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Bicyclic graphs with maximum general Randić index

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Abstract

The general Randić index $R_\alpha(G)$ of a graph G is defined as $R_\alpha(G) = \sum_{uv \in E} [d(u)d(v)]^\alpha$, where $d(u)$ denotes the degree of a vertex u in G and α is an arbitrary real number. A graph with n vertices and $n+1$ edges is called a bicyclic graph. In this paper, we characterize the bicyclic graphs with maximum general Randić index for $\alpha \geq 1$.

1 Introduction

Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The Randić index $R(G)$ of a graph G was introduced by chemist Milan Randić in 1975 that is defined as $R = \sum_{uv \in E} [d(u)d(v)]^{-\frac{1}{2}}$, where $d(u)$ denotes the degree of a vertex u in G, and the summation goes over all edges uv of G. In 1998, Bollobás and Erdös generalized this index as the general Randić index $R_\alpha(G)$ of G, defined as

$$R_\alpha(G) = \sum_{uv \in E} [d(u)d(v)]^\alpha,$$

where α is any real number. Evidently, the Randić index is a special case of the general Randić index for $\alpha = -\frac{1}{2}$. More data and information about the research background of the Randić index and its generalization can be found in literatures (see [1] and [10]). There are many results concerning Randić index and general Randić index in recent years. For a survey of these results and their mathematical properties, we refer to the book of Li and Gutman: *Mathematical Aspects of Randić-Type Molecular Structure Descriptors* [6].

A simple connected graph G with n vertices and $n+1$ edges is called bicyclic graph. For $n \geq 6$, let B_n denote the bicyclic graph obtained by inserting an edge between two non-adjacent vertices of the n-vertex cycle (or n-cycle) C_n and B'_n denote the bicyclic graph obtained by connecting two disjoint cycles C_a and C_b, $a+b=n$, by means of a new edge. Caporossi et all [3] showed that for a bicyclic graph G, $R(G) \leq \frac{n-4}{2} + \frac{4}{\sqrt{6}} + \frac{1}{3}$, and the equality holds if and only if $G \cong B_n$ or $G \cong B'_n$. Moreover, for $\alpha > 0$, Liu and Huang [9] gave a lower bound for the general Randić index of G: $R_\alpha(G) \geq 6 \cdot 6^\alpha + (n-5) \cdot 4^\alpha$, and they characterized the extremal bicyclic graphs that reach the bound.

In this paper, we consider bicyclic graphs with the maximum general Randić index for $\alpha \geq 1$. To state our results, we give some further notations and terminologies. For notations and terminologies not definded here, see Bondy and Murty [2]. Denote by $N(u)$ the neighborhood of the vertex u. 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 leaves is called a leaf branch. We define a class $\mathcal{F}$ of graphs as follows: $\mathcal{F}$ consists of bicyclic graphs each of which has two triangles sharing two common vertices, and the vertices not on the cycles are leaves adjacent to two common vertices of the triangles and to another vertex of one of the triangles. We use $\mathcal{F}_{a,\ b,\ c}$ to denote a graph in class $\mathcal{F}$, where a, c and b are nonnegative integers that denote the number of leaves adjacent to the two common vertices and to another leaf branch of the triangles, respectively. And we have $a+b+c=n-4$. Particularly, let $S_n^{++} = \{\mathcal{F}_{a,\ b,\ c} |\ a=b=0\ and\ c \neq 0\}$ and $\mathcal{F}_n = \{\mathcal{F}_{a,\ b,\ c} |\ a=c=0\ and\ b \neq 0\}$. If $b=0$, we write $\mathcal{F}_{a,\ b,\ c}$ simply as $\mathcal{F}_{a,\ c}$. $\mathcal{F}_{a,\ c}$ is balanced if $|a-c| \leq 1$, i.e, $\mathcal{F}_{a,\ c} = \mathcal{F}_{\lceil \frac{n-4}{2} \rceil,\ \lfloor \frac{n-4}{2} \rfloor}$ (see Fig. 1).

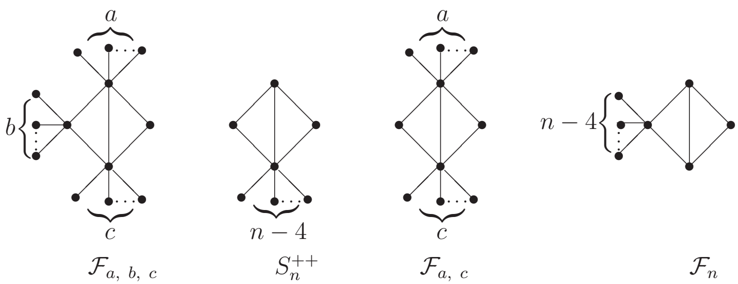


*Fig.*1

The main results of this paper are stated in the following theorems.

