Unicyclic Graphs with Maximum General Randić Index for $\alpha > 0$ *

Xueliang Li, Yongtang Shi, Tianyi Xu

Center for Combinatorics and LPMC

Nankai University, Tianjin 300071, P.R. China

(Received March 16, 2006)

Dedicated to Prof. Fuji Zhang on the occasion of his 70th birthday

Abstract

The general Randić index $R_\alpha(G)$ of a graph G is defined as the sum of the weights $(d(u)d(v))^\alpha$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G and α is an arbitrary real number. In this paper, we show that among all unicyclic graphs with n vertices, S_n^+ has the maximum general Randić index for $0 < \alpha < 1$, where S_n^+ denotes the unicyclic graph obtained from the star S_n on n vertices by joining its two vertices of degree one; $T_{\lceil \frac{n+1}{2} \rceil, \lfloor \frac{n+1}{2} \rfloor}$ has the maximum general Randić index for $\alpha > 2$ and $n \geq 7$, where $T_{\lceil \frac{n+1}{2} \rceil, \lfloor \frac{n+1}{2} \rfloor}$ is a triangle with two balanced leaf branches. For $1 < \alpha \leq 2$, we also give the structure description for the graphs with maximum general Randić index. The case for $\alpha < 0$ is much more complicated and left for further study.

*Supported by National Science Foundation of China.

1 Introduction

For a (molecular) graph $G = (V, E)$, the *general Randić index* $R_\alpha(G)$ of G is defined as the sum of $(d(u)d(v))^\alpha$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u of G, i.e., $R_\alpha(G) = \sum_{uv\in E}(d(u)d(v))^\alpha$, where α is an arbitrary real number.

It is well known that $R_{-\frac{1}{2}}$ was introduced by Randić [9] in 1975 as one of the many graph-theoretical parameters derived from the graph underlying some molecule. Later, in 1998 Bollobás and Erdös [1] generalized this index by replacing $-\frac{1}{2}$ with any real number α, which is called the general Randić index. The research background of Randić index together with its generalization appears in chemistry or mathematical chemistry and can be found in the literature (see [1],[2], [9]). Recently, finding bounds for the general Randić index of a given class of graphs, as well as related problem of finding the graphs with maximum or minimum general Randić index, attracted the attention of many researchers, and many results have been obtained (see [1]-[2], [4]-[10]).

A simple connected graph G is called *unicyclic* if it contains exactly one cycle. From this definition, one can see that a unicyclic graph has the same number of vertices and edges, and it is a cycle or a cycle with trees attached to its vertices. For $n \geq 3$, let S_n^+ denote the unicyclic graph obtained from the star S_n on n vertices by joining its two vertices of degree one. For $\alpha = -\frac{1}{2}$, Gao and Lu [4] showed that for a unicyclic graph G, $R_{-\frac{1}{2}}(G) \geq (n-3)(n-1)^{-\frac{1}{2}} + 2(2n-2)^{-\frac{1}{2}} + \frac{1}{2}$, and the equality holds if and only if $G \cong S_n^+$. For general α, Wu and Zhang [10] showed that among unicyclic graphs on n vertices, the cycle C_n for $\alpha > 0$ and S_n^+ for $-1 \leq \alpha < 0$, respectively, has the minimum general Randić index. For $\alpha < -1$, they gave the structure description of the unicyclic graphs with minimum general Randić index. But, unfortunately, they could not determine which of them can achieve the minimum value. Li, Wang and Zhang [7] completely solved the case for $\alpha < -1$, which was left unsolved by Wu and Zhang [10].

In this paper, we focus on investigating the unicyclic graphs with maximum general Randić index for $\alpha > 0$. The case for $\alpha < 0$ is much more complicated and left for further study. For convenience, we need some additional notations and terminologies. Denote by $d(u)$ and $N(u)$ the degree and neighborhood of the vertex u, respectively. A vertex of degree 1 in a graph is called a *leaf vertex* (or simply, a *leaf*) and the edge incident with the leaf is called a *leaf edge*. A vertex adjacent to some leaf vertices is called a *leaf branch*. The class $\mathcal{G}$ of graphs is defined as follows: $\mathcal{G}$ consists of the unicyclic graphs each of which has a triangle as its unique cycle, and the vertices not on the cycle are leaves. A graph in class $\mathcal{G}$ is called a *triangle with leaves*, denoted by $T_{a,b,c}$, where a, b and c are nonnegative integers that denote the degrees of the vertices on the triangle, respectively. And we have $a+b+c=n+3$. Obviously, if two of the three numbers a,b,c are 2, then the graph is S_n^+. Particularly, if $c=2$, a triangle with two leaf branches $T_{a,b,2}$ is simply $T_{a,b}$. $T_{a,b}$ is balanced if $|a-b|\leq 1$, i.e., $T_{a,b}=T_{\lceil\frac{n+1}{2}\rceil,\lfloor\frac{n+1}{2}\rfloor}$. Undefined notations and terminologies can be found in [3].

2 The case for $0<\alpha<1$

Following the proof idea and technique completely similar to those in [10], we can show the following lemmas and get our Theorem 2.6. Their proofs are omitted.

