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On Quotient of Geometric–Arithmetic Index and Square of Spectral Radius

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Abstract

Let $r \geq 2$ be a fixed integer, and x_r the largest positive root of the equation

$$(x-3+2\sqrt{2})\cos^r \frac{\pi}{x+1} = x-3+\frac{4\sqrt{2}}{3}.$$

For a connected graph G on $n > x_r$ vertices with geometric–arithmetic index GA, Randić index Ra and spectral radius λ_1, it is proved that

$$\frac{GA}{\lambda_1^r} \leq \frac{Ra}{2^{r-1}}$$

with equality if and only if G is a cycle. In particular, when $r = 2$, this settles a conjecture of Aouchiche and Hansen [Comparing the geometric–arithmetic index and the spectral radius of graphs, *MATCH Commun. Math. Comput. Chem.* **84** (2020) 473–482].

1 Introduction

Graphs considered in this paper are finite, undirected, simple, and connected. For a graph G, denote by $V(G)$ the vertex set and $E(G)$ the edge set of G. For $u \in V(G)$, denote by $d_G(u)$ or simply d_u the degree of u in G.

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The geometric–arithmetic index of a graph G, proposed by Vukicević and Furtula [11], is defined as

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

The Randić index (or product–connectivity index), proposed by Randić [8], is defined as

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

The Randić index is one of the most studied molecular descriptors in mathematical chemistry, see, e.g., [5, 6]. Vukicević and Furtula [11] observed that the geometric–arithmetic index shows somewhat better predictive power for physico–chemical properties than the Randić index. Since then, the geometric–arithmetic index received much attention, see, e.g., [4, 7, 12].

The spectral radius of a graph G, denoted by $\lambda_1 = \lambda_1(G)$, is the largest eigenvalue of its adjacency matrix $A(G)$, where $A(G) = (a_{uv})_{u,v \in V(G)}$ with $a_{uv} = 1$ if $uv \in E(G)$ and $a_{uv} = 0$ otherwise. The spectral radius has been comprehensively studied, see, e.g., [3, 10].

In the rest of the paper, we denote by GA the geometric–arithmetic index, Ra the Randić index, and λ_1 the spectral radius, of a graph G, respectively.

Aouchiche and Hansen [1] gave a upper bound on $\frac{GA}{\lambda_1}$ in terms of Ra, by combining two inequalities: $GA \le m$ and $Ra \cdot \lambda_1 \ge m$, where $m = |E(G)|$.

Lemma 1.1. *[1, Proposition 2.2] For any nontrivial connected graph G,*

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

with equality if and only if G is regular.

They also gave another upper bound on $\frac{GA}{\lambda_1^2}$ in terms of the number of vertices.

Lemma 1.2. *[1, Theorem 2.5] Let G be a connected graph on $n \ge 7$ vertices. Then*

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

with equality if and only if G is a cycle.

Using AutoGraphiX, they proposed the following conjecture, and showed that it is true for cyclic graphs.

Conjecture 1.1. *[1] For any connected graph G on $n \geq 8$ vertices,*

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

with equality if and only if G is a cycle.

As $Ra \leq \frac{n}{2}$ for a graph on n vertices, Conjecture 1.1 would imply Lemma 1.2.

In this note, we will prove the following generalized version of Conjecture 1.1.

Theorem 1.1. *Let $r \geq 2$ be a fixed integer, and x_r the largest positive root of the equation*

$$(x - 3 + 2\sqrt{2}) \cos^r \frac{\pi}{x+1} = x - 3 + \frac{4\sqrt{2}}{3}.$$

For any connected graph G on $n > x_r$ vertices, we have

$$\frac{GA}{\lambda_1^r} \leq \frac{Ra}{2^{r-1}}$$

with equality if and only if G is a cycle.

Remark 1.1. *Set $r = 2$. Note that $x_2 \approx 7.66251$. It is then reduced to the solution of Conjecture 1.1.*

For a better illustration, we list the values of x_r for $2 \leq r \leq 10$:

r	2	3	4	5	6	7	8	9	10
x_r	7.66251	12.9669	18.2289	23.478	28.7215	33.962	39.2008	44.4385	49.6754

2 Lemmas

Before proving Theorem 1.1, let us establish two auxiliary numerical results first.

