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On a Conjecture Between Randić Index and Average Distance of Unicyclic Graphs

Zhifu You[a], Bolian Liu[b]

[a] *School of Computer Science, Guangdong Polytechnic Normal University, Guangzhou, 510665, P.R. China*
[b] *School of Mathematical Science, South China Normal University, Guangzhou, 510631, P.R. China*

Abstract. The Randić index $R(G)$ of a graph G is defined as $R(G) = \sum_{uv\in E}(d(u)d(v))^{-\frac{1}{2}}$, where the summation goes over all edges of G. In 1988, Fajtlowicz proposed a conjecture: For all connected graphs G with average distance $ad(G)$, then $R(G) \geq ad(G)$. In this paper, we prove that this conjecture is true for unicyclic graphs.

1. Introduction

Let $G = (V(G), E(G))$ be a simple graph with $n = |V(G)|$ vertices and $m = |E(G)|$ vertices. A connected graph is a unicyclic graph if $m = n$. $d(v)$ (or d_v) denotes the degree of a vertex v. A vertex of degree one is called a leaf. Denote the number of leaves in G by n_1. Let $\mathcal{T}(n, n_1)$ and $\mathcal{U}(n, n_1)$ be the sets of trees and unicyclic graphs with n vertices and n_1 leaves, respectively. The distance $d_G(u, v)$ is the number of edges in a shortest path from u to v in G. And the average distance $ad(G)$ of graph G is the average value of the distances between all pairs of vertices in G. Recall that the Wiener index $W(G)$ is equal to $\sum_{u,v\in V} d_G(u, v)$. Then $ad(G) = W(G)/\binom{n}{2}$. For terminology and notation not defined here, we refer the readers to [1].

The Randić index is a graph invariant defined as

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

where uv denotes an edge of G.

Recently many researches on extremal aspects of the theory of Randić index have been reported (see [2]). Some problems are still open. In [3], S. Fajtlowicz proposed the following conjecture:

Conjecture 1.1 [3] *For all connected graphs G, $R(G) \geq ad(G)$.*

In [4], Li and Shi have proved that Conjecture 1.1 is true when $\delta(G) \geq \frac{n}{5}$ and $n \geq 15$. In [5], Cygan, Pilipczuk and Škrekovski have shown that Conjecture 1.1 holds for trees.

In this paper, we prove that Conjecture 1.1 is true for unicyclic graphs.

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Email address: liubl@scnu.edu.cn (Bolian Liu)

2. Main result

Lemma 2.1 [6] *Let G be a unicyclic graph and v_1v_2 be an edge in a cycle of G with $d(v_1) = d_1$, $d(v_2) = d_2$. Then the minimum value for the difference $R(G) - R(G - v_1v_2)$ is reached when $d_1 = d_2 = \frac{n+1}{2}$.*

$$\text{Thus } R(G) - R(G - v_1v_2) \geq 2\left(\frac{n+1}{2} - 2 + \frac{1}{\sqrt{2}}\right)\left(\sqrt{\frac{2}{n+1}} - \sqrt{\frac{2}{n-1}}\right) + \frac{2}{n+1}$$
$$\geq \sqrt{2} \cdot (n-1) \cdot \left(\sqrt{\frac{1}{n+1}} - \sqrt{\frac{1}{n-1}}\right) + \frac{2}{n+1}.$$

Lemma 2.2 *The function $f(x) = \sqrt{2} \cdot (x-1) \cdot \left(\sqrt{\frac{1}{x+1}} - \sqrt{\frac{1}{x-1}}\right) + \frac{2}{x+1}$ is increasing on $x \geq 11$. Then $f(x) \geq -0.23$ for $x \geq 6$.*

Proof. Let $\frac{1}{\sqrt{2}} f(x) = (x-1) \cdot \left(\sqrt{\frac{1}{x+1}} - \sqrt{\frac{1}{x-1}}\right) + \frac{\sqrt{2}}{x+1} = m(x)$ and $t = x - 1$.

Then $m(x) = m(1+t) = t \cdot \left(\sqrt{\frac{1}{t+2}} - \sqrt{\frac{1}{t}}\right) + \frac{\sqrt{2}}{t+2} = \frac{t}{\sqrt{t+2}} - \sqrt{t} + \frac{\sqrt{2}}{t+2}$.

