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The first three largest Randić indices of unicyclic graphs

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Abstract

The Randić index of a simple connected graph G is defined as $\sum_{uv\in E(G)}(d(u)d(v))^{-\frac{1}{2}}$. In this paper, we give the first three largest Randić indices of unicyclic graphs and characterize the extreme graphs that achieve those bounds.

1 Introduction

A single number that can be used to characterize some property of the graph of a molecule is called a *topological index*. For quite some time there has been rising interest in the field of computational chemistry in topological indices that capture the structural essence of compounds. The interest in topological indices is mainly related to their use in nonempirical quantitative structure-property relationships and quantitative structure-activity relationships.

One of the most important topological indices is the well-known branching index introduced by Randić [6] which is defined as the sum of certain bond contributions calculated from the vertex degree of the hydrogen suppressed molecular graphs.

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The Randić index, which is the sum of all relative accessibility areas in the molecule, is the relative molecular accessibility area expressed in R^2. These areas represent the total area which are accessible from the environment surrounding the molecules. This explains why the Randić index has been so successful in modeling very diverse physical and biological properties. The molecules can be represented as molecular graphs, namely as hydrogen depleted graphs in which vertices represent atoms and edges represent covalent bonds. For a molecular graph $G = (V(G), E(G))$ where $V(G)$ and $E(G)$ denote the the set of vertices and the set of edges of G respectively, the *Randić index* of G is defined as

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-\frac{1}{2}},$$

where $d(\cdot)$ denotes the degree of the corresponding vertex. The Randić index has received intensive attention recently. Much effort has been spent to derive nontrivial bounds for the Randić index of molecular graphs. For general graphs, a lower bound of $R(G)$ was given by Bollobás and Erdös [1], while an upper bound was recently presented in [4]. A lot of research focused on special classes of graphs. For example, trees with the largest and the smallest Randić index were considered in [3, 7, 8]. In [2], Lu et. al. gave a sharp lower bound for the Randić index of trees with n vertices and k pendants where $2 \leq k \leq n-1$. An upper bound of the Randić index of trees with n vertices and k pendants where $n \geq 3k-2$ was given in [9].

Here, we will investigate the Randić index of unicyclic graphs. Gao and Lu [2] obtained sharp lower and upper bounds for the Randić index of unicyclic graphs. Pan et. al. [5] gave a sharp lower bound for unicyclic graphs with k pendants. In this paper, we will obtain the first three largest Randić indices of unicyclic graphs. We will also characterize extreme unicyclic graphs which achieve those bounds.

Before proceeding, we introduce some notations. A *pendant* of a graph is a vertex with degree 1. We use $\mathcal{U}_n$ to denote the set of all unicyclic graphs of order n. We use $\mathcal{U}_{n,p}$ to denote the subset of $\mathcal{U}_n$ consisting of all graphs with p pendants. We use $\mathcal{U}_n^k$ to denote another subset of $\mathcal{U}_n$ consisting of all graphs with a k-cycle. For any $G \in \mathcal{U}_n$, we denote its unique cycle by $C(G)$. The maximum degree of G is denoted by $\Delta(G)$. An i-vertex of G means a vertex with degree i. We let $n_i(G)$ denote the number of i-vertices of G. As usual, C_n denotes the cycle on n vertices, P_n denotes the path on n vertices, and S_n denotes the star on n vertices. Let $G_n^k \in \mathcal{U}_n^k$ denote the graph obtained by attaching P_{n-k+1} to C_k. Let $G_{n,n-k}$ denote the graph obtained by identifying the center of S_{n-k+1} with a vertex of C_k.

Pan et. al. gave the following sharp lower bound on the Randić index of $\mathcal{U}_{n,p}$ with p pendants.

Theorem 1.1 *(Pan et. al. [5]) Let $G \in \mathcal{U}_{n,p}$. Then*

$$R(G) \geq \frac{n-p-2}{2} + \frac{p+\sqrt{2}}{\sqrt{p+2}},$$

where equality holds if and only if $G = G_{n,p}$.

Guo and Lu [2] showed that the largest Randić index is achieved by the graph C_n, a cycle on n-vertices.

Theorem 1.2 *(Gao and Lu [2]) Let G be a unicyclic graph on n vertices. Then*

$$\frac{1}{2} + \frac{n-3+\sqrt{2}}{\sqrt{n-1}} \leq R(G) \leq \frac{n}{2}$$

with left equality if and only if $G = G_{n,n-3}$ and with right equality if and only if $G = C_n$.