Lemma 2.1 *Suppose that the star S_n, $n\geq 2$, is disjoint from a graph G and v is its center. For a vertex $u\in V(G)$, let $G_1=G\bigcup S_n+uv$, and G_2 be the graph obtained from G by attaching a star S_{n+1} to the vertex u with u as its center as shown in Figure 2.1. If u is not an isolated vertex, then $R_\alpha(G_2)>R_\alpha(G_1)$ for $0<\alpha<1$.*

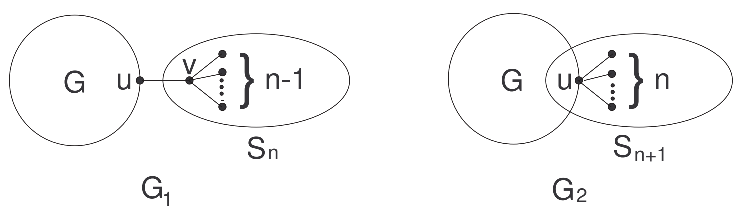

Figure 2.1

By Lemma 2.1, we have the following Lemma.

Lemma 2.2 *Assume G has the maximum general Randić index among unicyclic graphs of order n. If T is a tree attached to a vertex v of the unique cycle in G, then T must be a star with v as its center.*

Let G_1 be a unicyclic graph with the unique cycle C and S_{a+1}, S_{b+1} are the two stars attached to two vertices u and w of C, respectively. Assume the two paths between u

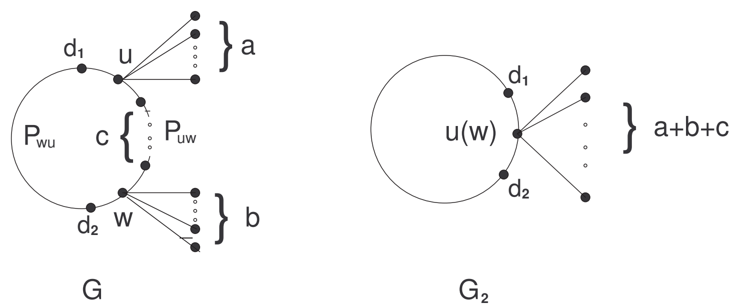

Figure 2.2

and w on C are P_{uw} and P_{wu}. Suppose the degrees of all vertices on P_{uw} are two (if there exists such vertex) in G, $|E(P_{uw})| = c$ and $|E(P_{wu})| \geq 3$. Now transform G_1 into a new unicyclic graph G_2 as follows: contract the path P_{uw} into one vertex $u(w)$, and attach a star $S_{a+b+c+1}$ to it (see Figure 2.2). Next we show that this transformation will increase the value of the general Randić index of the graph for $0 < \alpha < 1$.

Lemma 2.3 *Let G_1 and G_2 be the two unicyclic graphs described above. If $a, b \geq 1$, then $R_\alpha(G_2) > R_\alpha(G_1)$ for $0 < \alpha < 1$.*

It is easy to verify the following lemma.

Lemma 2.4 *Let G_1 and G_2 be two unicyclic graphs with the same order n, and their unique cycles are i-cycle and $(i-1)$-cycle respectively, $i \geq 4$. Furthermore, for each of the two graphs, the vertices not on the cycle are leaves adjacent to exactly one vertex of the cycle. Then $R_\alpha(G_2) > R_\alpha(G_1)$ for $0 < \alpha < 1$.* ∎

Lemma 2.5 *Let H_1, H_2, H_3 be three unicyclic graphs, each of which has a 4-cycle as its unique cycle, and the vertices not on the cycle are leaves that are neighbors of two nonadjacent vertices of the cycle, as shown in Figure 2.3. If $a \geq b \geq 1$, then $R_\alpha(H_3) > R_\alpha(H_1)$ for $0 < \alpha < 1$.*

From Lemmas 2.2, 2.3, 2.4 and 2.5, we conclude that

Theorem 2.6 *For $0 < \alpha < 1$, the unicyclic graph with maximum general Randić index must be in $\mathcal{G}$.* ∎

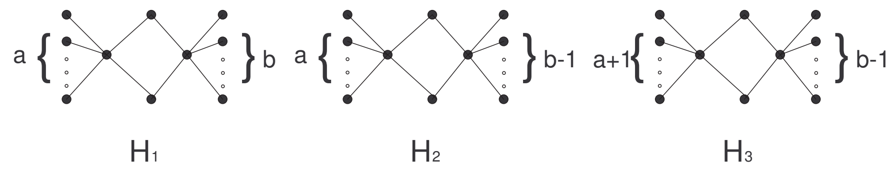

Figure 2.3

It is easy to show the following lemma by elementary calculus.

Lemma 2.7 *Let $f(x) = x^{\alpha-1}(x + b^{\alpha} - 2)$, $0 < \alpha < 1$, $b^{\alpha} > 2$. Then $f(x)$ is monotonously increasing for $x \geq b-1$.* ∎

Theorem 2.8 *Among all the unicyclic graphs, S_n^+ has the maximum general Randić index for $0 < \alpha < 1$.*

Proof. Suppose that G is the unicyclic graph with maximum general Randić index, but not S_n^+. By Theorem 2.6, $G = T_{a,b,c}$ for some integers a, b, c, and without lose of generality, suppose $a \geq c = n+3-a-b \geq b$, then $c \geq 3$. We have

$$\begin{aligned} R_\alpha(T_{a,b,c}) &= R_\alpha(T_{a,b,n+3-a-b}) = (a-2)a^\alpha + (b-2)b^\alpha \\ &\quad +(n+1-a-b)(n+3-a-b)^\alpha + \ a^\alpha b^\alpha + (a^\alpha + b^\alpha)(n+3-a-b)^\alpha. \end{aligned}$$

Define $f(x) = (x-2)x^\alpha + (b-2)b^\alpha + (n+1-b-x)(n+3-b-x)^\alpha + x^\alpha b^\alpha + (x^\alpha + b^\alpha)(n+3-b-x)^\alpha$, where $x \geq n+3-b-x$ and $x \geq b$. Then

$$\begin{aligned} f'(x) &= (\alpha+1)[x^\alpha - (n+3-b-x)^\alpha] - \alpha(b^\alpha - 2)[(n+3-b-x)^{\alpha-1} - x^{\alpha-1}] \\ &\quad -\alpha x^{\alpha-1}(n+3-b-x)^{\alpha-1}[x-(n+3-b-x)]. \end{aligned}$$

Case 1: $b^\alpha \leq 2$.

