

On the Randić index of unicyclic graphs with girth g *

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Abstract

The Randić index $R(G)$ of a graph G is the sum of the weights $(d(u)d(v))^{-1/2}$ of all edges uv of G , where $d(u)$ denotes the degree of the vertex u . In this paper, we give sharp lower bounds of Randić index of unicyclic graphs with girth g which partly confirms a conjecture by Aouchiche, Hansen and Zheng.

1 Introduction

The Randić index of an organic molecule whose molecular graph is G was introduced by the chemist Milan Randić in 1975 [14] as

$$R(G) = \sum_{uv} \frac{1}{\sqrt{d(u)d(v)}},$$

where $d(u)$ and $d(v)$ stand for the degrees of the vertices u and v , respectively, and the summation goes over all edges uv of G . This topological index, sometimes called connectivity index, has been successfully related to physical and chemical properties of organic molecules

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and become one of the most popular molecular descriptors. This is the only topological index to which two books [7, 8] are devoted.

A simple connected graph G is called unicyclic if it contains exactly one cycle, it is a cycle or a cycle with trees attached to its vertices. A pendant vertex is a vertex of degree 1. The girth of a graph is the length of a shortest cycle. Let $\mathcal{U}_{n,g} = \{G: G \text{ is a unicyclic graph with } n \text{ vertices and girth } g\}$, where $3 \leq g \leq n$. In this paper, unicyclic graphs with girth g are considered, and the lower bounds of their Randić index are given.

Let n be a positive integer with $n \geq 3$. We define an unicyclic graph $\mathcal{U}^0(n)$ with n vertices as follows: $\mathcal{U}^0(n)$ is obtained from the star graph $K_{1,n-1}$ by connecting two pendant vertices of $K_{1,n-1}$ (see Figure 1.1).

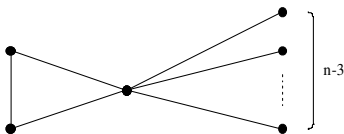


Figure 1.1

In this paper, we only consider finite, undirected and simple graphs. Undefined terminologies and notations may refer to [3].

There are many results concerning Randić index. B. Bollobás and P. Erdős [2] gave the sharp lower bound of $R(G) \geq \sqrt{n-1}$ when G is a graph of order n without isolated vertices. Pan, Xu and Yang [13] gave the sharp lower bounds on the Randić index of unicyclic graphs with n vertices and k pendant vertices. For more references, see [4, 5, 6, 9, 10, 11, 12, 15].

In [1], Aouchiche, Hansen and Zheng proposed a conjecture:

Conjecture. For any connected graph on $n \geq 3$ vertices with Randić index R and girth g ,

$$R \geq \frac{n-3+\sqrt{2}}{\sqrt{n-1}} + \frac{7}{2} - g \quad \text{and} \quad R \geq \frac{3n-9+3\sqrt{2}}{g\sqrt{n-1}} + \frac{3}{2g},$$

with equalities if and only if G is $\mathcal{U}^0(n)$.

In this paper, we give sharp lower bounds of Randić index of unicyclic graphs with girth g which partly confirms the conjecture.

2 Some Lemmas

In this section, we will give some lemmas which will be used in Section 3.

Lemma 2.1 *Let x be a positive integer. Denote*

$$f(x) = \left(\frac{1}{\sqrt{x+1}} - \frac{1}{\sqrt{x}} \right) (x - 2 + \sqrt{2}) + \frac{1}{\sqrt{x+1}}.$$

Then $f(x)$ is monotonously decreasing in x .

Proof. Note that $\frac{df(x)}{dx} = \frac{x+3-\sqrt{2}}{2(x+1)\sqrt{x+1}} - \frac{x+2-\sqrt{2}}{2x\sqrt{x}} = \frac{\sqrt{2}(3\sqrt{2}-6-\xi)}{4\xi^3} < 0$ where $x < \xi < x+1$. Thus $f(x)$ is monotonously decreasing in x . ■

Lemma 2.2 *For $x \geq 5$, $\frac{x-4+\sqrt{2}}{\sqrt{x-2}} + \frac{1}{2} > \frac{x-3+\sqrt{2}}{\sqrt{x-1}}$.*