It is sufficient to show that $f(x)$ is monotonously increasing in x, i.e., $m'(x) > 0$ for $x \geq 11$. Consider the first derivative
$$m'(x) = \frac{d}{dt}\left(\frac{t}{\sqrt{t+2}} - \sqrt{t} + \frac{\sqrt{2}}{t+2}\right) \cdot \frac{dt}{dx}$$
$$= \frac{\sqrt{t+2} - t \cdot \frac{1}{2\sqrt{t+2}}}{t+2} - \frac{1}{2\sqrt{t}} - \frac{\sqrt{2}}{(t+2)^2}$$
$$= \frac{\frac{1}{2}t + 2}{(t+2)\sqrt{t+2}} - \frac{1}{2\sqrt{t}} - \frac{\sqrt{2}}{(t+2)^2}.$$

Then $2\sqrt{t}(t+2)^2 m'(x) = (t+4)\sqrt{t}\sqrt{t+2} - (t+2)^2 - 2\sqrt{2}\sqrt{t} = n(t)$. (1)

Claim : $n(t) = (t+4)\sqrt{t}\sqrt{t+2} - (t+2)^2 - 2\sqrt{2}\sqrt{t} > 0$ for $t \geq 10$.

It is sufficient to prove that $\left[(t+4)\sqrt{t}\sqrt{t+2} - 2\sqrt{2}\sqrt{t}\right]^2 > (t+2)^4$, i.e.,

$2t^3 + 8t^2 - 4\sqrt{2}t(t+4)\sqrt{t+2} + 8t > 16$.

Then it is only needed to prove that $2t^3 + 8t^2 - 4\sqrt{2}t(t+4)\sqrt{t+2} > 0$, namely, $t > 2\sqrt{2}\sqrt{t+2}$.

In fact, $t^2 > 8(t+2)$ for $t \geq 10$.

Hence from (1), $2\sqrt{t}(t+2)^2 m'(x) > 0$. We have $m'(x) > 0$ for $x \geq 11$.

Note that $\frac{1}{\sqrt{2}} f(x) = m(x)$. Then $f(x)$ is monotonically increasing for $x \geq 11$ and $f(x) \geq f(11) = \sqrt{2} \cdot (11-1) \cdot \left(\sqrt{\frac{1}{11+1}} - \sqrt{\frac{1}{11-1}}\right) + \frac{2}{11+1} \geq -0.23$. It is easy to check that $f(10) \geq -0.23$, $f(9) \geq -0.23$, $f(8) \geq -0.22$, $f(7) \geq -0.22$ and $f(6) \geq -0.21$. Then $f(x) \geq -0.23$ for $x \geq 6$. □

Lemma 2.3 [5] *For any tree T with n vertices and n_1 leaves, the following inequality holds:*
$$R(T) \geq ad(T) + max\{0, \sqrt{n_1} - 2\}.$$

By using Theorem 5 from [7], Cygan et al. [5] obtained that:

Lemma 2.4 *Let T be a tree with n vertices and n_1 leaves, where $3 \leq n_1 \leq n-2$. Then $R(T) \geq \frac{n - n_1}{2} + \sqrt{n_1} - 0.462$.*

Let $DC(n, a, b)$ be a double comet obtained from the Path P_{n-a-b} by attaching a and b pendent vertices to two ends of P_{n-a-b}, respectively. In [5], Cygan et al. calculated $ad(DC(n, a, b))$ as:

$\binom{n}{2} ad(DC(n, a, b)) = ab(n - n_1 + 1) + 2\binom{a}{2} + 2\binom{b}{2} + (a+b)(n - n_1)(n - n_1 + 1)\big/2 + \binom{n - n_1 + 1}{3}$.