Theorem 1.1. *For $\alpha \geq 1$, the bicyclic graph with maximum general Randić index must be in $\mathcal{F}$.*

Theorem 1.2. *For $\alpha = 1$, S_n^{++} has the maximum general Randić index among bicyclic graphs with $n \geq 5$ vertices .*

Theorem 1.3. *Let $\alpha \geq 2$ and α' be the root of the equation $R_\alpha(\mathcal{F}_{1,\ 1}) = R_\alpha(S_6^{++})$. Among all bicyclic graphs with n vertices,*
(1) for $n \geq 7$, $\mathcal{F}_{\lceil \frac{n-4}{2} \rceil,\ \lfloor \frac{n-4}{2} \rfloor}$ has the maximum general Randić index ;
(2) for $n = 6$, $\mathcal{F}_{1,\ 1}$ has the maximum general Randić index when $\alpha \geq \alpha'$, S_6^{++} has the maximum general Randić index when $2 \leq \alpha < \alpha'$;
(3) for $n = 5$, S_5^{++} has the maximum general Randić index.

2 Preliminaries and the proof of Theorem 1.1 and 1.2

The proof ideas and techniques of the following lemmas are completely similar to those in [7].

Lemma 2.1. *Suppose a bicyclic 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 $N(v_1) \cap N(v_3) \backslash \{v_2\} = \emptyset$. Let $N(v_1)\backslash\{v_2\} = \{u_1, u_2, \ldots, u_{i-1}\}$ and $N(v_3)\backslash\{v_2\} = \{w_1, w_2, \ldots, w_{q-1}\}$. By deleting the edges $v_3w_1, v_3w_2, \ldots, v_3w_{q-1}$ and adding the new edges $v_1w_1, v_1w_2, \ldots, v_1w_{q-1}$, we get a new bicyclic graph G' (see Fig 2). Then $R_\alpha(G') > R_\alpha(G)$ for $\alpha \geq 1$.* □

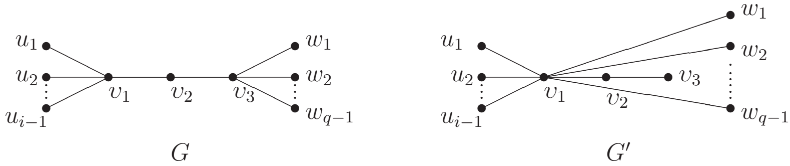


*Fig.*2

From lemma 2.1 we conclude that

Lemma 2.2. *Let G be a bicyclic graph with maximum general Randić index. Then both the two cycles of G must be 3-cycle having 2 common vertices or 4-cycle having 3 common vertices, and the vertices not on the cycles are leaves.* □

Proof of Theorem 1.1. By contradiction, suppose that G is a bicyclic graph with the maximum general Randić index and G is not in $\mathcal{F}$. By lemma 2.2, we only need to consider the following two cases.

Case 1. Two cycles of G are 3-cycle having 2 common vertices.

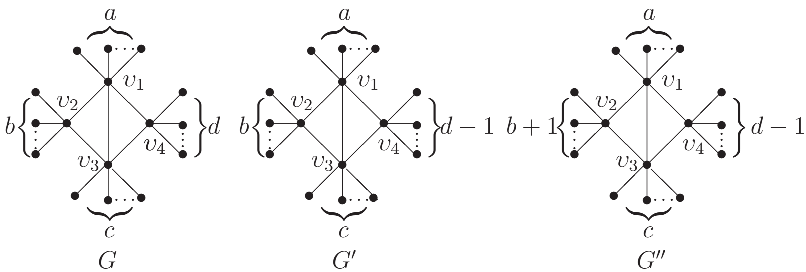


*Fig.*3

We denote the leaf branches of two cycles by $v_1v_2v_3v_4$. Denote by a, b, c and d the number of leaves adjacent to v_1, v_2, v_3 and v_4, respectively, as shown in Fig 3. Assume $b \geq d > 0$. Let G' and G'' be the bicyclic graphs as shown in Fig 3. We have

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

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

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

Let $f(x) = (x+2)^\alpha[x + (a+3)^\alpha + (c+3)^\alpha]$. Then

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

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

where $\xi_1 \in (d-1, d)$ and $\xi_2 \in (b, b+1)$. By $b \geq d \geq 1$, $\alpha \geq 1$ and since

$$f''(x) = \alpha(x+2)^{\alpha-2}\{(\alpha-1)[x + (a+3)^\alpha + (c+3)^\alpha] + 2(x+2)\} > 0,$$

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

Case 2. Two cycles of G are 4-cycle having 3 common vertices.