Proof. Let $f(x) = \frac{x-3+\sqrt{2}}{\sqrt{x-1}} - \frac{x-4+\sqrt{2}}{\sqrt{x-2}} - \frac{1}{2}$. Since $f(x) = \frac{\xi+1-\sqrt{2}}{2(\xi-1)^{\frac{3}{2}}} - \frac{1}{2}$ where $x-1 < \xi < x$, we have $\frac{df(x)}{dx} = \frac{-(\xi-1)^{\frac{3}{2}} - (6-3\sqrt{2})(\xi-1)^{\frac{1}{2}}}{4(\xi-1)^3} < 0$. So $f(x)$ is monotonously decreasing in x . Then $f(x) \leq f(5) = \frac{3+3\sqrt{2}-2\sqrt{3}-2\sqrt{6}}{6} < 0$. That is, $\frac{x-4+\sqrt{2}}{\sqrt{x-2}} + \frac{1}{2} > \frac{x-3+\sqrt{2}}{\sqrt{x-1}}$. ■

Lemma 2.3 *Let x be a positive integer. Denote*

$$f(x) = \frac{\sqrt{2} + 2x}{2\sqrt{x+1}} - \frac{\sqrt{2} - 2 + 2x}{2\sqrt{x}}.$$

Then $f(x)$ is monotonously decreasing in x .

Proof. Note that $f(x) = \frac{2\xi-\sqrt{2}+2}{4\xi\sqrt{\xi}}$ where $x < \xi < x+1$. Hence $\frac{df(x)}{dx} = \frac{\sqrt{2}(-2\xi+3\sqrt{2}-6)}{8\xi^3} < 0$. So $f(x)$ is monotonously decreasing in x . ■

Lemma 2.4 *Let x, y, n be positive integers with $2 \leq x \leq n-2$ and $2 \leq y \leq n-2$. Denote*

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

Then $f(x, y) \geq -\frac{1}{n-2} + \frac{2}{\sqrt{2(n-2)}}$.

Proof. Note that $\frac{\partial f(x, y)}{\partial x} = -\frac{1}{2\sqrt{2x^3}} + \frac{y}{2\sqrt{x^3y^3}} < 0$ and $\frac{\partial f(x, y)}{\partial y} = -\frac{1}{2\sqrt{2y^3}} + \frac{x}{2\sqrt{x^3y^3}} < 0$. Since $x \leq n-2$ and $y \leq n-2$, we have $f(x, y) \geq -\frac{1}{n-2} + \frac{2}{\sqrt{2(n-2)}}$. ■

3 Main results

Denote $\varphi(n, g) = \frac{n-3+\sqrt{2}}{\sqrt{n-1}} + \frac{7}{2} - g$, $\psi(n, g) = \frac{3n-9+3\sqrt{2}}{g\sqrt{n-1}} + \frac{3}{2g}$. We have the following results.

Theorem 3.1 *Let $G \in \mathcal{U}_{n,3}$. Then $R(G) \geq \varphi(n, 3)$ and $R(G) \geq \psi(n, 3)$ with equalities if and only if G is $\mathcal{U}^0(n)$.*

Proof. Note that $\varphi(n, 3) = \psi(n, 3) = \frac{n-3+\sqrt{2}}{\sqrt{n-1}} + \frac{1}{2}$, we apply induction on n . For $n = 3$, $G \cong C_3$, then $R(G) = \frac{3}{2} = \varphi(3, 3)$. For $n = 4$, $G \cong \mathcal{U}^0(4)$, then $R(G) = \frac{\sqrt{6}+\sqrt{3}}{3} + \frac{1}{2} = \varphi(4, 3)$. So in the following proof, we assume that $n \geq 5$. Let $G' \in \mathcal{U}_{n-1,3}$. Assume the Theorem is true when $G \in \mathcal{U}_{n-1,3}$. In the following four cases, we get a new graph $G \in \mathcal{U}_{n,3}$ from G' by adding a vertex v . For convenience, we denote $u, w, s \in C_3$.

Case 1. $d_G(v) = 1$ and v is adjacent to any vertex of the cycle C_3 .

