* and defined as

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

where d_u denotes the degree (number of neighbors) of u in G. The Randić index is probably the most studied molecular descriptor in mathematical chemistry. Actually, there are more than two thousand papers and five books devoted to that index and its generalizations (see, *e.g.*, [18, 22–25] and the references therein).

Motivated by the definition of Randić connectivity index, Vukičević and Furtula [38] recently proposed the *geometric-arithmetic index*. It is so-called since its definition involves both geometric and arithmetic means of the endpoints degrees of the edges in a graph. For a simple graph G with edge set E, the geometric-arithmetic index GA of a graph G is defined [38] by

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

where d_u denotes the degree of u in G.

It is noted in [38] that the predictive power of GA for physico-chemical properties is somewhat better than the predictive power of the Randić connectivity index. In [38], Vukičević and Furtula gave lower and upper bounds for GA, identified the trees with the minimum and the maximum GA indices, which are the star S_n and the path P_n, respectively. In [40] Yuan, Zhou and Trinajsić gave lower and upper bounds for the GA index of molecular graphs using the numbers of vertices and edges. They also determined the n-vertex molecular trees with the minimum, the second, and the third minimum values of GA, as well as its second and third maximum values. The chemical applicability of the geometric-arithmetic index was highlighted in [14, 17, 38]. Lower and upper bounds on the geometric-arithmetic index in terms of order n, size m, minimum degree δ and/or maximum degree were proved in [30]. Also in [30], GA was compared to other well known topological indices such as the Randić index, the first and second Zagreb indices, the harmonic index and the sum connectivity index. Other lower and upper bounds, on the geometric-arithmetic index, involving the order n the size m, the minimum and the maximum degrees and the second Zagreb index were proved in [13]. In [1], several bounds and comparisons, involving the geometric-arithmetic index and several other graph parameters, are proved. The problem of lower bounding GA over the class of connected graphs with fixed number of vertices and minimum degree was discussed in [15, 33].

The *adjacency matrix* A of G is a 0–1 $n \times n$–matrix indexed by the vertices of G and defined by $a_{ij} = 1$ if and only if $ij \in E$. The (adjacency) eigenvalues of G are those of its adjacency matrix A. According to *Hückel's molecular orbital* (HMO) theory, energy levels of electrons in a molecule correspond to the eigenvalues of the graph representing the molecule. Many chemical properties, such as stability, of a molecule are closely connected to its corresponding eigenvalues (see e.g. [11, ch. 8] and [21]). The largest eigenvalue of the adjacency matrix A of a graph G is called *the spectral radius* of G and denote $\lambda_1 = \lambda_1(G)$. In particular, Lovász and Pelikán [26] suggested the spectral radius of a molecular graph as a measure of branching of the underlying molecule (see also [10, 12]). Many papers and books were devoted to the study of mathematical properties and application of the spectral radius of a graphs. Among these publications, we cite the books [11, 34, 35] and the papers [2, 5–7, 9, 12, 16, 26, 27, 36] as well as the references therein. For results related to spectral properties of the geometric-arithmetic index see [31, 32].

Note that all results proved in the present paper were first obtained as conjectures, or at least tested, with the help of the conjecture-making system in graph theory AutoGraphiX [3, 4, 8].

2 Main results

We first prove an upper bound on the ratio GA/λ_1, over the class of all connected graphs, in terms of the order n.

Proposition 2.1. *For any connected graph G on $n \geq 3$ vertices with spectral radius λ_1*

and geometric-arithmetic index GA,

$$\frac{GA}{\lambda_1} \leq \frac{n}{2}$$

with equality if and only if G is regular.

Proof : Using the fact that $\lambda_1 \geq \overline{d}$ with equality if and only if G is regular (see *e.g.* [11]), we have

$$\frac{GA}{\lambda_1} \leq \frac{GA}{\overline{d}} = \frac{\sum_{ij\in E} \frac{2\sqrt{d_i d_j}}{d_i+d_j}}{\frac{2}{n}\sum_{ij\in E} 1} \leq \frac{\sum_{ij\in E} 1}{\frac{2}{n}\sum_{ij\in E} 1} = \frac{n}{2}.$$

Equality being reached if and only if $d_i = d_j$ for all edges $ij \in E$, *i.e.*, if and only if G is regular. ■

The next bound we prove, which is an improvement of the above proposition, involves the well-known molecular descriptor called *Randić* (*connectivity*) *index.*

Proposition 2.2. *For any connected graph G with spectral radius λ_1, Randić index Ra and geometric-arithmetic index GA,*

$$\frac{GA}{\lambda_1} \leq Ra$$

with equality if and only if G is regular.