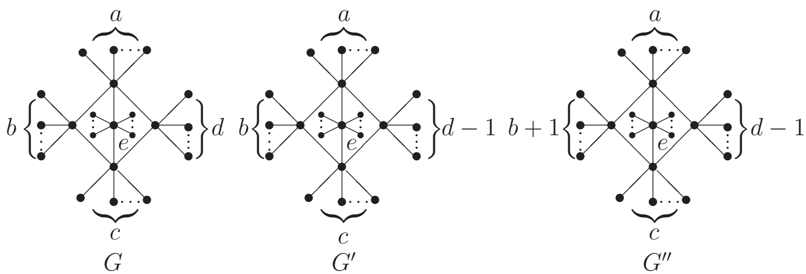


Fig.4

Let G, G', G'' be graphs depicted in Fig 4. First suppose $b \geq d > 0$, $e \geq 0$. Then by a fully analogous arguments used in case 1, we can prove that $R_\alpha(G'') > R_\alpha(G)$. Next suppose $d = e = 0$.

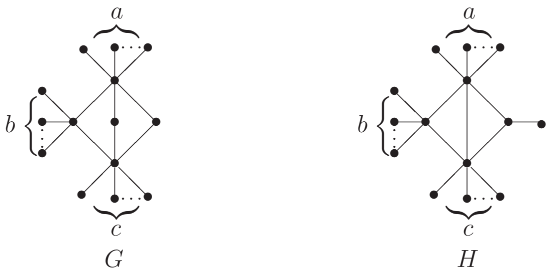


*Fig.*5

Let H be the bicyclic graph as shown in Fig 5. For $\alpha \geq 1$, we have

$$\begin{aligned} R_\alpha(H) - R_\alpha(G) &= (3^\alpha - 2^\alpha)[(a+3)^\alpha + (c+3)^\alpha] + (a+3)^\alpha(c+3)^\alpha \\ &\quad +3^\alpha - 2^\alpha[(a+3)^\alpha + (c+3)^\alpha] := f(a,c). \end{aligned}$$

Since $\dfrac{\partial f(a,c)}{\partial a} > 0$ and $\dfrac{\partial f(a,c)}{\partial c} > 0$, we have for $\alpha \geq 1$

$$f(a,c) > f(0,c) > f(0,0) = 3 \cdot 9^\alpha - 4 \cdot 6^\alpha + 3^\alpha > 0,$$

a contradiction. □

Proof of Theorem 1.2. By contradiction, assume G is a bicyclic graph with the maximum general Randić index, but G is not S_n^{++}. By Theorem 1.1, G must be in $\mathcal{F}$ with $a \neq 0$ or $b \neq 0$, a simple calculation shows

$$\begin{aligned} R_1(S_n^{++}) - R_1(G) &= R_1(S_{a+b+c+4}^{++}) - R_1(G) \\ &= ab + bc + ac + 2b > 0, \end{aligned}$$

again a contradiction. □

3 The case for $\alpha \geq 2$

In this section, in the proofs of lemmas and theorems, we use Maple program to deduce some inequalities involving exponential functions. To be more concise, we omit the tedious details of the deduction, and give the final inequalities.

Firstly, we present some lemmas.

Lemma 3.1. *Let $\alpha \geq 2$. Then $R_\alpha(\mathcal{F}_n) < R_\alpha(\mathcal{F}_{\lceil \frac{n-4}{2} \rceil,\ \lfloor \frac{n-4}{2} \rfloor})$ for $n \geq 6$, and $R_\alpha(\mathcal{F}_5) < R_\alpha(S_5^{++})$ for $n = 5$.*

Proof. We only consider the case when $n-4$ is odd, the case when $n-4$ is even is similar. Set $n-4 = 2k-1$ and let $f(k) = R_\alpha(\mathcal{F}_{k,\ k-1}) - R_\alpha(\mathcal{F}_{2k+3}) = k(k+3)^\alpha + (k-1)(k+2)^\alpha + 2^{\alpha+1}[(k+3)^\alpha + (k+2)^\alpha] + (k+3)^\alpha(k+2)^\alpha - (2k-1)(2k+1)^\alpha - 2\cdot 3^\alpha(2k+1)^\alpha - 2\cdot 6^\alpha - 9^\alpha$. It suffices to show $f(k) > 0$. Indeed, for $k \geq 2$