Lemma 2.5 [5] *Suppose that T is a tree with n vertices and n_1 leaves, where $3 \le n_1 \le n-2$. There exists a double comet $T' = DC(n,a,b)$ for some $a, b \ge 1$, $a+b = n_1$ such that $ad(T) \le ad(T')$.*

Proposition 2.6 *Let $T \in \mathcal{T}(n, n_1)$. If $n \ge 7$ and $n_1 = 3$, then $R(T) \ge ad(T) + 0.25$.*

Proof. By Lemmas 2.4 and 2.5,

$$\begin{aligned} R(T) - ad(T) - 0.25 &\ge R(T) - ad(DC(n,a,b)) - 0.25 \\ &\ge \frac{n-n_1}{2} + \sqrt{n_1} - 0.462 - ad(DC(n,a,b)) - 0.25 \\ &= \frac{n-3}{2} + \sqrt{3} - 0.462 - ad(DC(n,1,2)) - 0.25 \\ &= \frac{n-3}{2} + \sqrt{3} - 0.462 - \frac{2}{n(n-1)}\Big[2(n-1) + \frac{3}{2}(n-3)(n-2) + \frac{1}{6}(n-2)(n-3)(n-4)\Big] - 0.25 \\ &= \frac{n-3}{2} + \sqrt{3} - 0.462 - \frac{4}{n} - 2\frac{(n-2)(n-3)}{n(n-1)}\Big(\frac{3}{2} + \frac{n-4}{6}\Big) - 0.25 \\ &\ge \frac{n-3}{2} + \sqrt{3} - 0.462 - \frac{4}{n} - 3\frac{(n-2)(n-3)}{n(n-1)} - \frac{n-4}{3} - 0.25 \\ &\ge \frac{n}{6} - \frac{4}{n} - 3\frac{(n-2)(n-3)}{n(n-1)} + 0.85. \end{aligned}$$

Let $g(x) = \frac{x}{6} - \frac{4}{x} - 3\frac{(x-2)(x-3)}{x(x-1)} + 0.85$.

Consider the first derivative $g'(x) = \frac{1}{6} + \frac{4}{x^2} - 3 \cdot \frac{4x^2-12x+6}{x^2(x-1)^2} = \frac{x^2(x-1)^2 - 48x^2 + 168x - 84}{6x^2(x-1)^2} > 0$ for $x \ge 7$. Then $g(x)$ is increasing on $x \ge 7$ and $g(x) \ge g(7) = \frac{7}{6} - \frac{4}{7} - 3\frac{(7-2)(7-3)}{7(7-1)} + 0.85 \approx 0.016 > 0$.

Hence $R(T) - ad(T) - 0.25 \ge R(T) - ad(DC(n,a,b)) - 0.25 > 0$.

The result holds. □

Proposition 2.7 *Let $T \in \mathcal{T}(n, n_1)$. If $n \ge 9$ and $n_1 = 4$, then $R(T) \ge ad(T) + 0.25$.*

Proof. By Lemma 2.4,

$R(T) - ad(T) - 0.25 \ge R(T) - ad(DC(n,a,b)) - 0.25$. There are two cases:

Case 1: $DC(n,a,b) \cong DC(n,1,3)$.

$$\begin{aligned} R(T) - ad(T) - 0.25 &\ge \frac{n-n_1}{2} + \sqrt{n_1} - 0.462 - ad(DC(n,a,b)) - 0.25 \\ &= \frac{n-4}{2} + \sqrt{4} - 0.462 - ad(DC(n,1,3)) - 0.25 \\ &= \frac{n-4}{2} + \sqrt{4} - 0.462 - \frac{2}{n(n-1)}\Big[3(n-3) + 6 + 2(n-3)(n-4) + \frac{1}{6}(n-3)(n-4)(n-5)\Big] - 0.25 \\ &= \frac{n-4}{2} + \sqrt{4} - 0.462 - \frac{6}{n} - 2\frac{(n-3)(n-4)}{n(n-1)}\Big(2 + \frac{n-5}{6}\Big) - 0.25 \\ &\ge \frac{n-4}{2} + \sqrt{4} - 0.462 - \frac{6}{n} - 4\frac{(n-3)(n-4)}{n(n-1)} - \frac{n-5}{3} - 0.25 \\ &\ge \frac{n}{6} - \frac{6}{n} - 4\frac{(n-3)(n-4)}{n(n-1)} + 0.95. \end{aligned}$$

Let $h(x) = \frac{x}{6} - \frac{6}{x} - 4\frac{(x-3)(x-4)}{x(x-1)} + 0.95$.