Proof : It is proved in [16] that $\lambda_1 \cdot Ra \geq m$. Also, it is easy to see that $GA \leq m$ with equality if and only if G is regular.

Combining these two inequalities, we get

$$\frac{GA}{\lambda_1} \leq \frac{m}{\lambda_1} \leq Ra,$$

which proves the bound.

Equality implies $GA = m$, *i.e*, G is a regular graph. ■

Note that Proposition 2.2 is an improvement of Proposition 2.1 since for any graph G on $n \geq 2$ vertices, $Ra \leq n/2$ with equality if and only if G is regular (see e.g. [28]).

To prove our next result, we need the following Lemma from [27].

Lemma 2.3 ([27]). *If G is a graph on n vertices and m edges with spectral radius λ_1, then $\lambda_1 \leq \sqrt{2m-n+1}$ with equality if and only if G is the star graph S_n or the complete graph K_n.*

We next prove a lower bound on the ratio GA/λ_1 in terms of the number of vertices n. We also characterize the extremal graphs.

Theorem 2.4. *For any connected graph $G = (V, E)$ on $n \geq 3$ vertices with spectral radius λ_1 and geometric-arithmetic index GA,*

$$\frac{GA}{\lambda_1} \geq \frac{2(n-1)}{n}$$

with equality if and only if G is the star S_n.

Proof : We know that (see e.g. [38]) for any edge v_iv_j in G

$$\frac{2\sqrt{d_id_j}}{d_i+d_j} \geq \frac{2\sqrt{n-1}}{n}.$$

Combining this with Lemma 2.3, we get

$$\frac{GA(G)}{\lambda_1} \geq \frac{1}{\sqrt{2m-n+1}} \sum_{ij\in E} \frac{2\sqrt{n-1}}{n} = \frac{2m}{\sqrt{2m-n+1}} \cdot \frac{\sqrt{n-1}}{n}.$$

Now, consider the function $f(x) = 2x/\sqrt{2x-n+1}$. It is increasing (using the derivative) for all $x \geq n-1$, thus reaches its minimum for $x = n-1$. Therefore

$$\frac{GA(G)}{\lambda_1} \geq \frac{2(n-1)}{n}$$

with equality if and only if $m = n-1$ and $\lambda_1 = \sqrt{2m-n+1}$.

From Lemma 2.3, G is the star S_n. ■

We now use λ_1^2 instead of λ_1, and prove an upper bound on the ratio of the geometric-arithmetic index GA to the spectral radius squared λ_1^2. We also characterize the extremal graphs.

Theorem 2.5. *For any connected graph G on $n \geq 7$ vertices with spectral radius λ_1 and geometric-arithmetic index GA,*

$$\frac{GA}{\lambda_1^2} \leq \frac{n}{4}$$

with equality if and only if G is the cycle C_n. Moreover if $2 \leq n \leq 6$, we have

$$\frac{GA}{\lambda_1^2} \leq \frac{n-3+\frac{4\sqrt{2}}{3}}{4\cos^2\frac{\pi}{n+1}}$$

with equality if and only if G is the path P_n.

Proof : If $m \geq n$, where m denotes the number of edges in G, using the inequality $GA \leq m$, and the well-known result (see *e.g.* [11]) $\lambda_1 \geq 2m/n$ with equality if and only if G is regular, we have

$$\frac{GA}{\lambda_1^2} \leq \frac{m}{(2m/n)^2} = \frac{n}{4} \cdot \frac{n}{m} \leq \frac{n}{4}$$

with equality if and only if $m = n$ and G is regular, i.e., G is the cycle C_n.

If $m = n-1$, it is well-known that the path P_n maximizes GA (see [38]), and minimizes λ_1 (see *e.g.* [11]). Recall that

$$GA(P_n) = n - 3 + \frac{4\sqrt{2}}{3} \quad \text{and} \quad \lambda_1(P_n) = 2\cos\frac{\pi}{n+1}.$$

Thus

$$\frac{GA}{\lambda_1^2} \leq \frac{n-3+\frac{4\sqrt{2}}{3}}{4\cos^2\frac{\pi}{n+1}}$$

Now we need to compare both bounds:

$$\frac{n}{4} \qquad \text{and} \qquad \frac{n-3+\frac{4\sqrt{2}}{3}}{4\cos^2\frac{\pi}{n+1}}.$$

Using the Taylor series

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots$$

we get

$$\cos x \geq 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!}$$

and therefore

$$\frac{n-3+\frac{4\sqrt{2}}{3}}{4\cos^2\frac{\pi}{n+1}} \leq \frac{n-3+\frac{4\sqrt{2}}{3}}{4\left(1-\frac{\pi^2}{2!(n+1)^2}+\frac{\pi^4}{4!(n+1)^4}-\frac{\pi^6}{6!(n+1)^6}\right)^2}.$$