In this paper, we give the first three largest Randić indices of unicyclic graphs.

Theorem 1.3 *Among all the unicyclic graphs on n vertices,*

(1) The first largest Randić index of unicyclic graphs on n vertices is $\frac{n}{2}$, which is achieved only by the graph C_n;

(2) The second largest Randić index of unicyclic graphs on n vertices is $\frac{n-4}{2} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{2}}$ and it is achieved only by each graph in $\{G_n^k : 3 \leq k \leq n-2\}$;

(3) The third largest Randić index of unicyclic graphs on n vertices is $\frac{n-3}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}}$ and G_n^{n-1} is the only graph that has the second largest Randić index.

In order to prove Theorem 1.3, we need to look at a partition of all unicyclic graphs on n vertices. In our proof, we partition $\mathcal{U}_n$ according to the length of the cycles. Precisely, we partition $\mathcal{U}_n$ into $\mathcal{U}_n^3, \mathcal{U}_n^4, \cdots, \mathcal{U}_n^{n-1}, \mathcal{U}_n^n$, where $\mathcal{U}_n^k$ is the set of unicyclic graphs on n vertices with a k-cycle. We then investigate the largest and smallest Randić indices within each subclass $\mathcal{U}_n^k$. We prove the following theorem (Theorem 1.4). Theorem 1.3 follows straightly from Theorem 1.4.

Theorem 1.4 *Let G be a unicyclic graph with a k-cycle, i.e., $G \in \mathcal{U}_n^k$. Then*
(1) $\frac{k-2}{2} + \frac{n-k+\sqrt{2}}{\sqrt{n-k+2}} \leq R(G)$ with equality if and only if $G = G_{n,n-k}$;
(2) $R(G) \leq \frac{n-4}{2} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{2}}$ if $k \leq n-2$ with equality if and only if G is in $\{G_n^k : 3 \leq k \leq n-2\}$;
(3) $R(G) = R(G_n^{n-1}) = \frac{n-3}{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}}$ if $k = n-1$;
(4) $R(G) = R(C_n) = \frac{n}{2}$ if $k = n$.

Clearly, $\mathcal{U}_n^n = \{C_n\}$ and $\mathcal{U}_n^{n-1} = \{G_n^{n-1}\} = \{G_{n,1}\}$. So we only need to prove our theorem for $k \leq n-2$. In the following we always assume $3 \leq k \leq n-2$. The proofs of Theorem 1.4 will be given in Sections 2 and 3. We will prove the upper bound in Section 2 and the proof of lower bound is presented in Section 3.

2 Upper bound of the Randić index of unicyclic graphs with a k-cycle

In this section we show that G_n^k has the largest Randić index among the graphs in $\mathcal{U}_n^k$.

For any $G \in \mathcal{U}_n$, a ray of G is a path $v_0v_1\cdots v_t$ such that $d(v_t)=1$, $v_0 \in C(G)$, and $v_i \notin C(G)$ for each $i = 1, 2, \cdots, t$. Define $Ray(G) = \max\{|P| : P \text{ is a ray of } G\}$ where $|P|$ is the number of edges in P. If $|P| = Ray(G)$, we say P is a maximum ray.

Theorem 2.1 *Let $G \in \mathcal{U}_n^k$ where $3 \le k \le n-2$ and $G \ne G_n^k$. Then $R(G) < R(G_n^k) = \frac{n-4}{2} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{2}}$.*

Proof. It is not hard to check that the theorem is true if $n-k \le 3$.

Let $G \in \mathcal{U}_n^k$ be a counterexample to the theorem such that

(1) $n-k$ is as small as possible;

(2) subject to (1), $Ray(G)$ is as large as possible;

(3) subject to (1) and (2), $n_1(G)$ is as small as possible.

Then we have the following two easy observations.

Observation 1 $R(G) \ge R(G_n^k)$, and for any graph $H \in \mathcal{U}_n^k$, $R(H) \le R(G_n^k) \le R(G)$ if $Ray(H) > Ray(G)$, or if $Ray(H) \ge Ray(G)$ and $n_1(H) < n_1(G)$.

Observation 2 For any $H \in \mathcal{U}_{n-1}^k$ and $H \ne G_{n-1}^k$, $R(H) < R(G_{n-1}^k) = R(G_n^k) - \frac{1}{2}$.

Now we derive some properties of G in order to draw a contradiction.