If $x = n+3-b-x$, i.e., $x = (n+3-b)/2$, then $f'(x) = 0$.

If $x > n+3-b-x$, by the mean-value theorem, $x^\alpha - (n+3-b-x)^\alpha = \alpha\xi^{\alpha-1}[x-(n+3-b-x)]$, where $\xi \in (n+3-b-x, x)$.

$$\begin{aligned} f'(x) &= \alpha\xi^{\alpha-1}[x-(n+3-b-x)] - \alpha x^{\alpha-1}(n+3-b-x)^{\alpha-1}[x-(n+3-b-x)] \\ &\quad +\alpha[x^\alpha - (n+3-b-x)^\alpha] + \alpha(2-b^\alpha)[(n+3-b-x)^{\alpha-1} - x^{\alpha-1}] \\ &> \alpha[x-(n+3-b-x)](\xi^{\alpha-1} - x^{\alpha-1}) + \alpha[x^\alpha - (n+3-b-x)^\alpha] \\ &\quad +\alpha(2-b^\alpha)[(n+3-b-x)^{\alpha-1} - x^{\alpha-1}]. \end{aligned}$$

Since $0 < \alpha < 1$, $n+3-b-x < \xi < x$ and $b^\alpha \leq 2$, we have $f'(x) > 0$.

Therefore, $R_\alpha(T_{a+1,b,c-1}) > R_\alpha(T_{a,b,c})$, a contradiction.

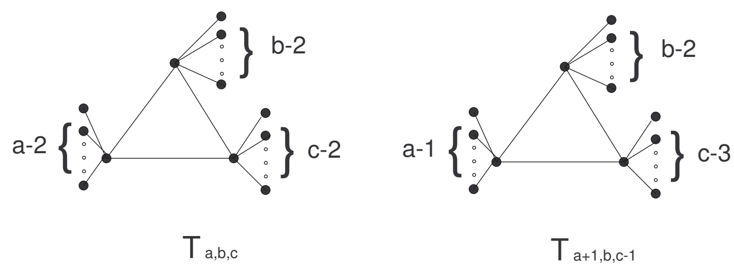

Figure 2.4

Case 2: $b^\alpha > 2$.

If $x = n+3-b-x$, i.e., $x = (n+3-b)/2$, then $f'(x) = 0$.

If $x > n+3-b-x$, by the mean-value theorem, $x^\alpha - (n+3-b-x)^\alpha = \alpha\xi^{\alpha-1}[x - (n+3-b-x)]$, where $\xi \in (n+3-b-x, x)$.

$$\begin{aligned} f'(x) &= \alpha\xi^{\alpha-1}[x-(n+3-b-x)] - \alpha x^{\alpha-1}(n+3-b-x)^{\alpha-1}[x-(n+3-b-x)] \\ &\quad +\alpha[x^\alpha - (n+3-b-x)^\alpha] + \alpha(2-b^\alpha)[(n+3-b-x)^{\alpha-1} - x^{\alpha-1}] \\ &> \alpha[x-(n+3-b-x)](\xi^{\alpha-1} - x^{\alpha-1}) \\ &\quad +\alpha[x^{\alpha-1}(x+b^\alpha-2) - (n+3-b-x)^{\alpha-1}(n+3-b-x+b^\alpha-2)]. \end{aligned}$$

By Lemma 2.7, we have $x^{\alpha-1}(x+b^\alpha-2)-(n+3-b-x)^{\alpha-1}(n+3-b-x+b^\alpha-2) > 0$, thus $f'(x) > 0$. Hence, $R_\alpha(T_{a+1,b,c-1}) > R_\alpha(T_{a,b,c})$, a contradiction. The proof is complete.▮

3 The case for $\alpha > 1$

Lemma 3.1 *Suppose a unicyclic graph G has a path $v_1v_2v_3$ such that $d(v_1) = i > 1$, $d(v_3) = q > 1$, $v_1v_3 \notin E(G)$ and $N(v_1) \cap N(v_3) = \emptyset$. Let $N(v_1) \setminus v_2 = \{u_1, u_2, \cdots, u_{i-1}\}$, $N(v_3) \setminus v_2 = \{w_1, w_2, \cdots, w_{q-1}\}$. By deleting the edges v_3w_1, v_3w_2, $\cdots$, v_3w_{q-1}, and adding the new edges v_1w_1, v_1w_2, $\cdots$, v_1w_{q-1}, we get a new unicyclic graph G', as shown in Figure 3.1. Then $R_\alpha(G') > R_\alpha(G)$.*