Consider the first derivative $h'(x) = \frac{1}{6} + \frac{6}{x^2} - 4 \cdot \frac{6x^2-24x+12}{x^2(x-1)^2} = \frac{x^2(x-1)^2 - 108x^2 + 504x - 252}{6x^2(x-1)^2} > 0$ for $x \ge 8$. Then $h(x)$ is increasing on $x \ge 8$ and $h(x) \ge h(8) = \frac{8}{6} - \frac{6}{8} - 4\frac{(8-4)(8-3)}{8(8-1)} + 0.95 \approx 0.1 > 0$.

Case 2: $DC(n,a,b) \cong DC(n,2,2)$.

$$R(T) - ad(T) - 0.25 \ge \frac{n-n_1}{2} + \sqrt{n_1} - 0.462 - ad(DC(n,a,b)) - 0.25$$

$$= \frac{n-4}{2} + \sqrt{4} - 0.462 - ad(DC(n,2,2)) - 0.25$$
$$= \frac{n-4}{2} + \sqrt{4} - 0.462 - \frac{2}{n(n-1)}\Big[4(n-3) + 4 + 2(n-3)(n-4) + \frac{1}{6}(n-3)(n-4)(n-5)\Big] - 0.25$$
$$= \frac{n-4}{2} + \sqrt{4} - 0.462 - \frac{8(n-2)}{n(n-1)} - 2\frac{(n-3)(n-4)}{n(n-1)}\Big(2 + \frac{n-5}{6}\Big) - 0.25$$
$$\geq \frac{n-4}{2} + \sqrt{4} - 0.462 - \frac{8(n-2)}{n(n-1)} - 4\frac{(n-3)(n-4)}{n(n-1)} - \frac{n-5}{3} - 0.25$$
$$\geq \frac{n}{6} - \frac{8(n-2)}{n(n-1)} - 4\frac{(n-3)(n-4)}{n(n-1)} + 0.95$$
$$= \frac{n}{6} - \frac{4n^2 - 20n + 32}{n(n-1)} + 0.95.$$

Let $l(x) = \frac{x}{6} - \frac{4x^2 - 20x + 32}{x(x-1)} + 0.95$.

Consider the first derivative $l'(x) = \frac{1}{6} - \frac{16x^2 - 64x + 32}{x^2(x-1)^2} = \frac{x^2(x-1)^2 - 96x^2 + 384x - 192}{6x^2(x-1)^2} > 0$ for $x \geq 9$.
Then $l(x)$ is increasing on $x \geq 9$ and $l(x) \geq l(9) = \frac{9}{6} - \frac{176}{72} + 0.95 > 0$.

The result holds. □

Theorem 2.8 *Let $U \in \mathcal{U}(n, n_1)$. If $n_1 \geq 5$, then $R(U) \geq ad(U)$.*

Proof. Let U be a unicyclic graph with n vertices and $n_1 \geq 5$ leaves, and uv an edge in the cycle of U. Then $n \geq 8$. Note that removing the edge uv strictly increases its Wiener index, namely, $W(U) - W(U - uv) < 0$.

By Lemmas 2.1 and 2.2, $R(U) - R(U - uv) - [W(U) - W(U - uv)]/\binom{n}{2} \geq R(U) - R(U - uv) \geq -0.23$.

By Lemma 2.3, $R(U) - W(U)/\binom{n}{2} \geq R(U - uv) - W(U - uv)/\binom{n}{2} - 0.23$,

i.e.,
$$\begin{aligned} R(U) - ad(U) &\geq R(U - uv) - ad(U - uv) - 0.23 \\ &\geq \sqrt{n_1} - 2 - 0.23 \\ &\geq \sqrt{5} - 2 - 0.23 \\ &> 0. \end{aligned}$$

The theorem follows. □

Theorem 2.9 *Let $U \in \mathcal{U}(n, n_1)$. If $n_1 = 4$, then $R(U) \geq ad(U)$.*

Proof. Let uv be an edge in the cycle of U. Similar to the proof of Theorem 2.8, we have
$R(U) - ad(U) \geq R(U - uv) - ad(U - uv) - 0.23$.