$$\begin{aligned}
f'(k) &= (k+3)^\alpha + \alpha k(k+3)^{\alpha-1} + (k+2)^\alpha + \alpha(k-1)(k+2)^{\alpha-1} \\
&+ \alpha 2^{\alpha+1}[(k+3)^{\alpha-1} + (k+2)^{\alpha-1}] + \alpha(k+3)^{\alpha-1}(k+2)^\alpha \\
&+ \alpha(k+3)^\alpha(k+2)^{\alpha-1} - \alpha(2k-1)(2k+1)^{\alpha-1} - 2(2k+1)^\alpha \\
&- 4\alpha\cdot 3^\alpha(2k+1)^{\alpha-1} \\
&> 8\alpha[(2k+4)^{\alpha-1} - (2k+1)^{\alpha-1}] + \alpha(k+3)^{\alpha-1}(k+2)^{\alpha-1}(2k+5) \\
&- 2(2k+1)^\alpha - \alpha(2k-9)(2k+1)^{\alpha-1} - 12\alpha(6k+3)^{\alpha-1} \\
&> \alpha(2k+5)(k^2+5k+6)^{\alpha-1} - 2(2k+1)^\alpha - \alpha(2k-9)(2k+1)^{\alpha-1} \\
&- 12\alpha(6k+3)^{\alpha-1} \\
&> (k^2+5k+6)^{\alpha-2}[\alpha(2k+5)(k^2+5k+6) - 2(2k+1)^2 \\
&- \alpha(2k-9)(2k+1) - 12\alpha(6k+3)] \\
&> 2\alpha k^3 + (11\alpha-8)k^2 - (19\alpha+8)k + 3\alpha - 2 := h(k,\alpha).
\end{aligned}$$

Since $\dfrac{\partial h(k,\alpha)}{\partial \alpha} = 2k^3 + 11k^2 - 19k + 3 > 0$, we have $h(k,\alpha) \geq h(k,2) = 4k^3 + 14k^2 - 46k + 4 > 0$ for $k \geq 2$.

Therefore, $f(k) \geq f(2) = 4^\alpha + 2\cdot 8^\alpha + 2\cdot 10^\alpha + 20^\alpha - 5^\alpha - 2\cdot 6^\alpha - 9^\alpha - 2\cdot 15^\alpha > 10^\alpha + 20^\alpha - 2\cdot 15^\alpha > 0$. It is not difficult to verify that $f(1) > 0$, which implies $R_\alpha(\mathcal{F}_5) < R_\alpha(S_5^{++})$. □

Lemma 3.2. *Let $\alpha \geq 2$ and α' be the root of the equation $R_\alpha(\mathcal{F}_{1,\ 1}) = R_\alpha(S_6^{++})$. Then*
(1)for $n \geq 7$, $R_\alpha(S_n^{++}) < R_\alpha(\mathcal{F}_{\lceil \frac{n-4}{2} \rceil,\ \lfloor \frac{n-4}{2} \rfloor})$;
(2) for $n = 6$, $R_\alpha(S_6^{++}) < R_\alpha(\mathcal{F}_{1,\ 1})$ when $\alpha > \alpha'$; $R_\alpha(\mathcal{F}_{1,\ 1}) < R_\alpha(S_6^{++})$ when $2 \leq \alpha < \alpha'$.

Proof. We only prove the case when $n-4$ is even, the case when $n-4$ is odd is similar. Let $n-4 = 2k$ and $f(k) = R_\alpha(\mathcal{F}_{k,\ k}) - R_\alpha(S_{2k+4}^{++}) =$

$2k(k+3)^\alpha + 4(2k+6)^\alpha + (k+3)^{2\alpha} - 2k(2k+3)^\alpha - 2(4k+6)^\alpha - 3^\alpha(2k+3)^\alpha - 2\cdot 6^\alpha$.
Then, when $k \geq 3$

$$\begin{aligned} f'(k) &= 2(k+3)^\alpha + \alpha 2k(k+3)^{\alpha-1} + 8\alpha(2k+6)^{\alpha-1} + 2\alpha(k+3)^{2\alpha-1} \\ &- 2(2k+3)^\alpha - \alpha 4k(2k+3)^{\alpha-1} - 8\alpha(4k+6)^{\alpha-1} - 6\alpha(6k+9)^{\alpha-1} \end{aligned}$$

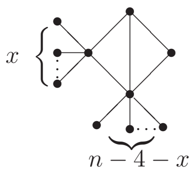
$$\begin{aligned} &> 8\alpha[(2k+6)^{\alpha-1} - (2k+3)^{\alpha-1}] + 8\alpha(2k+3)^{\alpha-1} + 2\alpha(k+3)^{2\alpha-1} \\ &- 2(2k+3)^\alpha - \alpha 4k(2k+3)^{\alpha-1} - 8\alpha(4k+6)^{\alpha-1} - 6\alpha(6k+9)^{\alpha-1} \\ &> 2\alpha(k+3)(k^2+6k+9)^{\alpha-1} - \alpha(4k-8)(2k+3)^{\alpha-1} \\ &- 2(2k+3)^\alpha - 8\alpha(4k+6)^{\alpha-1} - 6\alpha(6k+9)^{\alpha-1} \\ &> (k^2+6k+9)^{\alpha-2}[2\alpha(k+3)(k^2+6k+9) - 2(2k+3)^2 \\ &- \alpha(4k-8)(2k+3) - 8\alpha(4k+6) - 6\alpha(6k+9)] \\ &> 2\alpha k^3 + (10\alpha-8)k^2 - (10\alpha+24)k - 24\alpha - 18 \\ &\geq 4k^3 + 12k^2 - 44k - 66 > 0. \end{aligned}$$