Using an online symbolic computational tool, such as *WolframAlpha* (available at *https://www.wolframalpha.com*), we get

$$\frac{n-3+\frac{4\sqrt{2}}{3}}{4\left(1-\frac{\pi^2}{2!(n+1)^2}+\frac{\pi^4}{4!(n+1)^4}-\frac{\pi^6}{6!(n+1)^6}\right)^2} < \frac{n}{4}$$

for all $n \geq 7$. For $2 \leq n \leq 6$, direct calculation shows that

$$\frac{n}{4} < \frac{n-3+\frac{4\sqrt{2}}{3}}{4\cos^2\frac{\pi}{n+1}}.$$

This completes the proof. ■

We next state two conjectures, obtained using AutoGraphiX.

Conjecture 1. *For any connected graph G on $n \geq 13$ vertices with spectral radius λ_1 and geometric-arithmetic index GA,*

$$\frac{GA}{\lambda_1^2} \geq \frac{2\sqrt{n-1}}{n}$$

with equality if and only if G is the star S_n. Moreover, if $2 \leq n \leq 12$, then

$$\frac{GA}{\lambda_1^2} \geq \frac{n}{2(n-1)}$$

with equality if and only if G is the complete graph K_n.

Note that the above conjecture is true over the class of bipartite graphs as well as for regular graphs, as the following results show.

Proposition 2.6. *Let G be a bipartite graph on n vertices. Then*

$$\frac{GA}{\lambda_1^2} \geq \frac{2\sqrt{n-1}}{n}$$

with equality only for the star S_n.

Proof : Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the spectrum of G. It is well-known (see e.g. [11]) that the spectrum of bipartite graph is symmetric with respect to 0, and that (for any graph) $\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_n^2 = 2m$. Thus, we have $\lambda_1^2 \leq m$. In addition as mentioned above, for any edge v_iv_j in G

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} \geq \frac{2\sqrt{n-1}}{n}.$$

Therefore,

$$\frac{GA}{\lambda_1^2} \geq \frac{2m\sqrt{n-1}}{m \cdot n} = \frac{2\sqrt{n-1}}{n}$$

with equality if and only if $\lambda_1 = \sqrt{m}$ and

$$\frac{2\sqrt{d_i d_j}}{d_i + d_j} = \frac{2\sqrt{n-1}}{n}$$

for every edge v_iv_j in G, which corresponds to the star S_n. ■

Proposition 2.7. *Let G be a regular graph on n vertices. Then*

$$\frac{GA}{\lambda_1^2} \geq \frac{n}{2(n-1)}$$

with equality only for the complete graph K_n.

Proof : It is well-known that for a k-regular graph $\lambda_1 = k = 2m/n$ and $GA = m$. Thus

$$\frac{GA}{\lambda_1^2} = \frac{mn^2}{4m^2} = \frac{n}{2k} \geq \frac{n}{2(n-1)}$$

with equality if and only if $k = n-1$, which corresponds to the complete graph K_n. ■

The following conjecture, if true, improves Theorem 2.5.

Conjecture 2. *For any connected graph G on $n \geq 8$ vertices with spectral radius λ_1, Randić index Ra and geometric-arithmetic index GA,*

$$\frac{GA}{\lambda_1^2} \leq \frac{Ra}{2}$$

with equality if and only if G is the cycle C_n.

Note that for $2 \le n \le 7$, the maximum of $GA/(\lambda_1^2 \cdot Ra)$ seems to be attained for the path P_n. In this case, the value of the bound corresponding to the path P_n exceeds that corresponding to the cycle C_n.

The above conjecture is true for connected cyclic graphs, that is, graphs with n vertices and m edges such that $m \ge n$. To show that, we the inequality $\lambda_1 \cdot Ra \ge m$ proved in [16].

Proposition 2.8. *For any connected graph G on $n \ge 3$ vertices and $m \ge n$ edges with spectral radius λ_1, Randić index Ra and geometric-arithmetic index GA,*

$$\frac{GA}{\lambda_1^2} \le \frac{Ra}{2}$$

with equality if and only if G is the cycle C_n.

Proof : We have $GA \le m$ and, from [16], $Ra \ge m/\lambda_1$. Combining both inequalities, we get

$$\frac{GA}{\lambda_1} \le \frac{m}{\lambda_1} \le Ra,$$

therefore

$$\frac{GA}{\lambda_1^2} \le \frac{m}{\lambda_1^2} \le \frac{Ra}{\lambda_1}.$$

It is well know that $\lambda_1 \ge 2m/n$ with equality if and only if G is regular.

Thus, the equality holds if and if G is the cycle C_n.

Then the result follows. ■

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