Without loss of generality, we assume that v is adjacent to u . Let $d_{G'}(u) = d$. Denote $N(u) \setminus \{w, s\} = \{y_1, y_2, \dots, y_{d-2}\}$. We have $2 \leq d \leq n-2$, $d(s) \geq 2$, $d(w) \geq 2$, $d(y_i) \geq 1$. Thus

$$\begin{aligned}
 R(G) &= R(G') + \left(\frac{1}{\sqrt{d+1}} - \frac{1}{\sqrt{d}}\right)\left(\frac{1}{\sqrt{d(s)}} + \frac{1}{\sqrt{d(w)}}\right) + \left(\frac{1}{\sqrt{d+1}} - \frac{1}{\sqrt{d}}\right)\sum_{i=1}^{d-2} \frac{1}{\sqrt{d(y_i)}} + \frac{1}{\sqrt{d+1}} \\
 &\geq \varphi(n-1, 3) + \left(\frac{1}{\sqrt{d+1}} - \frac{1}{\sqrt{d}}\right)\left(\frac{1}{\sqrt{d(s)}} + \frac{1}{\sqrt{d(w)}}\right) + \left(\frac{1}{\sqrt{d+1}} - \frac{1}{\sqrt{d}}\right)\sum_{i=1}^{d-2} \frac{1}{\sqrt{d(y_i)}} + \frac{1}{\sqrt{d+1}} \\
 &\geq \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} + \left(\frac{1}{\sqrt{d+1}} - \frac{1}{\sqrt{d}}\right)\left[\left(\frac{1}{\sqrt{d(s)}} + \frac{1}{\sqrt{d(w)}}\right) + (d-2)\right] + \frac{1}{\sqrt{d+1}} \\
 &\geq \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} + \left(\frac{1}{\sqrt{d+1}} - \frac{1}{\sqrt{d}}\right)(d-2+\sqrt{2}) + \frac{1}{\sqrt{d+1}}. \\
 &\geq \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} + \left(\frac{1}{\sqrt{n-2+1}} - \frac{1}{\sqrt{n-2}}\right)(n-2-2+\sqrt{2}) + \frac{1}{\sqrt{n-2+1}} \\
 &= \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} + \frac{1}{\sqrt{n-1}} + \frac{n-4+\sqrt{2}}{\sqrt{n-1}} - \frac{n-4+\sqrt{2}}{\sqrt{n-2}} \\
 &= \varphi(n, 3).
 \end{aligned}$$

The last inequality follows by Lemma 2.1 as $d \leq n-2$.

In order for the equality to hold, all inequalities in the above argument should be equalities. Thus we have

$$R(G') = \varphi(n-1, 3), \quad d(s) = d(w) = 2, \quad d(y_i) = 1, \quad d = n-2.$$

By the induction hypothesis, $G' \cong \mathcal{U}^0(n-1)$. Hence $G \cong \mathcal{U}^0(n)$ and it is easy to check $R(\mathcal{U}^0(n)) = \varphi(n, 3)$.

Case 2. $d_G(v) = 1$. The vertex adjacent to v is a pendant vertex p of G' .

Denote the unique vertex adjacent to p is q . Let $d_{G'}(q) = d$. We have $d \geq 2$. Thus

$$\begin{aligned}
 R(G) &= R(G') - \frac{1}{\sqrt{d}} + \frac{1}{\sqrt{2d}} + \frac{\sqrt{2}}{2} \\
 &\geq \varphi(n-1, 3) + \frac{1-\sqrt{2}}{\sqrt{2d}} + \frac{\sqrt{2}}{2} \\
 &\geq \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} + \frac{1-\sqrt{2}}{2} + \frac{\sqrt{2}}{2} \\
 &= \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + 1. \\
 &> \varphi(n, 3).
 \end{aligned}$$

The last inequality follows by Lemma 2.2.

Case 3. $d_G(v) = 1$. The vertex adjacent to v is neither a pendant vertex of G' nor a vertex of the cycle C_3 .

Denote the vertex adjacent to v is r . Let $d_{G'}(r) = d$. We have $2 \leq d \leq n-4$. Denote $N_{G'}(r) = \{y_1, y_2, \dots, y_d\}$. Then there exists a vertex whose degree is at least 2 in these d vertices. Thus

$$\begin{aligned}
 R(G) &= R(G') + \left(\frac{1}{\sqrt{d+1}} - \frac{1}{\sqrt{d}}\right) \sum_{i=1}^d \frac{1}{\sqrt{d(y_i)}} + \frac{1}{\sqrt{d+1}} \\
 &\geq \varphi(n-1, 3) + \left(\frac{1}{\sqrt{d+1}} - \frac{1}{\sqrt{d}}\right) \left(\frac{1}{\sqrt{2}} + d-1\right) + \frac{1}{\sqrt{d+1}} \\
 &= \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} + \frac{\sqrt{2}+2d}{2\sqrt{d+1}} - \frac{\sqrt{2}-2+2d}{2\sqrt{d}}. \\
 &\geq \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} + \frac{2n-8+\sqrt{2}}{2\sqrt{n-3}} - \frac{2n-10+\sqrt{2}}{2\sqrt{n-4}}. \\
 &> \varphi(n, 3).
 \end{aligned}$$

The second inequality follows by Lemma 2.3 as $d \leq n-4$. To check that the last inequality holds, refer the readers to Appendix.