Lemma 2.1. *For $n > x_r$,*

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

Proof. Recall that x_r is the largest positive root of the equation

$$(x - 3 + 2\sqrt{2}) \cos^r \frac{\pi}{x+1} = x - 3 + \frac{4\sqrt{2}}{3}.$$

This, together with the fact that

$$\lim_{n\to\infty} \left((n - 3 + 2\sqrt{2}) \cos^r \frac{\pi}{n+1} - \left(n - 3 + \frac{4\sqrt{2}}{3} \right) \right) = \frac{2\sqrt{2}}{3} > 0,$$

implies that for $n > x_r$,

$$(n - 3 + 2\sqrt{2}) \cos^r \frac{\pi}{n+1} > n - 3 + \frac{4\sqrt{2}}{3},$$

as desired. ∎

Lemma 2.2. *For $n > x_r$,*

$$n-5+\frac{2\sqrt{6}}{5}+\sqrt{3}+\frac{2\sqrt{2}}{3} < \left(n-5+\frac{\sqrt{6}}{3}+\frac{4\sqrt{3}}{3}+\sqrt{2}\right)\cos^r\frac{\pi}{2n-2}.$$

Proof. Following a similar setting of x_r, we set y_r to be the largest positive root of the equation

$$\left(x-5+\frac{\sqrt{6}}{3}+\frac{4\sqrt{3}}{3}+\sqrt{2}\right)\cos^r\frac{\pi}{2x-2} = x-5+\frac{2\sqrt{6}}{5}+\sqrt{3}+\frac{2\sqrt{2}}{3}.$$

Notice that

$$\begin{aligned}&\lim_{n\to\infty}\left(\left(n-5+\frac{\sqrt{6}}{3}+\frac{4\sqrt{3}}{3}+\sqrt{2}\right)\cos^r\frac{\pi}{2n-2}-\left(n-5+\frac{2\sqrt{6}}{5}+\sqrt{3}+\frac{2\sqrt{2}}{3}\right)\right)\\ = \ &\frac{5\sqrt{2}+5\sqrt{3}-\sqrt{6}}{15} > 0.\end{aligned}$$

So, if $n > y_r$, then

$$n-5+\frac{2\sqrt{6}}{5}+\sqrt{3}+\frac{2\sqrt{2}}{3} < \left(n-5+\frac{\sqrt{6}}{3}+\frac{4\sqrt{3}}{3}+\sqrt{2}\right)\cos^r\frac{\pi}{2n-2}.$$

It suffices to show that $x_r > y_r$. In order to complete this task, we will involve with an intermediate value, say $\bar{y}_r$, such that $x_r \geq \bar{y}_r > y_r$.

It is easy to see that the main difficulty we face here is the existence of two cosine functions: $\cos^r\frac{\pi}{n+1}$ and $\cos^r\frac{\pi}{2n-2}$. For simplification, we resort to the following inequality about $\cos x$:

$$1-\frac{x^2}{2} < \cos x < 1-\frac{x^2}{2}+\frac{x^4}{24}$$

when $0 < x < \frac{\pi}{2}$. Another inequality is also helpful:

$$1-xr < (1-x)^r \leq 1-rx+\binom{r}{2}x^2$$

when $r \geq 2$ and $0 < x < 1$.

As a consequence, it follows that

$$\cos^r\frac{\pi}{2n-2} > \left(1-\frac{\pi^2}{2(2n-2)^2}\right)^r > 1-\frac{\pi^2 r}{2(2n-2)^2} \tag{2.1}$$

and

$$\begin{aligned}&\cos^r\frac{\pi}{n+1}\\ < \ &\left(1-\frac{\pi^2}{2(n+1)^2}+\frac{\pi^4}{24(n+1)^4}\right)^r\end{aligned}$$

$$\leq \quad 1 - r\left(\frac{\pi^2}{2(n+1)^2} - \frac{\pi^4}{24(n+1)^4}\right) + \binom{r}{2}\left(\frac{\pi^2}{2(n+1)^2} - \frac{\pi^4}{24(n+1)^4}\right)^2. \qquad (2.2)$$

Set the intermediate value $\bar{y}_r$ as

$$\begin{aligned}\bar{y}_r \quad = \quad & \frac{1}{16(5\sqrt{2}+5\sqrt{3}-\sqrt{6})} \\ & \cdot\Bigg(16(5\sqrt{2}+5\sqrt{3}-\sqrt{6}) + 15\pi^2 r \\ & +\sqrt{5\pi^2 r(2688 - 1824\sqrt{2} - 1792\sqrt{3} + 1504\sqrt{6} + 45\pi^2 r)}\Bigg).\end{aligned}$$

It is somewhat tedious but not hard to verify that: When $n > \bar{y}_r$, from (2.1), we always have

$$\begin{aligned} & \left(n - 5 + \frac{\sqrt{6}}{3} + \frac{4\sqrt{3}}{3} + \sqrt{2}\right)\cos^r\frac{\pi}{2n-2} \\ > \quad & \left(n - 5 + \frac{\sqrt{6}}{3} + \frac{4\sqrt{3}}{3} + \sqrt{2}\right)\left(1 - \frac{\pi^2 r}{2(2n-2)^2}\right) \\ > \quad & n - 5 + \frac{2\sqrt{6}}{5} + \sqrt{3} + \frac{2\sqrt{2}}{3},\end{aligned}$$

so $\bar{y}_r > y_r$.