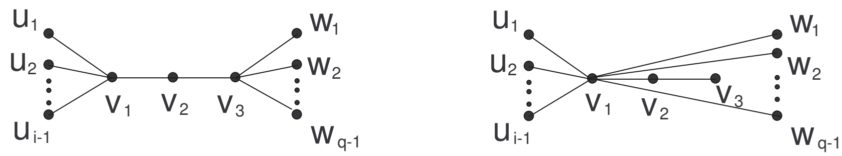

Figure 3.1

Proof. Let $d(v_2) = j$. Considering the values of the general Randić index of G and G', we have

$$\begin{aligned} R_\alpha(G') - R_\alpha(G) &= (i+q-1)^\alpha(\sum_{k=1}^{i-1} d(u_k)^\alpha + \sum_{k=1}^{q-1} d(w_k)^\alpha) + (i+q-1)^\alpha j^\alpha + j^\alpha \\ &\quad - i^\alpha \sum_{k=1}^{i-1} d(u_k)^\alpha - q^\alpha \sum_{k=1}^{q-1} d(w_k)^\alpha - (ij)^\alpha - (qj)^\alpha \\ &\geq (i+q-1)^\alpha j^\alpha + j^\alpha - (ij)^\alpha - (qj)^\alpha = j^\alpha((i+q-1)^\alpha - i^\alpha - q^\alpha + 1) = j^\alpha f(i,q). \end{aligned}$$

Without lose of generality, suppose $i \geq q$. $f(i,q) = ((i+q-1)^\alpha - i^\alpha) - (q^\alpha - 1) = \alpha(q-1)(\xi_1^{\alpha-1} - \xi_2^{\alpha-1}) > 0$, where $\xi_1 \in (i, i+q-1)$, $\xi_2 \in (1, q)$. ∎

From Lemma 3.1, we conclude that

Lemma 3.2 *Let G be the unicyclic graph with maximum general Randić index, then the unique cycle of G must be 3-cycle or 4-cycle, and the vertices not on cycle are leaves.*

Now we will show that the unique cycle of the extremal graph is not a 4-cycle.

Theorem 3.3 *For $\alpha > 1$, the unicyclic graph with the maximum general Randić index must be in $\mathcal{G}$.*

Proof. By contradiction, suppose that G is the unicyclic graph with the maximum general Randić index and the unique cycle of G is $v_1v_2v_3v_4$. Denote by a, b, c and d the numbers of the leaves of vertices v_1, v_2, v_3 and v_4, respectively, as shown in Figure 3.2.

Case 1: $a, c > 0$ or $b, d > 0$

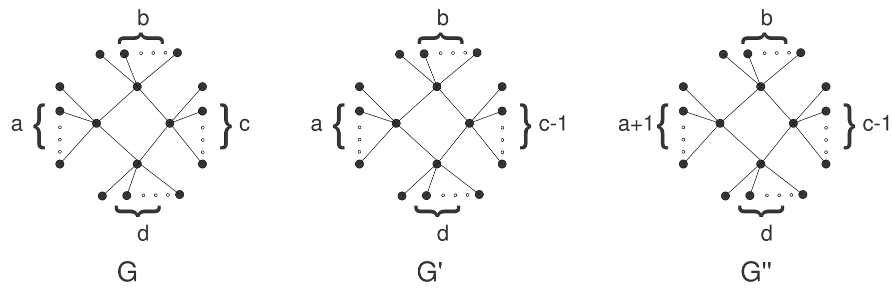

Figure 3.2

Assume $a \geq c > 0$. Let G' and G'' be the unicyclic graphs as shown in Figure 3.2. We have

$$\begin{aligned}
R_\alpha(G) &= a(a+2)^\alpha + b(b+2)^\alpha + c(c+2)^\alpha + d(d+2)^\alpha \\
&\quad +(a+2)^\alpha((b+2)^\alpha + (d+2)^\alpha) + (c+2)^\alpha((b+2)^\alpha + (d+2)^\alpha) \\
R_\alpha(G') &= a(a+2)^\alpha + b(b+2)^\alpha + (c-1)(c+1)^\alpha + d(d+2)^\alpha \\
&\quad +(a+2)^\alpha((b+2)^\alpha + (d+2)^\alpha) + (c+1)^\alpha((b+2)^\alpha + (d+2)^\alpha) \\
R_\alpha(G'') &= (a+1)(a+3)^\alpha + b(b+2)^\alpha + (c-1)(c+1)^\alpha + d(d+2)^\alpha \\
&\quad +(a+3)^\alpha((b+2)^\alpha + (d+2)^\alpha) + (c+1)^\alpha((b+2)^\alpha + (d+2)^\alpha)
\end{aligned}$$

Let $f(x) = (x + (b+2)^\alpha + (d+2)^\alpha)(x+2)^\alpha$. Thus,

$$\begin{aligned}
R_\alpha(G) - R_\alpha(G') &= (c + (b+2)^\alpha + (d+2)^\alpha)(c+2)^\alpha \\
&\quad -(c - 1 + (b+2)^\alpha + (d+2)^\alpha)(c+1)^\alpha \\
&= f(c) - f(c-1) = f'(\xi_1), \\
R_\alpha(G'') - R_\alpha(G') &= (a + 1 + (b+2)^\alpha + (d+2)^\alpha)(a+3)^\alpha \\
&\quad -(a + (b+2)^\alpha + (d+2)^\alpha)(a+2)^\alpha \\
&= f(a+1) - f(a) = f'(\xi_2),
\end{aligned}$$

where $\xi_1 \in (c-1, c)$ and $\xi_2 \in (a, a+1)$. By $a \geq c \geq 1$, $\alpha > 1$ and since

$$\begin{aligned}
f''(x) &= \alpha(x+2)^{\alpha-2}(2(x+2) - (1-\alpha)(x + (b+2)^\alpha + (d+2)^\alpha)) \\
&= \alpha(x+2)^{\alpha-2}((1+\alpha)x + 4 + (\alpha-1)((b+2)^\alpha + (d+2)^\alpha)) > 0
\end{aligned}$$

for any $x > 0$, we know that $f'(\xi_2) > f'(\xi_1)$, which implies that $R_\alpha(G'') > R_\alpha(G)$ for $\alpha > 1$, a contradiction.