Since $f(3) = 4\cdot 6^\alpha + 4\cdot 12^\alpha + 36^\alpha - 6\cdot 9^\alpha - 2\cdot 18^\alpha - 27^\alpha > 36^\alpha - 2\cdot 18^\alpha - 27^\alpha > 0$, we have $f(k) \geq f(3) > 0$. For $k = 2$, using the same arguments we can verify that $f(2) > 0$.

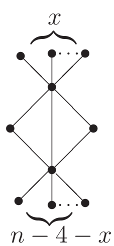
Hence for $k \geq 2$, i.e, $n \geq 7$, we have $R_\alpha(S_n^{++}) < R_\alpha(\mathcal{F}_{\lceil \frac{n-4}{2} \rceil,\ \lfloor \frac{n-4}{2} \rfloor})$.

For $k = 1$, $f(1) = 2(4^\alpha - 5^\alpha) + 2(8^\alpha - 6^\alpha) + 2(8^\alpha - 10^\alpha) + 16^\alpha - 15^\alpha > \alpha(15^{\alpha-1} - 4\cdot 10^{\alpha-1})$. When $\alpha \geq 5$, $15^{\alpha-1} - 4\cdot 10^{\alpha-1} \geq 0$, so $f(1) > 0$. Let $2 \leq \alpha < 5$. Using Maple program, we can verify that $f(1) > 0$ when $\alpha' < \alpha < 5$, and $f(1) < 0$ when $2 \leq \alpha < \alpha'$. This yields (2) and completes the proof of the lemma. □

Lemma 3.3. *For $\alpha \geq 2$, $x \geq 1$ and $n-4-x \geq 1$, $R_\alpha(\mathcal{F}_{0,\ x,\ n-4-x}) < R_\alpha(\mathcal{F}_{x,\ n-4-x})$.*



$\mathcal{F}_{0,\ x,\ n-4-x}$



$\mathcal{F}_{x,\ n-4-x}$

Fig. 6

Proof. Let $f(n) = R_\alpha(\mathcal{F}_{x,\ n-4-x}) - R_\alpha(\mathcal{F}_{0,\ x,\ n-4-x}) = x(x+3)^\alpha - x(x+2)^\alpha + 2^\alpha(x+3)^\alpha - 3^\alpha(x+2)^\alpha + 2^\alpha(n-x-1)^\alpha - (x+2)^\alpha(n-x-1)^\alpha + 2^\alpha(x+3)^\alpha - 6^\alpha + (x+3)^\alpha(n-x-1)^\alpha - 3^\alpha(n-x-1)^\alpha$. Since $\alpha \geq 1$ and $x \geq 1$, we have

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

Thus $R_\alpha(\mathcal{F}_{x,\ n-4-x}) - R_\alpha(\mathcal{F}_{0,\ x,\ n-4-x}) = f(n) \geq f(6) = 4^\alpha + 3\cdot 8^\alpha + 16^\alpha - 3^\alpha - 6^\alpha - 9^\alpha - 2\cdot 12^\alpha > 2\cdot 8^\alpha + 16^\alpha - 9^\alpha - 2\cdot 12^\alpha > 0$, which completes the proof. □

Lemma 3.4. *For* $\alpha \geq 2$ *and* $1 < x+1 < n-4-x$, $R_\alpha(\mathcal{F}_{x,\ n-4-x}) < R_\alpha(\mathcal{F}_{\lceil \frac{n-4}{2}\rceil,\ \lfloor \frac{n-4}{2}\rfloor})$.

Proof. **Case 1 .** $x = 1$ (see Fig. 7).