We are left to show that $x_r \geq \bar{y}_r$. Recall from Lemma 2.1 that when $n > x_r$,

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

So our proof will be completed if

$$\bar{y}_r - 3 + \frac{4\sqrt{2}}{3} > (\bar{y}_r - 3 + 2\sqrt{2})\cos^r\frac{\pi}{\bar{y}_r+1}.$$

This is indeed true as, from (2.2), one has

$$\begin{aligned} & (\bar{y}_r - 3 + 2\sqrt{2})\cos^r\frac{\pi}{\bar{y}_r+1} \\ < \quad & (\bar{y}_r - 3 + 2\sqrt{2})\Bigg(1 - r\left(\frac{\pi^2}{2(\bar{y}_r+1)^2} - \frac{\pi^4}{24(\bar{y}_r+1)^4}\right) \\ & +\binom{r}{2}\left(\frac{\pi^2}{2(\bar{y}_r+1)^2} - \frac{\pi^4}{24(\bar{y}_r+1)^4}\right)^2\Bigg) \\ < \quad & \bar{y}_r - 3 + \frac{4\sqrt{2}}{3},\end{aligned}$$

in which the last inequality follows from a series of somewhat tedious (but standard) calculations.

The result follows finally. ∎

3 $r = 2$

First we prove the case $r = 2$ (Conjecture 1.1). The proof is partitioned into three subcases: $\lambda_1 > 2$, $\lambda_1 = 2$, and $\lambda_1 < 2$.

Lemma 3.1. *For any connected graph G, if $\lambda_1 > 2$, then*

$$\frac{GA}{\lambda_1^2} < \frac{Ra}{2}.$$

Proof. From Lemma 1.1, we have

$$\frac{GA}{\lambda_1^2} = \frac{GA}{\lambda_1} \cdot \frac{1}{\lambda_1} < Ra \cdot \frac{1}{2},$$

as desired. ■

Let us recall the characterization of graphs whose spectral radii are no more than 2. Let $K_{1,4}$ be the 5–vertex star. Let C_n be the cycle on $n \geq 3$ vertices. Let W_n be the n–vertex tree obtained from a path $v_1 \ldots v_{n-2}$ by adding a vertex of degree one adjacent to v_2 and a vertex of degree one adjacent to v_{n-3}, where $n \geq 6$. Let T_7 be the 7–vertex tree consisting of three paths of length two at a common vertex, T_8 the 8–vertex tree consisting of two paths of length three and one path of length one at a common vertex, and T_9 the 9–vertex tree consisting of one path of length five, one path of length two and one path of length one at a common vertex. The illustrations about W_n, T_7, T_8, and T_9 are given in Fig. 1.

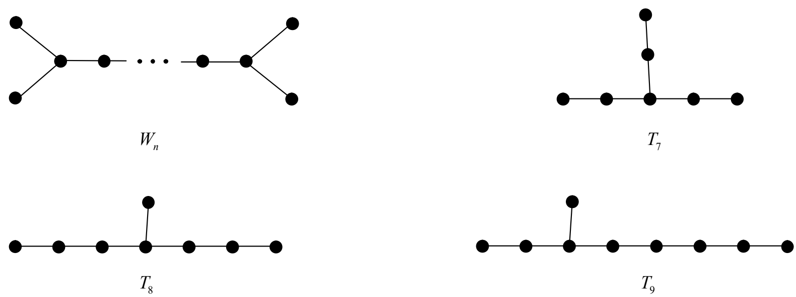

Figure 1. The illustrations about W_n, T_7, T_8, and T_9.

Lemma 3.2. *[9] If G is a connected graph with $\lambda_1 = 2$, then G is one of $K_{1,4}$, C_n, W_n, T_7, T_8, T_9. If G is a connected graph with $\lambda_1 < 2$, then G is a proper induced (connected) subgraph of one of $K_{1,4}$, C_n, W_n, T_7, T_8, T_9.*

Lemma 3.3. *For any connected graph G on $n \geq 8$ vertices, if $\lambda_1 = 2$, then*

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

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

Proof. From Lemma 3.2, G is C_n, W_n, T_8, or T_9. The result follows from direct calculations. ■

Lemma 3.4. *For any connected graph G on $n \geq 8$ vertices, if $\lambda_1 < 2$, then*

$$\frac{GA}{\lambda_1^2} < \frac{Ra}{2}.$$

Proof. From Lemma 3.2 again, we may assume that G is a proper induced (connected) subgraph of C_ℓ, W_ℓ, or T_9 for some $\ell > n$.