Claim 1. Each vertex of G is adjacent to at most one 1-vertex.

Proof of Claim 1. Suppose on the contrary that a vertex y is adjacent to two 1-vertices, say x, z. Let $N(y) = \{x, z, y_3, \cdots, y_d\}$ where $d = d(y) \ge 3$, and let $G' = G - yz + xz \in \mathcal{U}_n^k$. Then

$$\begin{aligned} R(G) - R(G') &= \sum_{i=3}^{d} \frac{1}{\sqrt{d(y_i)d(y)}} + \frac{2}{\sqrt{d(y)}} - \left(\sum_{i=3}^{d} \frac{1}{\sqrt{d(y_i)(d(y)-1)}} + \frac{1}{\sqrt{2(d(y)-1)}} + \frac{1}{\sqrt{2}} \right) \\ &\le \frac{2}{\sqrt{d(y)}} - \frac{1}{\sqrt{2(d(y)-1)}} - \frac{1}{\sqrt{2}} \\ &= f(d(y)), \end{aligned}$$

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

Now we show $f(x) < 0$ for any integer $x \ge 3$. First $f(3) = \frac{2}{\sqrt{3}} - \frac{1}{2} - \frac{1}{\sqrt{2}} < 0$. If $x \ge 4$, then

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

$$
\begin{aligned}
&= \left(2-\frac{1}{\sqrt{2}}\right)\frac{1}{\sqrt{x}}-\frac{1}{\sqrt{2}} \le \left(2-\frac{1}{\sqrt{2}}\right)\frac{1}{\sqrt{4}}-\frac{1}{\sqrt{2}} \\
&= 1-\frac{3\sqrt{2}}{4} < 0.
\end{aligned}
$$

Therefore, $R(G)-R(G') < 0$, i.e., $R(G) < R(G')$. This is a contradiction to Observation 1 since $Ray(G') \ge Ray(G)$ and $n_1(G) = n_1(G')+1 > n_1(G')$. This contradiction proves Claim 1.

Claim 2. If $u \in V(G)$ is adjacent to a 1-vertex, then $d(u) \le 3$.
Proof of Claim 2. Assume on the contrary that $d(u) \ge 4$. Let $s = d(u)$ and v be the 1-vertex that is adjacent to u. Let $N(u) = \{v, u_2, \cdots, u_s\}$ and $G' = G - v \in \mathcal{U}_{n-1}^k$. Then

$$
\begin{aligned}
R(G)-R(G') &= \sum_{i=2}^{s}\frac{1}{\sqrt{d(u_i)d(u)}}+\frac{1}{\sqrt{d(u)}}-\sum_{i=2}^{s}\frac{1}{\sqrt{d(u_i)(d(u)-1)}} \\
&< \frac{1}{\sqrt{d(u)}} \le \frac{1}{2}.
\end{aligned}
$$

Hence, $R(G) < R(G')+\frac{1}{2}$. Since $G' \in \mathcal{U}_{n-1}^k$, by Observation 2 we have $R(G') \le R(G_{n-1}^k) = R(G_n^k)-\frac{1}{2}$. Therefore, $R(G) < R(G_n^k)$, a contradiction to Observation 1. This proves Claim 2.

Claim 3. $Ray(G) \ge 2$.
Proof of Claim 3. Since $n_1(G) \ge 2$, we have $Ray(G) \ge 1$. By contradiction, assume $Ray(G) = 1$. Then each 1-vertex is adjacent to some vertex of $C(G)$. By Claim 1, the degree of each vertex of $C(G)$ is either 2 or 3. Since $n_1(G) \ge 2$, let x, u be two 1-vertices and y, v be the neighbors of x, u, respectively. Then $d(v) = d(y) = 3$. Let $N(y) = \{y_1, y_2, x\}$ and $N(v) = \{v_1, v_2, u\}$. Clearly, $y_1, y_2 \in C(G)$, so $d(y_1) \le 3$ and $d(y_2) \le 3$. Consider $G' = G - xy + xu \in \mathcal{U}_n^k$. We have