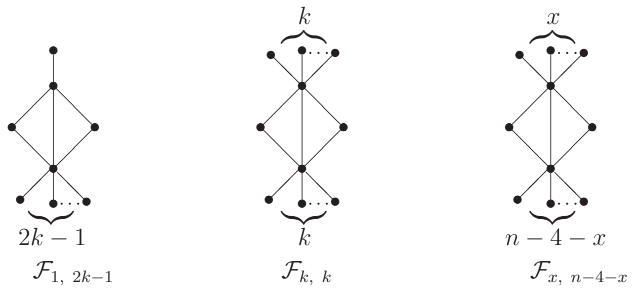


Fig.7

Again we only consider the case for $n-4 = 2k$, since the case when $n-4$ is odd is similar. Let $f(k) = R_\alpha(\mathcal{F}_{k,\ k}) - R_\alpha(\mathcal{F}_{1,\ 2k-1})$. By using the same method as in the proof of lemma 3.2, we obtain the following results: $f'(k) > 0$ when $k \geq 4$. Since $f(4) > 0$, we have $f(k) \geq f(4) > 0$. For $k = 2$ and $k = 3$, it is not difficult to verify that $R_\alpha(\mathcal{F}_{x,\ n-4-x}) < R_\alpha(\mathcal{F}_{\lceil \frac{n-4}{2}\rceil,\ \lfloor \frac{n-4}{2}\rfloor})$.

Case 2. $x \geq 2$.

Let $f(x) = R_\alpha(\mathcal{F}_{x,\ n-4-x}) = (x+3)^{\alpha+1} + (n-x-1)^{\alpha+1} +$

$(2^{\alpha+2}-3)[(x+3)^\alpha+(n-x-1)^\alpha]+(x+3)^\alpha(n-x-1)^\alpha$. Consider

$$\begin{aligned} f'(x) &= (\alpha+1)[(x+3)^\alpha-(n-x-1)^\alpha]+\alpha(2^{\alpha+2}-3)[(x+3)^{\alpha-1} \\ &- (n-x-1)^{\alpha-1}]+\alpha(x+3)^{\alpha-1}(n-x-1)^{\alpha-1}(n-2x-4) \\ &= \alpha(x+3)^{\alpha-1}(n-x-1)^{\alpha-1}(n-2x-4) \\ &- \alpha(\alpha+1)(n-2x-4)\xi_1^{\alpha-1}-\alpha(\alpha-1)(2^{\alpha+2}-3)(n-2x-4)\xi_2^{\alpha-2}, \end{aligned}$$

where $\xi_1,\xi_2\in(x+3,n-x-1)$. Since $\alpha\geq 2$ and $2\leq x<n-4-x$, we have

$$\begin{aligned} f'(x) &= \alpha(n-2x-4)[(x+3)^{\alpha-1}(n-x-1)^{\alpha-1}-(\alpha+1)\xi_1^{\alpha-1} \\ &- (\alpha-1)(2^{\alpha+2}-3)\xi_2^{\alpha-2}] \\ &> (x+3)^{\alpha-1}(n-x-1)^{\alpha-1}-(\alpha+1)(n-x-1)^{\alpha-1} \\ &- (\alpha-1)(2^{\alpha+2}-3)(n-x-1)^{\alpha-2} \\ &= (n-x-1)^{\alpha-2}[(n-x-1)(x+3)^{\alpha-1}-(\alpha+1)(n-x-1) \\ &- (\alpha-1)(2^{\alpha+2}-3)]. \end{aligned}$$

Let $g(x)=(n-x-1)(x+3)^{\alpha-1}-(\alpha+1)(n-x-1)-(\alpha-1)(2^{\alpha+2}-3)$. Since

$$\begin{aligned} g'(x) &= -(x+3)^{\alpha-1}+(\alpha-1)(n-x-1)(x+3)^{\alpha-2}+(\alpha+1) \\ &> -(x+3)^{\alpha-1}+(\alpha-1)(x+3)^{\alpha-1}+(\alpha+1)>0, \end{aligned}$$

we have $g(x)\geq g(2)=(n-3)\cdot 5^{\alpha-1}-(\alpha+1)(n-3)-(\alpha-1)(2^{\alpha+2}-3)\geq 7\cdot 5^{\alpha-1}-(\alpha+1)\cdot 7-(\alpha-1)(2^{\alpha+2}-3)>0$. Then $f'(x)>0$ for $x+1<n-4-x$, and this implies $R_\alpha(\mathcal{F}_{x,\ n-4-x})<R_\alpha(\mathcal{F}_{\lceil\frac{n-4}{2}\rceil,\ \lfloor\frac{n-4}{2}\rfloor})$. □

Lemma 3.5. *For $\alpha\geq 2$ and $1\leq x<n-4-2x$, $R_\alpha(\mathcal{F}_{x,\ n-4-2x,\ x})<R_\alpha(\mathcal{F}_{\lceil\frac{n-4}{2}\rceil,\ \lfloor\frac{n-4}{2}\rfloor})$.*

Proof. As in the previous proofs, we may assume $n-4-2x=2k$ (see Fig. 8). Let $f(x,k)=R_\alpha(\mathcal{F}_{x+k,\ x+k})-R_\alpha(\mathcal{F}_{x,\ 2k,\ x})=2(x+k)(x+k+3)^\alpha+2^{\alpha+2}(x+k+3)^\alpha+(x+k+3)^{2\alpha}-2x(x+3)^\alpha-2k(2k+2)^\alpha-2(2k+2)^\alpha(x+3)^\alpha-2^{\alpha+1}(x+3)^\alpha-(x+3)^{2\alpha}$.