Case 4. $d_G(v) \geq 2$.

If $d_G(v) > 2$, then there exists more than one cycle in the graph G , which contradicts to the definition of unicyclic graph. So we only consider $d_G(v) = 2$. In this case, the vertex

v split one edge of G' , we assume that the edge is xy . If $d(x) = 1$ or $d(y) = 1$, it is equivalent to the case that v adjacent to a pendant vertex, as we have proved in Case 2. So $2 \leq d(x) \leq n-2$, $2 \leq d(y) \leq n-2$. Thus we have

$$\begin{aligned} R(G) &= R(G') - \frac{1}{\sqrt{d(x)d(y)}} + \frac{1}{\sqrt{2d(x)}} + \frac{1}{\sqrt{2d(y)}} \\ &\geq \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} - \frac{1}{\sqrt{d(x)d(y)}} + \frac{1}{\sqrt{2d(x)}} + \frac{1}{\sqrt{2d(y)}} \\ &\geq \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} - \frac{1}{n-2} + \frac{2}{\sqrt{2(n-2)}} \\ &= \frac{n-4+2\sqrt{2}-\frac{1}{\sqrt{n-2}}}{\sqrt{n-2}} + \frac{1}{2}. \end{aligned}$$

The second inequality follows by Lemma 2.4.

If $n \geq 8$, we have $\frac{1}{\sqrt{n-2}} < \sqrt{2} - 1$, then $R(G) \geq \frac{n-4+2\sqrt{2}-\frac{1}{\sqrt{n-2}}}{\sqrt{n-2}} + \frac{1}{2} > \frac{n-3+\sqrt{2}}{\sqrt{n-2}} + \frac{1}{2} > \frac{n-3+\sqrt{2}}{\sqrt{n-1}} + \frac{1}{2} = \varphi(n, 3)$. If $5 \leq n \leq 7$, there is only one graph (see Figure 3.1) satisfied this case.

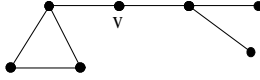


Figure 3.1 $R(G) = \frac{4\sqrt{6}+4\sqrt{3}+3}{6} > \varphi(7, 3)$

This completes the proof of our Theorem. ■

Theorem 3.2 *Let $G \in \mathcal{U}_{n,g}$. Then $R(G) \geq \varphi(n, g)$ and $R(G) \geq \psi(n, g)$ with equalities if and only if G is $\mathcal{U}^0(n)$.*

Proof. We apply induction on g . For $g = 3$, the theorem holds by Theorem 3.1. So in the following proof, we assume that $g \geq 4$. Let $G' \in \mathcal{U}_{n-1, g-1}$. Now, we add a vertex v on G' and consider the following two cases.

Case 1. We get a new graph $G \in \mathcal{U}_{n,g}$ by adding a vertex v on G' .

It is not difficult to see that v must split one of the edges of the cycle C_{g-1} . We assume that the edge is xy . Then $2 \leq d(x) \leq n-2$, $2 \leq d(y) \leq n-2$. Thus

$$\begin{aligned}
 R(G) &= R(G') - \frac{1}{\sqrt{d(x)d(y)}} + \frac{1}{\sqrt{2d(x)}} + \frac{1}{\sqrt{2d(y)}} \\
 &\geq \varphi(n-1, g-1) - \frac{1}{\sqrt{d(x)d(y)}} + \frac{1}{\sqrt{2d(x)}} + \frac{1}{\sqrt{2d(y)}} \\
 &\geq \varphi(n-1, g-1) - \frac{1}{n-2} + \frac{2}{\sqrt{2(n-2)}} \\
 &> \frac{n-4+\sqrt{2}}{\sqrt{n-2}} + \frac{7}{2} - g + 1 \\
 &\geq \frac{n-3+\sqrt{2}}{\sqrt{n-2}} + \frac{7}{2} - g \\
 &> \frac{n-3+\sqrt{2}}{\sqrt{n-1}} + \frac{7}{2} - g \\
 &= \varphi(n, g),
 \end{aligned}$$

as mentioned in Lemma 2.4, the second inequality holds.