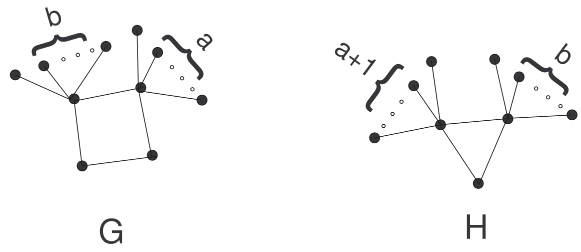

Figure 3.3

Case 2: Otherwise, suppose $c = d = 0$ and $a \geq b \geq 0$.

Let H be the unicyclic graph as shown in Figure 3.3. For $a \geq 1$, we have

$$\begin{aligned}
& R_\alpha(H) - R_\alpha(G) \\
= \ & (a+1)(a+3)^\alpha + b(b+2)^\alpha + (a+3)^\alpha(b+2)^\alpha + 2^\alpha((a+3)^\alpha + (b+2)^\alpha) \\
& -a(a+2)^\alpha - b(b+2)^\alpha - (a+2)^\alpha(b+2)^\alpha - 2^\alpha((a+2)^\alpha + (b+2)^\alpha) - 4^\alpha \\
> \ & (a+3)^\alpha - 4^\alpha \geq 0.
\end{aligned}$$

And it is easy to verify that the inequality holds for $a = b = 0$, a contradiction. ∎

In the following, we only consider the case $\alpha > 2$.

Lemma 3.4 *For $\alpha > 2$, we have*
(i) for $n \geq 7$, $R_\alpha(S_n^+) < R_\alpha(T_{\lceil \frac{n+1}{2} \rceil, \lfloor \frac{n+1}{2} \rfloor})$;
(ii) for $n = 5$ and $n = 6$, when $\alpha \geq \alpha'$, $R_\alpha(S_n^+) < R_\alpha(T_{\lceil \frac{n+1}{2} \rceil, \lfloor \frac{n+1}{2} \rfloor})$; when $2 < \alpha < \alpha'$, $R_\alpha(T_{\lceil \frac{n+1}{2} \rceil, \lfloor \frac{n+1}{2} \rfloor}) < R_\alpha(S_n^+)$, where α' is the root of equation $R_\alpha(T_{\lceil \frac{n+1}{2} \rceil, \lfloor \frac{n+1}{2} \rfloor}) = R_\alpha(S_n^+)$.

Proof. When $n-3$ is even, suppose that $n-3 = 2k$. Let $f(k) = R_\alpha(T_{k+2,k+2}) - R_\alpha(S_n^+) = 2(k+2)^{\alpha+1} + (2^{\alpha+1}-4)(k+2)^\alpha + (k+2)^{2\alpha} - [2^{\alpha+1}(k+1)^{\alpha+1} + 2^\alpha(2^{\alpha+1} - 2)(k+1)^\alpha + 4^\alpha]$. We have

$$\begin{aligned}
& f'(k) = 2(\alpha+1)(k+2)^\alpha + \alpha(2^{\alpha+1}-4)(k+2)^{\alpha-1} + 2\alpha(k+2)^{2\alpha-1} \\
& \qquad -[(\alpha+1)2^{\alpha+1}(k+1)^\alpha + \alpha 2^\alpha(2^{\alpha+1}-2)(k+1)^{\alpha-1}] \\
> \ & [\alpha(k+2)^\alpha(k+2)^{\alpha-1} - (\alpha+1)2^{\alpha+1}(k+1)^\alpha] \\
& +[\alpha(k+2)^\alpha(k+2)^{\alpha-1} - \alpha 2^\alpha(2^{\alpha+1}-2)(k+1)^{\alpha-1}] \\
> \ & [\alpha(k+2)^{\alpha-1} - (\alpha+1)2^{\alpha+1}] + \alpha[(k+2)^\alpha - 2^\alpha(2^{\alpha+1}-1)].
\end{aligned}$$

We consider the case of $k \geq 4$. Since $\alpha > 2$,

$$\begin{aligned} f'(k) &> \alpha 6^{\alpha-1} - (\alpha+1)2^{\alpha+1} + \alpha 6^{\alpha} - \alpha 2^{\alpha}(2^{\alpha+1}-1) \\ &= 7\alpha 6^{\alpha-1} - \alpha 2^{\alpha+1} - \alpha 2^{2\alpha+1} + (\alpha 2^{\alpha} - 2^{\alpha+1}) \\ &> \alpha 2^{\alpha-1}[7 \cdot 3^{\alpha-1} - 4 - 2^{\alpha+2}] = \alpha 2^{\alpha-1}[(2 \cdot 3^{\alpha} - 2^{\alpha+2}) + (3^{\alpha-1} - 4)] \\ &\geq \alpha 2^{\alpha-1}[2-1] > 0. \end{aligned}$$

Since $f(4) > 0$, then $f(k) > f(4) > 0$ when $k \geq 4$. For $k = 2$ and $k = 3$, we can verify $f(k) > 0$.

So, for $k \geq 2$, i.e., $n \geq 7$, $f(k) > 0$, and we have $R_\alpha(S_n^+) < R_\alpha(T_{\lceil \frac{n+1}{2} \rceil, \lfloor \frac{n+1}{2} \rfloor})$.