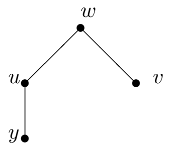
$$
\begin{aligned}
R(G)-R(G') &= \frac{1}{\sqrt{d(y_1)d(y)}}+\frac{1}{\sqrt{d(y_2)d(y)}}+\frac{1}{\sqrt{d(y)}}+\frac{1}{\sqrt{d(v)}} \\
&\quad -\frac{1}{\sqrt{d(y_1)(d(y)-1)}}-\frac{1}{\sqrt{d(y_2)(d(y)-1)}}-\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{2d(v)}} \\
&= \left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{d(y_1)}}+\frac{1}{\sqrt{d(y_2)}}\right)+\frac{2}{\sqrt{3}}-\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{6}} \\
&\le \frac{2}{\sqrt{3}}\left(\frac{1}{\sqrt{3}}-\frac{1}{\sqrt{2}}\right)+\frac{2}{\sqrt{3}}-\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{6}} \\
&< 0.
\end{aligned}
$$

Therefore $R(G) < R(G')$. Since $Ray(G') = Ray(G)+1 > Ray(G)$, by Observation 1 we have $R(G) \ge R(G')$, a contradiction. This proves Claim 3.

Claim 4. For each maximum ray $P = v_0v_1\cdots v_t$ of G, we have $d(v_{t-1}) = 2$.

It follows from Claims 2 and 3 and the maximality of the ray.

Claim 5. G does not contain the configuration in Figure 1.



$d(v) = d(y) = 1,\ d(u) = 2$

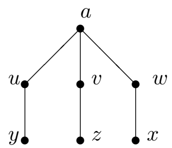
Figure 1

Proof of Claim 5. Suppose on the contrary that G contains the configuration in Figure 1. Then by Claim 2, $d(w) = 3$. Let $N(w) = \{z, u, v\}$. Let $G' = G - wv + yv \in \mathcal{U}_n^k$. We have

$$\begin{aligned} R(G) - R(G') &= \left(\frac{1}{\sqrt{3d(z)}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{\sqrt{2}}\right) - \left(\frac{1}{\sqrt{2d(z)}} + \frac{1}{2} + \frac{1}{2} + \frac{1}{\sqrt{2}}\right) \\ &< \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} - 1 < 0. \end{aligned}$$

Therefore $R(G) < R(G')$. Note that $Ray(G') \geq Ray(G)$ and $n_1(G') = n_1(G) - 1 < n_1(G)$. By Observation 1 we have $R(G') \leq R(G_n^k) \leq R(G)$. This contradiction proves Claim 5.

Claim 6. G does not contain the configuration in Figure 2.



$d(u) = d(v) = d(w) = 2,\ d(x) = d(y) = d(z) = 1$

Figure 2

Proof of Claim 6. Suppose on the contrary that G contains the configuration in Figure 2. Let $d = d(a)$. Clearly, $d \geq 4$. Let $N(a) = \{u, v, w, x_4, \ldots, x_d\}$. Let $G' = G - av - aw + vy + wz \in \mathcal{U}_n^k$. We have

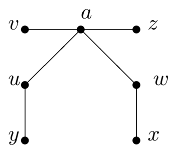
$$\begin{aligned} R(G') - R(G) &= \left(\frac{1}{\sqrt{2}} + 2 + \frac{1}{\sqrt{2(d-2)}} + \sum_{i=4}^{d} \frac{1}{\sqrt{d(x_i)(d-2)}}\right) \\ &\quad - \left(\frac{3}{\sqrt{2}} + \frac{3}{\sqrt{2d}} + \sum_{i=4}^{d} \frac{1}{\sqrt{d(x_i)d}}\right) \\ &> 2 - \sqrt{2} + \frac{1}{\sqrt{2(d-2)}} - \frac{3}{\sqrt{2d}} := g(d). \end{aligned}$$

Taking derivative of $g(d)$ we have

$$g'(d) = \frac{1}{2\sqrt{2}}\left(\frac{3}{\sqrt{d^3}} - \frac{1}{\sqrt{(d-2)^3}}\right) > 0,$$

when $d \geq 4$. It is easy to check that $g(4) > 0$. Hence $g(d) > 0$, i.e., $R(G') > R(G)$. Since $Ray(G') \geq Ray(G)$ and $n_1(G') < n_1(G)$, by Observation 1, we have $R(G') \leq R(G_n^k) \leq R(G)$. This contradiction proves Claim 6.

Claim 7. G does not contain the configuration in Figure 3.