There are two cases:

Case 1: $U - uv$ has at least 5 leaves.

By Lemma 2.3, $R(U - uv) - ad(U - uv) - 0.23 \geq \sqrt{5} - 2 - 0.23 > 0$.

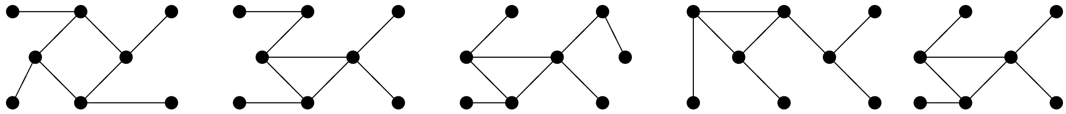
Then $R(U) \geq ad(U)$.

Case 2: $U - uv$ has 4 leaves.

Since U and $U - uv$ both have 4 leaves, the cycle of U is C_3 or C_4. Note that if $n \geq 9$, by Proposition 2.7, then $R(U) - ad(U) \geq R(U - uv) - ad(U - uv) - 0.23 \geq 0.25 - 0.23 > 0$. There remains three subcases:

Subcase 2.1: $n = 8$. And the cycle of U is C_4.

Then $U \cong U_1$, and $R(U_1) - ad(U_1) = \frac{4}{\sqrt{3}} + \frac{4}{3} - \frac{15}{7} > 0$.

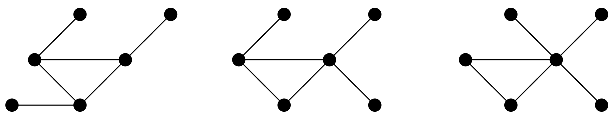


U_1 U_2 U_3 U_4 U_5

Figure 1. Unicyclic graphs which have order $n \le 8$ and 4 leaves, and every spanning trees with 4 leaves.

Subcase 2.2: $n = 8$. And the cycle of U is C_3.
Then $U \cong U_i$ $(i = 2, 3, 4)$.
By direct calculations, $R(U_2) - ad(U_2) = \frac{1}{\sqrt{2}} + \frac{4}{3} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{3}} - \frac{61}{28} > 0$; $R(U_3) - ad(U_3) = \sqrt{3} + \frac{5}{6} + \frac{3}{2\sqrt{2}} - \frac{15}{7} > 0$; $R(U_4) - ad(U_4) = \frac{4}{3} + \frac{4}{\sqrt{3}} - \frac{63}{28} > 0$.
Subcase 2.3: $n = 7$.
Then $U \cong U_5$, and $R(U_5) - ad(U_5) = \sqrt{3} + \frac{4}{3} - \frac{40}{21} > 0$.
The theorem follows. □

Theorem 2.10 *Let $U \in \mathcal{U}(n, n_1)$. If $n_1 = 3$, then $R(U) \ge ad(U)$.*
Proof. Similar to the proof of Theorem 2.9, for an edge in the cycle of U, we have
$R(U) - ad(U) \ge R(U - uv) - ad(U - uv) - 0.23$.
There are three cases:
Case 1: $U - uv$ has 5 leaves.
By Lemma 2.3, $R(U) - ad(U) \ge R(U - uv) - ad(U - uv) - 0.23 \ge \sqrt{5} - 2 - 0.23 > 0$.
Case 2: $U - uv$ has 3 leaves.
It remains two subcases.
Subcase 2.1: $n \ge 7$.
By Proposition 2.6, $R(U) - ad(U) \ge R(U - uv) - ad(U - uv) - 0.23 \ge 0.25 - 0.23 > 0$.
Subcase 2.2: $n = 6$.
Since U has three 3 leaves, $U \cong U_i$ $(i = 6, 7, 8)$.



U_6 U_7 U_8

Figure 2. Unicyclic graphs with order $n = 6$ and 3 leaves.