From Case 4 of Theorem 3.1, we also know that if $n \geq 8$, $-\frac{1}{\sqrt{d(x)d(y)}} + \frac{1}{\sqrt{2d(x)}} + \frac{1}{\sqrt{2d(y)}} \geq \frac{n-3+\sqrt{2}}{\sqrt{n-1}} - \frac{n-4+\sqrt{2}}{\sqrt{n-2}}$. Thus

$$\begin{aligned}
 R(G) &= R(G') - \frac{1}{\sqrt{d(x)d(y)}} + \frac{1}{\sqrt{2d(x)}} + \frac{1}{\sqrt{2d(y)}} \\
 &\geq \psi(n-1, g-1) + \frac{n-3+\sqrt{2}}{\sqrt{n-1}} - \frac{n-4+\sqrt{2}}{\sqrt{n-2}} \\
 &\geq \frac{\frac{3n-12+3\sqrt{2}}{\sqrt{n-2}} + \frac{3}{2}}{g-1} + \frac{n-3+\sqrt{2}}{\sqrt{n-1}} - \frac{n-4+\sqrt{2}}{\sqrt{n-2}}.
 \end{aligned}$$

So $R(G) - \psi(n, g) \geq \frac{\frac{3n-12+3\sqrt{2}}{\sqrt{n-2}} + \frac{3}{2}}{g-1} + \frac{n-3+\sqrt{2}}{\sqrt{n-1}} - \frac{n-4+\sqrt{2}}{\sqrt{n-2}} - \frac{3n-9+3\sqrt{2}}{g\sqrt{n-1}} - \frac{3}{2g}$. Let $f(n) = \frac{n-3+\sqrt{2}}{\sqrt{n-1}} - \frac{n-4+\sqrt{2}}{\sqrt{n-2}}$. It follows that $f(n)$ is strictly monotone decreasing from Lemma 2.2. Thus $f(n) \leq f(5) < \frac{3}{8}$. We have $R(G) - \psi(n, g) = \frac{1}{g(g-1)}[f(n)(g-2)^2 - 4f(n) + \frac{3}{2} + \frac{3n-9+3\sqrt{2}}{\sqrt{n-1}}] > 0$. That is, $R(G) > \psi(n, g)$ when $n \geq 8$.

If $n = 5, 6, 7$, $g \geq 4$, then the theorem holds clearly by the facts that the total 23 graphs are listed in Figure 3.2, and the following values maybe useful.

$$\begin{aligned}
 \psi(5, 4) &\doteq 1.655, \psi(5, 5) \doteq 1.324, \psi(6, 4) \doteq 1.856, \psi(6, 5) \doteq 1.484, \psi(6, 6) \doteq 1.237, \psi(7, 4) \doteq 2.033, \\
 \psi(7, 5) &\doteq 1.626, \psi(7, 6) \doteq 1.355, \psi(7, 7) \doteq 1.162.
 \end{aligned}$$

By all the above, for $g \geq 4$, we have $R(G) > \varphi(n, g)$ and $R(G) > \psi(n, g)$. Thus, it follows from Theorem 3.1 that $R(G) \geq \varphi(n, g)$ and $R(G) \geq \psi(n, g)$ with equalities if and only if G

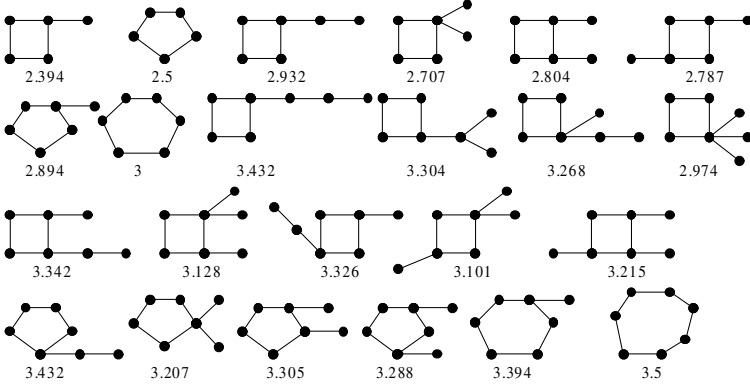


Figure 3.2

is $\mathcal{U}^0(n)$.