For $k = 1$, we have $f(1) = 2 \cdot 3^{\alpha} + (2 \cdot 6^{\alpha} - 3 \cdot 4^{\alpha}) + (9^{\alpha} - 2 \cdot 8^{a})$. When $\alpha \geq 6$, $9^{\alpha} - 2 \cdot 8^{a} > 0$, so $f(1) > 0$; when $2 < \alpha < 6$, by a Maple program, we can verify that when $\alpha' < \alpha < 6$, $f(1) > 0$, and when $2 < \alpha < \alpha'$, $f(1) < 0$, where α' is the root of equation $f(1) = 0$, i.e., when $\alpha \geq \alpha'$, $R_\alpha(S_5^+) < R_\alpha(T_{3,3})$; when $2 < \alpha < \alpha'$, $R_\alpha(T_{3,3}) < R_\alpha(S_5^+)$.

By the same method, we have similar conclusion for $n - 3$ odd. The details are omitted. ∎

Lemma 3.5 *For $\alpha > 2$ and $1 \leq x \leq y = n - x - 3$, $R_\alpha(T_{x+2,y+2}) < R_\alpha(T_{\lceil \frac{n+1}{2} \rceil, \lfloor \frac{n+1}{2} \rfloor})$.*

Proof. **Case 1:** $x = 1$ (see Figure 3.4)

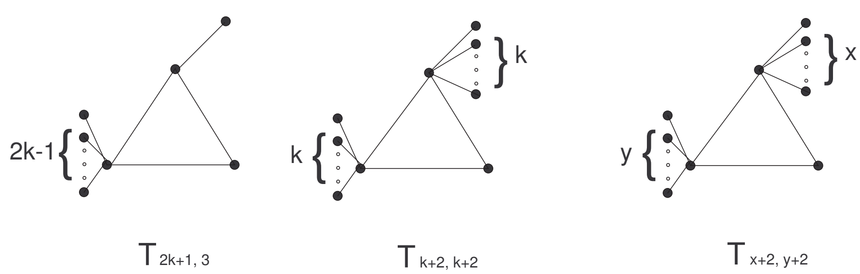

Figure 3.4

We only consider the case for $n - 3$ even, since the case for $n - 3$ odd is similar. In this case, let $f(k) = R_\alpha(T_{k+2,k+2}) - R_\alpha(T_{2k+1,3})$, by using the same method as Lemma 3.4, we have the following result: When $k \geq 5$, $f'(k) > 0$. Since $f(5) > 0$,

$f(k) > f(5) > 0$ when $k \geq 5$. For $k=2$, $k=3$ and $k=4$, we can directly verify that $R_\alpha(T_{n-1,2}) < R_\alpha(T_{\lceil \frac{n+1}{2} \rceil, \lfloor \frac{n+1}{2} \rfloor})$.

Case 2: $x \geq 2$ (see Figure 3.4)

Let $f(x) = R_\alpha(T_{x+2,y+2})$, i.e., $f(x) = (x+2)^{\alpha+1} + (n-x-1)^{\alpha+1} + (2^\alpha - 2)[(x+2)^\alpha + (n-x-1)^\alpha] + (x+2)^\alpha (n-x-1)^\alpha$. We have

$$
\begin{aligned}
f'(x) &= (\alpha+1)[(x+2)^\alpha - (n-x-1)^\alpha] + \alpha(2^\alpha-2)[(x+2)^{\alpha-1} - (n-x-1)^{\alpha-1}] \\
&\quad + \alpha(x+2)^{\alpha-1}(n-x-1)^{\alpha-1}(n-2x-3) \\
&= \alpha(x+2)^{\alpha-1}(n-x-1)^{\alpha-1}(n-2x-3) - \alpha(\alpha+1)(n-2x-3)\xi_1^{\alpha-1} \\
&\quad - \alpha(\alpha-1)(2^\alpha-2)(n-2x-3)\xi_2^{\alpha-2},
\end{aligned}
$$

where $\xi_1, \xi_2 \in (x+2, n-x-1)$. Since $\alpha > 2$ and $2 \leq x \leq y = n-x-3$, we have

$$f'(x) = \alpha(n-2x-3)[(x+2)^{\alpha-1}(n-x-1)^{\alpha-1} - (\alpha+1)\xi_1^{\alpha-1} - (\alpha-1)(2^\alpha-2)\xi_2^{\alpha-2}].$$

Let $g(x) = (x+2)^{\alpha-1}(n-x-1)^{\alpha-1} - (\alpha+1)\xi_1^{\alpha-1} - (\alpha-1)(2^\alpha-2)\xi_2^{\alpha-2}$, we have

$$
\begin{aligned}
g(x) &\geq (x+2)^{\alpha-1}(n-x-1)^{\alpha-1} \\
&\quad - (\alpha+1)(n-x-1)^{\alpha-1} - (\alpha-1)(2^\alpha-2)(n-x-1)^{\alpha-2} \\
&= (n-x-1)^{\alpha-2}[(n-x-1)((x+2)^{\alpha-1} - (\alpha+1)) - (\alpha-1)(2^\alpha-2)] \\
&\geq (n-x-1)^{\alpha-2}[(x+2)(4^{\alpha-1} - (\alpha+1)) - (\alpha-1)(2^\alpha-2)] \\
&\geq (n-x-1)^{\alpha-2}[4^\alpha - 4(\alpha+1) - (\alpha-1)(2^\alpha-2)] \\
&= (n-x-1)^{\alpha-2}[4^\alpha - \alpha 2^\alpha + 2^\alpha - 2\alpha - 6] > 0.
\end{aligned}
$$

Then $f'(x) > 0$ for $x < n-x-3 = y$. Therefore $R_\alpha(T_{x+2,y+2}) < R_\alpha(T_{\lceil \frac{n+1}{2} \rceil, \lfloor \frac{n+1}{2} \rfloor})$. The proof is thus complete. ∎