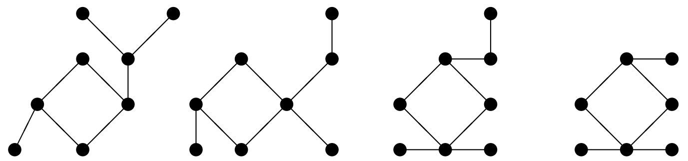
By direct calculations, $R(U_6) - ad(U_6) = \frac{3}{\sqrt{3}} + 1 - \frac{9}{5} > 0$; $R(U_7) - ad(U_7) = 1 + \frac{1}{2\sqrt{2}} + \frac{3}{2\sqrt{3}} + \frac{1}{\sqrt{6}} - \frac{26}{15} > 0$; $R(U_8) - ad(U_8) = \frac{3}{\sqrt{5}} + \frac{2}{\sqrt{10}} + \frac{1}{2} - \frac{8}{5} > 0$.
Case 3: $U - uv$ has 4 leaves.
It remains two subcases.
Subcase 3.1: $n \ge 9$.

By Proposition 2.7, $R(U) - ad(U) \geq R(U - uv) - ad(U - uv) - 0.23 \geq 0.25 - 0.23 > 0$.

Subcase 3.2: $n = 6, 7, 8$.

The cycle of U may be C_3, C_4, or C_5. Since $U - uv$ has 4 leaves by deleting any edge uv in the cycle of U, the cycle of U is C_4.

And $U \cong U_i$ $(i = 9, \ldots, 12)$.



U_9 U_{10} U_{11} U_{12}

Figure 3. Unicyclic graphs which have order $n \leq 8$ and 3 leaves, and every spanning trees with 4 leaves.

By direct calculations, $R(U_9) - ad(U_9) = \frac{1}{3} + \sqrt{3} + \frac{4}{\sqrt{6}} - \frac{33}{14} > 0$; $R(U_{10}) - ad(U_{10}) = \frac{5}{2\sqrt{2}} + \frac{1}{2} + \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}} - \frac{63}{28} > 0$; $R(U_{11}) - ad(U_{11}) = \sqrt{2} + \frac{3}{\sqrt{6}} + 1 - \frac{65}{28} > 0$; $R(U_{12}) - ad(U_{12}) = \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{2}} + 1 - 2 > 0$.

The theorem follows. □

Theorem 2.11 *Let $U \in \mathcal{U}(n, n_1)$. If $n_1 = 2$, then $R(U) \geq ad(U)$.*

Proof. There are two cases:

Case 1: The cycle of U has at least 5 vertices.

Then by deleting an edge uv in the cycle such that $U - uv$ has 3 leaves, and using Lemmas 2.1-2.3, and Proposition 2.6, we have

$R(U) - ad(U) \geq R(U - uv) - ad(U - uv) - 0.23 \geq 0.25 - 0.23 > 0$.

Case 2: The cycle of U has 3 or 4 vertices.

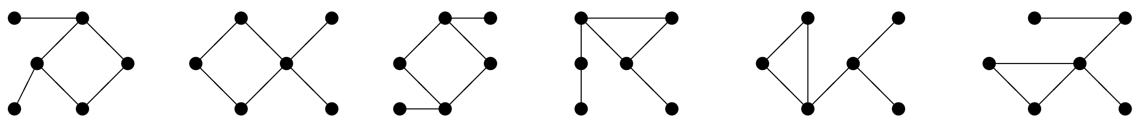
There are three subcases.

Subcase 2.1: $n \geq 7$.

Similar to Case 1, we also have $R(U) \geq ad(U)$.

Subcase 2.2: $n = 6$.

Then $U \cong U_i$ $(i = 13, \ldots, 18)$.



U_{13} U_{14} U_{15} U_{16} U_{17} U_{18}

Figure 4. Unicyclic graphs with order $n = 6$ and 2 leaves.