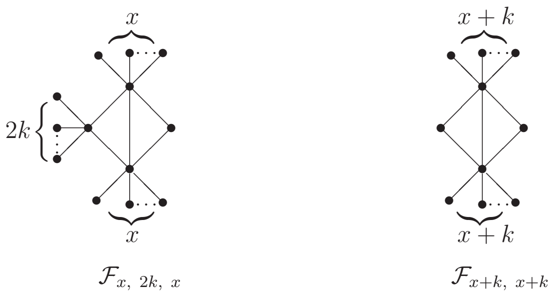


Fig. 8

Case 1. $k-1<x<2k$.

Note that for $x\geq 2$ and $k\geq 2$

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

Hence, for $k\geq 2$ and $k-1<x<2k$, we have $f(x,k)\geq f(x,2)=f(2,2)>0$ or $f(x,k)\geq f(x,2)=f(3,2)>0$, according as $x=k=2$ or $x=k+1=3$.

For $x=1$, $f(x,k)=f(1,k)=f(1,1)=4\cdot 5^{\alpha}+4\cdot 10^{\alpha}+25^{\alpha}-4\cdot 4^{\alpha}-3\cdot 16^{\alpha}-2\cdot 8^{\alpha}>2\cdot 10^{\alpha}+25^{\alpha}-3\cdot 16^{\alpha}>0$.

Thus, we have $R_{\alpha}(\mathcal{F}_{x,\ n-4-2x,\ x})<R_{\alpha}(\mathcal{F}_{\lceil\frac{n-4}{2}\rceil,\ \lfloor\frac{n-4}{2}\rfloor})$.

Case 2. $1\leq x\leq k-1$.

Note that

$$\begin{aligned}\frac{\partial f(x,k)}{\partial x} &= 2[(x+k+3)^{\alpha}-(x+3)^{\alpha}]+(2\alpha x+\alpha\cdot 2^{\alpha+1})[(x+k+3)^{\alpha-1}\\ &- (x+3)^{\alpha-1}]+(2\alpha k+\alpha\cdot 2^{\alpha+1})(x+k+3)^{\alpha-1}\\ &+ 2\alpha(x+k+3)^{2\alpha-1}-2\alpha[(2k+2)^{\alpha}(x+3)^{\alpha-1}+(x+3)^{2\alpha-1}]\\ &> 2\alpha[(x+k+3)^{2\alpha-1}-(2k+2)^{\alpha}(x+3)^{\alpha-1}+(x+3)^{2\alpha-1}]\\ &> (x+k+3)^{2\alpha-4}[(x+k+3)^3-(2k+2)^2(x+3)-(x+3)^3]\\ &> 3k(x+3)^2-(x+3)(k^2+8k+4)+k^3:=g(x,k).\end{aligned}$$

Since $\dfrac{\partial g(x,k)}{\partial k}>0$, we have $g(x,k)\geq g(x,2)=g(1,2)>0$. So $f(x,k)$ is monotonously increasing in x, and thus $f(x,k)\geq f(1,k)=(k+4)^{\alpha}(2+2k+2^{\alpha+2})+(k+4)^{2\alpha}-(2k+2\cdot 4^{\alpha})(2k+2)^{\alpha}-2\cdot 4^{\alpha}-2\cdot 8^{\alpha}-16^{\alpha}$.

By dropping out some positive items in $f'(1,k)$, for $k\geq 3$ we have

$$\begin{aligned}f'(1,k) &> 2\alpha(k+4)^{2\alpha-1}-2(2k+2)^{\alpha}-2\alpha(2k+2)^{\alpha-1}(2k+2\cdot 4^{\alpha})\\ &= 2[\alpha(k+4)^{2\alpha-1}-(2k+2)^{\alpha}-2k\alpha(2k+2)^{\alpha-1}-8\alpha(8k+8)^{\alpha-1}]\\ &> \alpha(k+4)^3-(2k+2)^2-2k\alpha(2k+2)-8\alpha(8k+8)\\ &> 2(k+4)^3-(2k+2)^2-4k(2k+2)-16(8k+8)>0.\end{aligned}$$

When $k = 2$, we can also verify $f'(1,2) > 0$.