Lemma 3.6 *For $\alpha > 2$ and $y \geq x \geq n+3-x-y > 2$, there exists an integer $2 \leq a \leq n-1$, such that $R_\alpha(T_{x,y,n+3-x-y}) < R_\alpha(T_{a,n+1-a})$.*

Proof. **Case 1:** $y - x \geq n+3-y-x$

Now we will prove that $f(x) = R_\alpha(T_{x,y,n+3-x-y})$ is an increasing function of x when $\alpha > 2$. Let $A = n+3-y$, we have

$$f(x) = (x-2)x^\alpha + (y-2)y^\alpha + (A-x-2)(A-x)^\alpha + x^\alpha(A-x)^\alpha + y^\alpha(x^\alpha + (A-x)^\alpha).$$

Consider

$$\begin{aligned}
f'(x) &= (\alpha+1)x^{\alpha} - 2\alpha x^{\alpha-1} - (\alpha+1)(A-x)^{\alpha} + 2\alpha(A-x)^{\alpha-1} \\
&\quad + \alpha x^{\alpha-1}(A-x)^{\alpha} - \alpha x^{\alpha}(A-x)^{\alpha-1} + \alpha y^{\alpha}(x^{\alpha-1} - (A-x)^{\alpha-1}) \\
&= \alpha(\alpha+1)(x-(A-x))\xi_1^{\alpha-1} \\
&\quad + \alpha(x-(A-x))[(\alpha-1)(y^{\alpha}-2)\xi_2^{\alpha-2} - x^{\alpha-1}(A-x)^{\alpha}],
\end{aligned}$$

where $\xi_1, \xi_2 \in (A-x, x)$. Since $\alpha > 2$ and $y \geq x \geq A-x$, we have

$$\begin{aligned}
f'(x) &> \alpha(\alpha+1)(x-(A-x))(A-x)^{\alpha-1} \\
&\quad + \alpha(x-(A-x))[(A-x)^{\alpha-2}(x^{\alpha} - 2 - x^{\alpha-1}(A-x))] \\
&= \alpha(x-(A-x))[(\alpha+1)(A-x)^{\alpha-1} + (A-x)^{\alpha-2}(x^{\alpha-1}(x-(A-x)) - 2)] \\
&\geq \alpha(x-(A-x))[(\alpha+1)(A-x)^{\alpha-1} - 2(A-x)^{\alpha-2}] \geq 0.
\end{aligned}$$

This means that $f(x) = R_{\alpha}(T_{x,y,n+3-x-y})$ is an increasing function of x.

Thus, $R_{\alpha}(T_{x,y,n+3-x-y}) < R_{\alpha}(T_{n+3-2x-y,y})$.

Case 2: $y - x < n+3-y-x$

By **Case 1**, we only need to prove the following proposition: for $x \geq n+3-2x > 2$, $R_{\alpha}(T_{x,x,n+3-2x})$ is an increasing function of x when $\alpha > 2$.

We have $f(x) = R_{\alpha}(T_{x,x,n+3-2x}) = 2(x-2)x^{\alpha} + (n+1-2x)(n+3-2x)^{\alpha} + x^{2\alpha} + 2x^{\alpha}(n+3-2x)^{\alpha}$, then

$$\begin{aligned}
f'(x) &= 2(\alpha+1)(x^{\alpha} - (n+3-2x)^{\alpha}) - 4\alpha(x^{\alpha-1} - (n+3-2x)^{\alpha-1}) \\
&\quad + 2\alpha x^{\alpha-1}[x(x^{\alpha-1} - (n+3-2x)^{\alpha-1}) - (n+3-2x)^{\alpha-1}(x-(n+3-2x))],
\end{aligned}$$

Since $x(x^{\alpha-1}-(n+3-2x)^{\alpha-1}) = x(x-(n+3-2x))(\alpha-1)\xi_1^{\alpha-2}$, where $\xi_1 \in (n+3-2x, x)$, we have

$$\begin{aligned}
& x(x^{\alpha-1} - (n+3-2x)^{\alpha-1}) - (n+3-2x)^{\alpha-1}(x-(n+3-2x)) \\
= \; & x(x-(n+3-2x))(\alpha-1)\xi_1^{\alpha-2} - (n+3-2x)^{\alpha-1}(x-(n+3-2x)) \\
> \; & (n+3-2x)(x-(n+3-2x))(n+3-2x)^{\alpha-2} \\
& -(n+3-2x)^{\alpha-1}(x-(n+3-2x)) = 0.
\end{aligned}$$

Then

$$\begin{aligned}
f'(x) &> 2(\alpha+1)(x^{\alpha} - (n+3-2x)^{\alpha}) - 4\alpha(x^{\alpha-1} - (n+3-2x)^{\alpha-1}) \\
&\geq 2(\alpha+1)x(x^{\alpha-1} - (n+3-2x)^{\alpha-1}) - 4\alpha(x^{\alpha-1} - (n+3-2x)^{\alpha-1}) \\
&= [2(\alpha+1)x - 4\alpha](x^{\alpha-1} - (n+3-2x)^{\alpha-1}) > 0.
\end{aligned}$$

Then $f(x) = R_\alpha(T_{x,x,n+3-2x})$ is an increasing function of x.

Subcase 1: If $n+3-2x$ is even, since $f(x)$ is an increasing function of x, we have $R_\alpha(T_{x,x,n+3-2x}) < R_\alpha(T_{\frac{n+1}{2},\frac{n+1}{2}})$.