Case 2. We get a new graph $G'' \in \mathcal{U}_{n,g-1}$ by adding a vertex v on G' .

Apply induction on n , we can easily conclude that $R(G'') \geq \varphi(n, g-1)$ by Theorem 3.1. So we only need to prove that $R(G'') \geq \psi(n, g-1)$. As proof methods similar to the cases of Theorem 3.1, we simplified the proof of the following subcases.

Subcase 2.1. $d_{G''}(v) = 1$ and v is adjacent to any vertex of the cycle C_{g-1} .

$$\begin{aligned}
 R(G'') &\geq R(G') + \frac{1}{2} + \left(\frac{1}{\sqrt{n-2+1}} - \frac{1}{\sqrt{n-2}} \right) (n-2-2+\sqrt{2}) + \frac{1}{\sqrt{n-2+1}} \\
 &\geq \frac{3n-12+3\sqrt{2}}{(g-1)\sqrt{n-2}} + \frac{3}{2(g-1)} + \frac{1}{2} + \frac{1}{\sqrt{n-1}} + \frac{n-4+\sqrt{2}}{\sqrt{n-1}} - \frac{n-4+\sqrt{2}}{\sqrt{n-2}} \\
 &> \psi(n, g-1).
 \end{aligned}$$

The last inequality follows as $g \geq 4$.

Subcase 2.2. $d_{G''}(v) = 1$. The vertex adjacent to v is a pendant vertex p of G' .

Denote the unique vertex adjacent to p is q . Let $d_{G'}(q) = d$. We have $d \geq 2$. Thus

$$\begin{aligned}
 R(G'') &= R(G') - \frac{1}{\sqrt{d}} + \frac{1}{\sqrt{2d}} + \frac{\sqrt{2}}{2} \\
 &\geq \frac{3n-12+3\sqrt{2}}{(g-1)\sqrt{n-2}} + \frac{3}{2(g-1)} + \frac{1-\sqrt{2}}{\sqrt{2d}} + \frac{\sqrt{2}}{2} \\
 &\geq \frac{3n-12+3\sqrt{2}}{(g-1)\sqrt{n-2}} + \frac{3}{2(g-1)} + \frac{1}{2} \\
 &> \psi(n, g-1).
 \end{aligned}$$

The last inequality follows as $n \geq 5$.

Subcase 2.3. $d_{G''}(v) = 1$. The vertex adjacent to v is neither a pendant vertex of G' nor a vertex of the cycle C_{g-1} .

Denote the vertex adjacent to v is r . Let $d_{G'}(r) = d$. We have $2 \leq d \leq n-4$. Denote $N_{G'}(r) = \{y_1, y_2, \dots, y_d\}$. Then there exists a vertex whose degree is at least 2 in these d vertices. Thus

$$\begin{aligned}
 R(G) &= R(G') + \left(\frac{1}{\sqrt{d+1}} - \frac{1}{\sqrt{d}}\right) \sum_{i=1}^d \frac{1}{\sqrt{d(y_i)}} + \frac{1}{\sqrt{d+1}} \\
 &\geq \frac{3n-12+3\sqrt{2}}{(g-1)\sqrt{n-2}} + \frac{3}{2(g-1)} + \frac{2n-8+\sqrt{2}}{2\sqrt{n-3}} - \frac{2n-10+\sqrt{2}}{2\sqrt{n-4}}. \\
 &> \psi(n, g-1).
 \end{aligned}$$

The last inequality follows as $g \geq 4$.

Subcase 2.4. $d_{G''}(v) \geq 2$.

$$\begin{aligned}
 R(G'') &\geq \frac{3n-12+3\sqrt{2}}{(g-1)\sqrt{n-2}} + \frac{3}{2(g-1)} - \frac{1}{n-2} + \frac{2}{\sqrt{2(n-2)}} \\
 &> \psi(n, g-1).
 \end{aligned}$$

The last inequality follows as $g \geq 4$.

It follows from Case 1 and Case 2 that the Theorem holds. ■

4 Remarks

Now we show that the conjecture by Aouchiche, Hansen and Zheng is true for unicyclic graphs. But we still do not know whether it is true for any connected graphs. The case maybe much more complicated.

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Appendix

Proposition 1. For $x > 3$, $\frac{-(12-6\sqrt{2})\sqrt{x(x-3)}+6x-12-3\sqrt{2}}{2\sqrt{x-3}} > 0$.