$d(u) = d(w) = 2$, $d(x) = d(y) = 1$, $d(a) = 4, d(v) \leq 4, d(z) \leq 4$

Figure 3

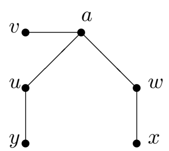
Proof of Claim 7. Suppose on that contrary that G contains a configuration in Figure 3. Let $G' = G - aw + yw$. We have

$$\begin{aligned}
R(G') - R(G) &= \left(\frac{1}{\sqrt{2}} + 1 + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}}\left(\frac{1}{\sqrt{d(v)}} + \frac{1}{\sqrt{d(z)}}\right)\right) \\
&\quad - \left(\sqrt{2} + \frac{1}{\sqrt{2}} + \frac{1}{2}\left(\frac{1}{\sqrt{d(v)}} + \frac{1}{\sqrt{d(z)}}\right)\right) \\
&= 1 + \frac{1}{\sqrt{6}} - \sqrt{2} + \left(\frac{1}{\sqrt{3}} - \frac{1}{2}\right)\left(\frac{1}{\sqrt{d(v)}} + \frac{1}{\sqrt{d(z)}}\right) \\
&\geq 1 + \frac{1}{\sqrt{6}} - \sqrt{2} + \left(\frac{1}{\sqrt{3}} - \frac{1}{2}\right)\left(\frac{1}{\sqrt{4}} + \frac{1}{\sqrt{4}}\right) \\
&= \frac{1}{2} + \frac{1}{\sqrt{6}} - \sqrt{2} + \frac{1}{\sqrt{3}} \\
&> 0,
\end{aligned}$$

so $R(G') > R(G)$.

On the other hand, notice that $Ray(G') \geq Ray(G)$ and $n_1(G') < n_1(G)$, by Observation 1, we also have $R(G') \leq R(G_n^k) \leq R(G)$. This contradiction proves Claim 7.

Claim 8. G does not contain the configuration in Figure 4.



$d(u) = d(w) = 2,\ d(x) = d(y) = 1,\ d(a) = 3, d(v) \le 30$

Figure 4

Proof of Claim 8. Assume that G contains a configuration in Figure 4. Let $G' = G - aw + yw \in \mathcal{U}_n^k$. We have

$$\begin{aligned} R(G') - R(G) &= \left(\frac{1}{\sqrt{2}} + \frac{3}{2} + \frac{1}{\sqrt{2d(v)}}\right) - \left(\sqrt{2} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3d(v)}}\right) \\ &= \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)\frac{1}{\sqrt{d(v)}} + \frac{1}{\sqrt{2}} + \frac{3}{2} - \sqrt{2} - \frac{2}{\sqrt{6}} \\ &\ge \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)\frac{1}{\sqrt{30}} + \frac{1}{\sqrt{2}} + \frac{3}{2} - \sqrt{2} - \frac{2}{\sqrt{6}} \\ &> 0, \end{aligned}$$

so $R(G') > R(G)$.

On the other hand, notice that $Ray(G') \ge Ray(G)$ and $n_1(G') < n_1(G)$, by Observation 1, we also have $R(G') \le R(G_n^k) \le R(G)$. This contradiction proves Claim 8.

Claim 9. $Ray(G) \ge 3$.

Proof of Claim 9. Suppose on the contrary that $Ray(G) \le 2$. Then by Claim 3, $Ray(G) = 2$.

We now argue that every vertex of $C(G)$ has degree ≤ 4. Let $v \in C(G)$. If $d(v) \ge 3$, then either v is adjacent to a 1-vertex or v is the initial vertex of $d(v) - 2$ maximum ray(s) (length= 2). For the first case, by Claim 2, we have $d(v) = 3$. For the second case, by Claim 6, we have $d(v) \le 4$.

Moreover, by Claim 1 and Claim 7, no two rays share a common vertex since $Ray(G) = 2$. Hence $\Delta(G) = 3$. If G has two maximum rays xyz and uvw where $x, u \in C(G)$, then $d(x) = d(u) = 3$, $d(y) = d(v) = 2$, and $d(z) = d(w) = 1$. Let $N(x) = \{y, x_1, x_2\}$ and $G' = G - xy + wy \in \mathcal{U}_n^k$. Note $Ray(G') > Ray(G)$, hence by Observation 1 $R(G') \le R(G_n^k) \le R(G)$. On the other hand, we also have

$$\begin{aligned} R(G') - R(G) &= \left(\frac{1}{\sqrt{2d(x_1)}} + \frac{1}{\sqrt{2d(x_2)}} + 1 + \frac{1}{\sqrt{2}}\right) - \left(\frac{1}{\sqrt{3d(x_1)}} + \frac{1}{\sqrt{3d(x_2)}} + \frac{1}{\sqrt{6}} + \frac{2}{\sqrt{2}}\right) \\ &= \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)\left(\frac{1}{\sqrt{d(x_1)}} + \frac{1}{\sqrt{d(x_2)}}\right) + 1 - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{6}} \end{aligned}$$

$$\begin{aligned}
&\geq \left(\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{3}}\right)\frac{2}{\sqrt{3}}+1-\frac{1}{\sqrt{2}}-\frac{1}{\sqrt{6}}\\
&> 0,
\end{aligned}$$

which is a contradiction. Thus G has only one maximum ray.