If G is a proper induced (connected) subgraph of C_ℓ, then $G \cong P_n$, where P_n represents the path on n vertices. Note that $\lambda_1 = 2\cos\frac{\pi}{n+1}$, see, e.g., [2]. Our desired inequality is equivalent to

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

for $n \geq 8$, which is a direct consequence of Lemma 2.1 with $r = 2$.

If G is a proper induced (connected) subgraph of W_ℓ, then either $G \cong P_n$, or the tree obtained from W_{n+1} by deleting a vertex of degree one (see Fig. 2). As above, we have verified the former case. For the latter case, we have $\lambda_1 = 2\cos\frac{\pi}{2n-2}$ (see, e.g., [2]), and we resort to Lemma 2.2 with $r = 2$, and get

$$\frac{n-5+\frac{2\sqrt{6}}{5}+\sqrt{3}+\frac{2\sqrt{2}}{3}}{\cos^2\frac{\pi}{2n-2}} < n-5+\frac{\sqrt{6}}{3}+\frac{4\sqrt{3}}{3}+\sqrt{2},$$

as desired.

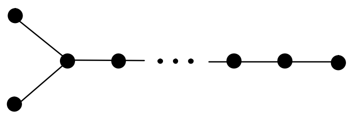

Figure 2. A proper induced (connected) subgraph of W_ℓ.

Suppose that G is a proper induced (connected) subgraph of T_9. Recall the T_9 is a tree on 9 vertices, and G has at least 8 vertices, it means that G contains exactly 8 vertices.

More precisely, G is obtained from T_9 by deleting one vertex of degree one, so we have three candidates, two of which are just the ones considered in last two paragraphs, and the remaining one is the 8–vertex tree consisting of one path of length four, one path of length two and one path of length one at a common vertex (see Fig. 3), it can be verified by direct calculation.

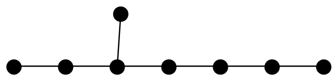

Figure 3. A proper induced (connected) subgraph of T_9.

The proof is completed. ■

Combining all the arguments as above, we may deduce that Conjecture 1.1 is true.

Theorem 3.1. *For any connected graph G on $n \geq 8$ vertices,*

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

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

4 General *r*

Finally, we give an extension to all positive integers $r \geq 2$ (Theorem 1.1), which comes from induction.

The case $r = 2$ is our basic case. Further, suppose that $r \geq 3$ and that Theorem 1.1 is true for $r - 1$. So

$$\frac{GA}{\lambda_1^{r-1}} \leq \frac{Ra}{2^{r-2}}$$

with equality if and only if G is the cycle C_n (in such case $\lambda_1 = 2$). Next we show that it is still valid for r.

If $\lambda_1 \geq 2$, then

$$\frac{GA}{\lambda_1^r} = \frac{GA}{\lambda_1^{r-1}} \cdot \frac{1}{\lambda_1} \leq \frac{Ra}{2^{r-2}} \cdot \frac{1}{\lambda_1} \leq \frac{Ra}{2^{r-2}} \cdot \frac{1}{2} = \frac{Ra}{2^{r-1}}$$

with equalities if and only if G is the cycle C_n (and $\lambda_1 = 2$).

Suppose that $\lambda_1 < 2$. Note that $x_r > 9$ for $r \geq 3$. As in the proof of the case $r = 2$ (Lemma 3.4), we may assume that either $G \cong P_n$, or the tree obtained from W_{n+1} by deleting a vertex of degree one. In the former case,

$$\frac{GA}{\lambda_1^r} < \frac{Ra}{2^{r-1}}$$

is equivalent to

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

for $n > x_r$, which is verified in Lemma 2.1. In the latter case, Lemma 2.2 guarantees the validity of

$$\frac{GA}{\lambda_1^r} < \frac{Ra}{2^{r-1}},$$

by considering its equivalent form:

$$n - 5 + \frac{2\sqrt{6}}{5} + \sqrt{3} + \frac{2\sqrt{2}}{3} < \left(n - 5 + \frac{\sqrt{6}}{3} + \frac{4\sqrt{3}}{3} + \sqrt{2}\right) \cos^r \frac{\pi}{2n-2}$$

for $n > x_r$.

Combining the above two cases, Theorem 1.1 follows.

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