Proof. It is easy to calculate that $-(\frac{7-\frac{13}{2}\sqrt{2}}{5-4\sqrt{2}})^2 - \frac{9+4\sqrt{2}}{10-8\sqrt{2}} > 0$, thus

$$(180 - 144\sqrt{2})[(x - \frac{7 - \frac{13}{2}\sqrt{2}}{5 - 4\sqrt{2}})^2] - (\frac{7 - \frac{13}{2}\sqrt{2}}{5 - 4\sqrt{2}})^2 - \frac{9 + 4\sqrt{2}}{10 - 8\sqrt{2}} < 0.$$

That is,

$$36x^2 - (144 + 36\sqrt{2})x + (162 + 72\sqrt{2}) > (216 - 144\sqrt{2})x(x - 3).$$

Hence $6x - 12 - 3\sqrt{2} > (12 - 6\sqrt{2})\sqrt{x(x - 3)}$. Clearly, the Proposition holds. ■

Proposition 2. Let n be a positive integer with $n \geq 5$. We will show that $\frac{2n-8+\sqrt{2}}{2\sqrt{n-3}} - \frac{2n-10+\sqrt{2}}{2\sqrt{n-4}} > \frac{n-3+\sqrt{2}}{\sqrt{n-1}} - \frac{n-4+\sqrt{2}}{\sqrt{n-2}}$.

Proof. Since $\frac{2n-8+\sqrt{2}}{2\sqrt{n-3}} - \frac{2n-10+\sqrt{2}}{2\sqrt{n-4}} = \frac{2\xi-\sqrt{2}+2}{4\xi\sqrt{\xi}}$ and $\frac{n-3+\sqrt{2}}{\sqrt{n-1}} - \frac{n-4+\sqrt{2}}{\sqrt{n-2}} = \frac{\xi-\sqrt{2}+2}{2\xi\sqrt{\xi}}$ where $n-4 < \zeta < n-3$, $n-2 < \xi < n-1$, we have

$$\begin{aligned} \frac{2n-8+\sqrt{2}}{2\sqrt{n-3}} - \frac{2n-10+\sqrt{2}}{2\sqrt{n-4}} - \frac{2\xi-\sqrt{2}+2}{4\xi\sqrt{\xi}} &= \frac{(\xi-\zeta)(4x+12-6\sqrt{2})\sqrt{x}}{16x^3} \\ &> \frac{(2x+6-3\sqrt{2})\sqrt{x}}{8x^3} \\ &= \frac{2x^{\frac{3}{2}} + (6-3\sqrt{2})x^{\frac{1}{2}}}{8x^3} \\ &> \frac{2(\xi-3)^{\frac{3}{2}} + (6-3\sqrt{2})(\xi-3)^{\frac{1}{2}}}{8\xi^3} \\ &= \frac{(2\xi-3\sqrt{2})\sqrt{\xi-3}}{8\xi^3}, \end{aligned}$$

where $\zeta < x < \xi$, the first inequality holds because $\xi - \zeta > 1$ and the second inequality holds because $\xi - 3 < x < \xi$. We also have

$$\frac{n-3+\sqrt{2}}{\sqrt{n-1}} - \frac{n-4+\sqrt{2}}{\sqrt{n-2}} - \frac{2\xi-\sqrt{2}+2}{4\xi\sqrt{\xi}} = \frac{2-\sqrt{2}}{4\xi\sqrt{\xi}} = \frac{4\xi^{\frac{3}{2}} - 2\sqrt{2}\xi^{\frac{3}{2}}}{8\xi^3}.$$

Let $f(\xi) = (2\xi - 3\sqrt{2})\sqrt{\xi - 3} - 4\xi^{\frac{3}{2}} + 2\sqrt{2}\xi^{\frac{3}{2}}$. In order to show the Proposition, it is sufficient to show that $f(\xi) \geq 0$. It is easy to check that $\frac{df(\xi)}{d\xi} = \frac{-(12-6\sqrt{2})\sqrt{\xi(\xi-3)}+6\xi-12-3\sqrt{2}}{2\sqrt{\xi-3}}$. Then by Proposition 1, $f(\xi)$ is strictly monotone increasing. Since $f(9) > 0$, it follows that $f(\xi) > 0$ for $\xi \geq 9$, that is, the Proposition holds for $n \geq 11$. When $5 \leq n \leq 10$, we can directly prove that the Proposition is correct. The proof is completed. ■