Since $n_1(G) \geq 2$, there exists a vertex $u \in C(G)$ that is adjacent to a 1-vertex, say v. Let xyz be a maximum ray with $d(y) = 2$, $d(z) = 1$, and $d(x) = 3$. Let $G'' = G - uv + zv \in \mathcal{U}_n^k$. Since $Ray(G'') = 3 > Ray(G)$, again by Observation 1 $R(G'') \leq R(G_n^k) \leq R(G)$. On the other hand, similarly to G', we can also show that $R(G'') > R(G)$. This contradiction proves Claim 9.

Claim 10. For each maximum ray $P = v_0v_1 \cdots v_{t-1}v_t$ of G, we have $d(v_{t-2}) = 3$ and $d(v_{t-3}) \geq 31$.

Proof of Claim 10. By Claim 9, $t \geq 3$, hence $v_{t-2} \notin C(G)$. Clearly $d(v_{t-2}) \geq 2$.

If $d(v_{t-2}) = 2$, we let G' be the graph obtained by identifying v_{t-2} with v_{t-1} and removing the loop. So $G' \in \mathcal{U}_{n-1}^k$. Since $G \neq G_n^k$, $G' \neq G_{n-1}^k$. Then by Observation 2 we have $R(G) - \frac{1}{2} = R(G') < R(G_{n-1}^k) = R(G_n^k) - \frac{1}{2} \leq R(G) - \frac{1}{2}$, a contradiction. So $d(v_{t-2}) \geq 3$.

Let $N(v_{t-2}) = \{v_{t-1}, v_{t-3}, x_3, \cdots, x_{d(v_{t-2})}\}$. By Claim 5, $d(x_i) \geq 2$ for each $i \geq 3$. For any $i \geq 3$, let $y \in N(x_i)$ and $y \neq v_{t-2}$. Then $v_0v_1 \cdots v_{t-2}x_iy$ must be a maximum ray since it has the same length as P does. Hence by Claim 4 we have $d(x_i) = 2$ and $d(y) = 1$. Moreover, by Claim 6 we have $d(v_{t-2}) = 3$ otherwise G contains a configuration in Figure 2.

Since $d(v_{t-2}) = 3$, by Claim 8 we have $d(v_{t-3}) \geq 31$.

Claim 11. Let $P = v_0v_1 \cdots v_t$ be a maximum ray of G. For each vertex $u \in N(v_{t-3})$ and $u \notin P \cup C(G)$, $d(u) \leq 3$.

Proof of Claim 11. For the sake of convenience, let $x = v_t$, $y = v_{t-1}$, $z = v_{t-2}$, and $w = v_{t-3}$. By Claims 4, 8, and 10, $d(x) = 1$, $d(y) = 2$, $d(z) = 3$, and $d(w) \geq 31$. Let $u \in N(w)$ and $u \notin P \cup C(G)$. Assume $d(u) \geq 4$. Then by Claim 2 we know that every neighbor of u has degree at least two. Let $N(u) = \{w, u_2, u_3, \cdots, u_{d(u)}\}$. Let $u_i' \in N(u_i)$ and $u_i' \neq u$ for $i = 2, \cdots d(u)$. Note that the path $v_0v_1 \cdots v_{t-3}uu_iu_i'$ is a maximum ray since it has the same length as P. Then by Claim 10, $d(u) = 3$, a contradiction. Therefore, $d(u) \leq 3$.

With all these preparations, now we can prove that such a counterexample G does not exist.