By direct calculations, $R(U_{13}) - ad(U_{13}) = \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{6}} + \frac{5}{6} - \frac{9}{5} > 0$; $R(U_{14}) - ad(U_{14}) = 2 + \frac{1}{\sqrt{2}} - \frac{26}{15} > 0$; $R(U_{15}) - ad(U_{15}) = \frac{2}{\sqrt{3}} + \frac{4}{\sqrt{6}} - \frac{28}{15} > 0$; $R(U_{16}) - ad(U_{16}) = \frac{1}{\sqrt{2}} + \frac{3}{\sqrt{6}} + \frac{1}{3} + \frac{1}{\sqrt{3}} - \frac{29}{15} > 0$; $R(U_{17}) - ad(U_{17}) = \frac{2}{\sqrt{3}} + \frac{5}{6} + \frac{2}{\sqrt{6}} - \frac{28}{15} > 0$; $R(U_{18}) - ad(U_{18}) = 1 + \frac{5}{2\sqrt{2}} - \frac{9}{5} > 0$.

Subcase 2.3: $n = 5$.

Then $U \cong U_i$ $(i = 19, 20)$.

U_{19} U_{20}

Figure 5. Unicyclic graphs with order $n = 5$ and 2 leaves.

By direct calculations, $R(U_{19}) - ad(U_{19}) = \frac{2}{\sqrt{3}} + \frac{2}{\sqrt{6}} + \frac{1}{3} - \frac{8}{5} > 0$; $R(U_{20}) - ad(U_{20}) = \frac{3}{2} + \frac{1}{\sqrt{2}} - \frac{3}{2} > 0$.

By this the proof of Theorem 2.11 is completed. □

Theorem 2.12 *Let $U \in \mathcal{U}(n, n_1)$. If $n_1 = 1$, then $R(U) \geq ad(U)$.*

Proof. If $n \geq 7$, by choosing an edge of the cycle of U and deleting uv such that $U - uv$ has 3 leaves, and using Proposition 2.6, then we have $R(U) - ad(U) \geq R(U - uv) - ad(U - uv) - 0.23 \geq 0.25 - 0.23 > 0$.

It remains three cases.

Case 1: $n = 6$.

Then $U \cong U_i$ $(i = 21, 22, 23)$, where U_{21}, U_{22} and U_{23} are the unicyclic graphs obtained from C_3, C_4 and C_5 by attaching P_4, P_3, and P_2 on the cycle, respectively.

By direct calculations, $R(U_{21}) - ad(U_{21}) = 1 + \frac{1}{\sqrt{2}} + \frac{3}{\sqrt{6}} - \frac{31}{15} > 0$; $R(U_{22}) - ad(U_{22}) = 1 + \frac{1}{\sqrt{2}} + \frac{3}{\sqrt{6}} - \frac{29}{15} > 0$; $R(U_{23}) - ad(U_{23}) = \frac{3}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{26}{15} > 0$.

Case 2: $n = 5$.

Then $U \cong U_i$ $(i = 24, 25)$, where U_{24} and U_{25} are the unicyclic graphs obtained from C_3 and C_4 by attaching P_3 and P_2 on the cycle, respectively.

By direct calculations, $R(U_{24}) - ad(U_{24}) = \frac{1}{2} + \frac{1}{\sqrt{2}} + \frac{3}{\sqrt{6}} - \frac{17}{10} > 0$; $R(U_{25}) - ad(U_{25}) = 1 + \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}} - \frac{8}{5} > 0$.

Case 3: $n = 4$.

Then $U \cong U_{26}$, where U_{26} is the unicyclic graph obtained from C_3 by attaching P_2 on the cycle.

By direct calculation, $R(U_{26}) - ad(U_{26}) = \frac{1}{2} + \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}} - \frac{4}{3} > 0$.

By this the proof of Theorem 2.12 is completed. □

Theorem 2.13 *Let $U \in \mathcal{U}(n, n_1)$ with $n_1 = 0$. Then $R(U) \geq ad(U)$.*

Proof. For a unicyclic graph with n vertices, if U has no leaves, then $U \cong C_n$ and $R(C_n) = \frac{1}{\sqrt{2 \times 2}} \times n = \frac{n}{2}$ and $ad(C_n) = \frac{n^2}{4(n-1)}$ when n is even; $ad(C_n) = \frac{n+1}{4}$ when n is odd. Thus $R(C_n) \geq ad(C_n)$. □

By Theorems 2.8-2.13, we have the main result:

Theorem 2.14 *Let U be a unicyclic graph with n vertices. Then $R(U) \geq ad(U)$.*

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