Subcase 2: If $n+3-2x$ is odd, since $f(x)$ is an increasing function of x, without loss of generality, we only need to prove for $x \geq 3$, $R_\alpha(T_{x,x,3}) < R_\alpha(T_{x+1,x})$ in the following. Let $f(x) = R_\alpha(T_{x+1,x}) - R_\alpha(T_{x,x,1}) = (x+1)^{\alpha+1} - 2(x+1)^\alpha + x^\alpha(x+1)^\alpha + 2^\alpha[x^\alpha + (x+1)^\alpha] - x^{\alpha+1} + 2x^\alpha - x^{2\alpha} - 3^\alpha(1+2x^\alpha)$. We have

$$\begin{aligned} f'(x) &= (\alpha+1)[(x+1)^\alpha - x^\alpha] + [\alpha(2^\alpha-2)(x+1)^{\alpha-1} - \alpha(2\cdot 3^\alpha - 2^\alpha - 2)x^{\alpha-1} \\ &\quad + \alpha(x+1)^{\alpha-1}x^{\alpha-1}] + 2\alpha x^\alpha[(x+1)^{\alpha-1} - x^{\alpha-1}] \\ &> \alpha x^{\alpha-1}[(2^\alpha-2) - (2\cdot 3^\alpha - 2^\alpha - 2) + (x+1)^{\alpha-1}] + 2\alpha x^\alpha \cdot x^{\alpha-2} \\ &= \alpha x^{\alpha-1}[2^{\alpha+1} - 2\cdot 3^\alpha + (x+1)^{\alpha-1} + 2x^{\alpha-1}], \end{aligned}$$

for $x \geq 4$, $2^{\alpha+1} - 2\cdot 3^\alpha + (x+1)^{\alpha-1} + 2x^{\alpha-1} > 0$. So $f'(x) > 0$, i.e., $f(x)$ is an increasing function in $x \geq 4$. And we can verify that $f(4) > 0$. Thus, $f(x) \geq f(4) > 0$. We can also see that $f(3) > 0$, therefore, $R_\alpha(T_{x,x,1}) < R_\alpha(T_{x+1,x})$. The proof is complete. ∎

From Lemma 3.4, Lemma 3.5 and Lemma 3.6, we conclude

Theorem 3.7 *For $\alpha > 2$, among all the unicyclic graphs, $T_{a,b} = T_{\lceil\frac{n+1}{2}\rceil,\lfloor\frac{n+1}{2}\rfloor}$ has the maximum general Randić index for $n \geq 7$; for $n = 5$ and $n = 6$, $T_{a,b} = T_{\lceil\frac{n+1}{2}\rceil,\lfloor\frac{n+1}{2}\rfloor}$ has the maximum general Randić index when $\alpha \geq \alpha'$, $T_{a,b} = S_n^+$ has the maximum general Randić index when $2 < \alpha < \alpha'$, where α' is the root of equation $R_\alpha(T_{\lceil\frac{n+1}{2}\rceil,\lfloor\frac{n+1}{2}\rfloor}) = R_\alpha(S_n^+)$.*

4 Concluding remarks

In this paper, we study unicyclic graphs with maximum general Randić index for $\alpha > 0$. We use the following table to summarize our main results.

α	$0 < \alpha < 1$	$1 < \alpha \leq 2$	$\alpha > 2$
extremal unicyclic graph	S_n^+	in $\mathcal{G}$	for $n \geq 7$, $T_{\lceil\frac{n+1}{2}\rceil,\lfloor\frac{n+1}{2}\rfloor}$

For $n=5$ and $n=6$, $T_{a,b}=T_{\lceil\frac{n+1}{2}\rceil,\lfloor\frac{n+1}{2}\rfloor}$ has the maximum general Randić index for $\alpha\geq\alpha'$, $T_{a,b}=S_n^+$ has the maximum general Randić index for $2<\alpha<\alpha'$, where α' is the root of equation $R_\alpha(T_{\lceil\frac{n+1}{2}\rceil,\lfloor\frac{n+1}{2}\rfloor})=R_\alpha(S_n^+)$. The case for $\alpha<0$ is much more complicated and left for further study.

References

[1] B. Bollobás and P. Erdös, Graphs of extremal weights, Ars Combin. 50(1998), 225-233.

[2] B. Bollobás, P. Erdös and A. Sarkar, Extremal graphs for weights, Discrete Math. 200(1999), 5-19.

[3] J.A. Bondy and U.S.R. Murty, Graph Theory With Applications, Macmllan Press Ltd. London, 1976.

[4] J. Gao and M. Lu, On the Randić index of unicyclic graphs, MATCH Commun. Math. Comput. Chem. 53(2)(2005), 377-384.

[5] Y. Hu, X. Li and Y. Yuan, Trees with minimum general Randić index, MATCH Commun. Math. Comput. Chem. 52(2004), 119-128

[6] Y. Hu, X. Li and Y. Yuan, Trees with maximum general Randić index, MATCH Commun. Math. Comput. Chem. 52(2004), 129-146.

[7] X. Li, L. Wang, and Y. Zhang, Complete solution for unicyclic graphs with minimum general Randić index, MATCH Commun. Math. Comput. Chem. 55(2)(2006), 391-408.

[8] M. Lu, H. Liu and F. Tian, The connectivity index, MATCH Commun. Math. Comput. Chem. 51(2004), 149-154.

[9] M. Randić, On characterization of molecular branching, J. Amer. Chem. Soc. 97(1975), 6609-6615.

[10] B. Wu and L. Zhang, Unicyclic graphs with minimum general Randić index, MATCH Commun. Math. Comput. Chem. 54(2)(2005), 455-464.