The final step. Let $P = v_0v_1 \cdots v_t$ be a maximum ray of G. Then by Claims 4 and 10, we have $d(v_t) = 1$, $d(v_{t-1}) = 2$, $d(v_{t-2}) = 3$, $d(v_{t-3}) \geq 31$. Let $w \in N(v_{t-3})$, and $w \notin C(G) \cup P$, then Claim 11 gives $d(w) \leq 3$. Since $d(v_{t-2}) = 3$, we let $N(v_{t-2}) = \{v_{t-1}, v_{t-3}, u\}$. By Claims 1, 5, and the maximality of P we know $d(u) = 2$. Let $N(u) = \{v_{t-2}, v\}$, then v must be a 1-vertex. Therefore, G contains a configuration in Figure 5

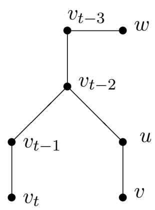


Figure 5

In this configuration, $d(v) = d(v_t) = 1$, $d(u) = d(v_{t-1}) = 2$, $d(v_{t-2}) = 3$, $d(v_{t-3}) \geq 31$, and $d(w) \leq 3$. Let $d = d(v_{t-3})$, $m = d(w)$, and $N(v_{t-3}) = \{v_{t-2}, w, x_3, \cdots x_d\}$. Let $G' = G - v_{t-3}w - v_{t-2}u + uv_t + v_{t-2}w \in \mathcal{U}_n^k$. We have

$$\begin{aligned} R(G') - R(G) &= \left(\sum_{i=3}^{d} \frac{1}{\sqrt{(d-1)d(x_i)}} + \frac{1}{\sqrt{3m}} + \frac{1}{\sqrt{3(d-1)}} + \frac{1}{\sqrt{6}} + \frac{2}{2} + \frac{1}{\sqrt{2}}\right) \\ &\quad - \left(\sum_{i=3}^{d} \frac{1}{\sqrt{dd(x_i)}} + \frac{1}{\sqrt{dm}} + \frac{1}{\sqrt{3d}} + \frac{2}{\sqrt{6}} + \frac{2}{\sqrt{2}}\right) \\ &> \frac{1}{\sqrt{3m}} - \frac{1}{\sqrt{dm}} + 1 - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} \\ &= \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{d}}\right)\frac{1}{\sqrt{m}} + 1 - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} \\ &\geq \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{31}}\right)\frac{1}{\sqrt{3}} + 1 - \frac{1}{\sqrt{6}} - \frac{1}{\sqrt{2}} \\ &> 0. \end{aligned}$$

On the other hand, it is clear that $Ray(G') > Ray(G)$, thus by Observation 1 we have $R(G') \leq R(G_n^k) \leq R(G)$.

This contradiction shows that such a counterexample does not exist, thus completes the proof of the theorem. ■

3 Lower bound of the Randić index of unicyclic graphs with a k-cycle

In this section we prove that $G_{n,n-k}$ has the smallest Randić index in $\mathcal{U}_n^k$.

Theorem 3.1 *Let $G \in \mathcal{U}_n^k$ where $3 \leq k \leq n$. If $G \neq G_{n,n-k}$, then $R(G) > R(G_{n,n-k}) = \frac{k-2}{2} + \frac{n-k+\sqrt{2}}{\sqrt{n-k+2}}$.*

Proof. With k fixed, we prove the theorem by doing induction on $n \geq k$.

When $n \leq k+2$ the claim can be easily checked to be true.

Now assume that it holds for $\mathcal{U}_{n-1}^k$.

Let $G \in \mathcal{U}_n^k$ and $G \neq G_{n,n-k}$.

If all pendant vertices of G are adjacent to $C(G)$, then G is a unicyclic graph with $n-k$ pendants. Thus by Theorem 1.1, we have $R(G) > R(G_{n,n-k})$.

Now suppose there are two vertices v_1 and u such that $d(v_1) = 1$, $u \in N(v_1)$, and $u \notin C(G)$. Let $d = d(u) \leq n-k$. Let $l \geq 1$ denote the number of non-pendant neighbors of u. Then $r = d - l - 1 \geq 0$ is the number of pendant neighbors of u except v_1.

Let $N(u) = \{v_1, v_2, \ldots, v_d\}$ such that $1 = d(v_1) = \ldots = d(v_{r+1}) < 2 \leq d(v_{r+2}) \leq \ldots \leq d(v_d)$.

Let $G' = G - v_1 \in \mathcal{U}_{n-1}^k$. By our induction hyperthesis, $R(G') \geq R(G_{n-1,n-k-1})$. We also have

$$\begin{aligned}
R(G) - R(G') &= \frac{1}{\sqrt{d}} + \sum_{i=2}^{d} \frac{1}{\sqrt{d(v_i)d}} - \sum_{i=2}^{d} \frac{1}{\sqrt{d(v_i)(d-1)}} \\
&= \frac{r+1}{\sqrt{d}} - \frac{r}{\sqrt{d-1}} + \sum_{i=2+r}^{d} \frac{1}{\sqrt{d(v_i)}} \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}} \right) \\
&\geq \frac{r+1}{\sqrt{d}} - \frac{r}{\sqrt{d-1}} + \frac{l}{\sqrt{2}} \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}} \right) \\
&= \frac{d-l}{\sqrt{d}} - \frac{d-1-l}{\sqrt{d-1}} + \frac{l}{\sqrt{2}} \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}} \right) \\
&= \sqrt{d} - \frac{l}{\sqrt{d}} - \sqrt{d-1} + \frac{l}{\sqrt{d-1}} + \frac{l}{\sqrt{2}} \left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}} \right) \\
&= \sqrt{d} - \sqrt{d-1} + l \left(\frac{1}{\sqrt{d-1}} - \frac{1}{\sqrt{d}} \right) - \frac{l}{\sqrt{2}} \left(\frac{1}{\sqrt{d-1}} - \frac{1}{\sqrt{d}} \right) \\
&= \sqrt{d} - \sqrt{d-1} + l \left(1 - \frac{1}{\sqrt{2}} \right) \left(\frac{1}{\sqrt{d-1}} - \frac{1}{\sqrt{d}} \right) \\
&> \sqrt{d} - \sqrt{d-1} \\
&= \frac{1}{\sqrt{d} + \sqrt{d-1}} \\
&\geq \frac{1}{\sqrt{n-k} + \sqrt{n-k-1}} \\
&= \sqrt{n-k} - \sqrt{n-k-1}.
\end{aligned}$$

So

$$\begin{aligned}
R(G) &> R(G') + \sqrt{n-k} - \sqrt{n-k-1} \\
&\geq R(G_{n-1,n-k-1}) + \sqrt{n-k} - \sqrt{n-k-1} \\
&= \frac{k-2}{2} + \frac{n-k-1+\sqrt{2}}{\sqrt{n-k+1}} + \sqrt{n-k} - \sqrt{n-k-1}
\end{aligned}$$

$$\begin{aligned}
&= \frac{k-2}{2} + \frac{n-k+\sqrt{2}}{\sqrt{n-k+2}} - \frac{n-k+\sqrt{2}}{\sqrt{n-k+2}} + \frac{n-k-1+\sqrt{2}}{\sqrt{n-k+1}} + \sqrt{n-k} - \sqrt{n-k-1} \\
&= R(G_{n,n-k}) - \frac{n-k+2-2+\sqrt{2}}{\sqrt{n-k+2}} + \frac{n-k+1-2+\sqrt{2}}{\sqrt{n-k+1}} + \sqrt{n-k} - \sqrt{n-k-1} \\
&= R(G_{n,n-k}) + \left(\sqrt{n-k} - \sqrt{n-k-1}\right) - \left(\sqrt{n-k+2} - \sqrt{n-k+1}\right) \\
&\quad -(2-\sqrt{2})\left(\frac{1}{\sqrt{n-k+1}} - \frac{1}{\sqrt{n-k+2}}\right).
\end{aligned}$$

Consider $f(x) = \sqrt{x} - \sqrt{x-1}$ where $x \geq 2$. Clearly

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

is an increasing function.

By the mean value theorem we have

$$\begin{aligned}
&\left(\sqrt{n-k} - \sqrt{n-k-1}\right) - \left(\sqrt{n-k+2} - \sqrt{n-k+1}\right) \\
&= f(n-k) - f(n-k+2) \\
&= -2f'(\xi) \qquad \xi \in (n-k, n-k+2) \\
&\geq -2f'(n-k+2) \\
&= \frac{1}{\sqrt{n-k+1}} - \frac{1}{\sqrt{n-k+2}}.
\end{aligned}$$

Hence

$$\begin{aligned}
R(G) &> R(G_{n,n-k}) + \frac{1}{\sqrt{n-k+1}} - \frac{1}{\sqrt{n-k+2}} - (2-\sqrt{2})\left(\frac{1}{\sqrt{n-k+1}} - \frac{1}{\sqrt{n-k+2}}\right) \\
&= R(G_{n,n-k}) + (\sqrt{2}-1)\left(\frac{1}{\sqrt{n-k+1}} - \frac{1}{\sqrt{n-k+2}}\right) \\
&> R(G_{n,n-k}),
\end{aligned}$$

which completes the proof. ■

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