It means that $f(1,k)$ is monotonously increasing in k, and hence $f(1,k) \geq f(1,2) = 2 \cdot 6^\alpha + 4 \cdot 12^\alpha + 36^\alpha - 2 \cdot 4^\alpha - 2 \cdot 8^\alpha - 16^\alpha - 2 \cdot 24^\alpha > 2 \cdot 12^\alpha + 36^\alpha - 2 \cdot 24^\alpha - 16^\alpha > 0$. Therefore, $R_\alpha(\mathcal{F}_{x,\ n-4-2x,\ x}) < R_\alpha(\mathcal{F}_{\lceil \frac{n-4}{2} \rceil,\ \lfloor \frac{n-4}{2} \rfloor})$. □

Proof of Theorem 1.3. After considering special cases which are stated in the above lemmas, next we will prove that $\mathcal{F}_{a,\ c}$ has the greater general Randić index than $\mathcal{F}_{a',\ b',\ c'}$, where $b' \neq 0$ and at least one of a' and c' is not zero, moreover $a + c = a' + b' + c'$. Let $f(x,y,n) = R_\alpha(\mathcal{F}_{x,\ y,\ n-4-x-y}) = x(x+3)^\alpha + y(y+2)^\alpha + (n-4-x-y)(n-x-y-1)^\alpha + [2^\alpha + (y+2)^\alpha][(x+3)^\alpha + (n-x-y-1)^\alpha] + (x+3)^\alpha(n-x-y-1)^\alpha$. We need to consider the following three cases.

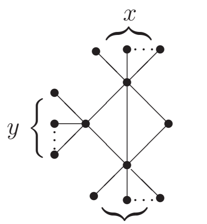


Fig. 9

Case 1. $y \leq n-4-x-y \leq x$.

In this case we will prove that $f(x,y,n)$ monotonously decreases in y for $\alpha \geq 2$. Note that

$$
\begin{aligned}
\frac{\partial f(x,\ y,\ n)}{\partial y} &= (y+2)^\alpha + \alpha y(y+2)^{\alpha-1} - (n-x-y-1)^\alpha \\
&- \alpha(n-4-x-y)(n-x-y-1)^{\alpha-1} \\
&+ \alpha(y+2)^{\alpha-1}[(x+3)^\alpha + (n-x-y-1)^\alpha] \\
&- \alpha(n-x-y-1)^{\alpha-1}[(y+2)^\alpha + 2^\alpha + (x+3)^\alpha] \\
&< \alpha(y+2)^{\alpha-1}[(x+3)^\alpha + (n-x-y-1)^\alpha] \\
&- \alpha(n-x-y-1)^{\alpha-1}[(y+2)^\alpha + (x+3)^\alpha] \\
&= -\alpha(\alpha-1)(n-x-2y-3)(x+3)^\alpha \xi_1^{\alpha-2} \\
&+ \alpha(y+2)^{\alpha-1}(n-x-2y-3)(n-x-y-1)^{\alpha-1} \\
&= \alpha(n-x-2y-3)[-(\alpha-1)(x+3)^\alpha \xi_1^{\alpha-2} \\
&+ (y+2)^{\alpha-1}(n-x-y-1)^{\alpha-1}],
\end{aligned}
$$

where $\xi_1 \in (y+2, n-x-y-1)$. Since $\alpha \geq 2$ and $y \leq n-4-x-y \leq x$, we have

$$\begin{aligned}\frac{\partial f(x,\ y,\ n)}{\partial y} &< -(\alpha-1)(x+3)^{\alpha}(n-x-y-1)^{\alpha-2}\\ &+ (y+2)^{\alpha-1}(n-x-y-1)^{\alpha-1}\\ &< (y+2)^{\alpha-2}[(n-x-y-1)^{\alpha}-(x+3)^{\alpha}] < 0.\end{aligned}$$

It means $R_\alpha(\mathcal{F}_{x,\ y,\ n-4-x-y}) < R_\alpha(\mathcal{F}_{x,\ y-1,\ n-3-x-y}) < \cdots < R_\alpha(\mathcal{F}_{x,\ n-4-x})$ for $1 \leq y \leq n-4-x-y \leq x$.

Case 2. $n-4-x-y < y \leq x$.

In order to obtain the same result as in case 1, consider

$$\begin{aligned}\frac{\partial^2 f(x,\ y,\ n)}{\partial n\,\partial y} &= -2\alpha(n-x-y-1)^{\alpha-1}-\alpha(\alpha-1)2^{\alpha}(n-x-y-1)^{\alpha-2}\\ &- \alpha(\alpha-1)(n-4-x-y)(n-x-y-1)^{\alpha-2}\\ &- \alpha(\alpha-1)(n-x-y-1)^{\alpha-2}[(y+2)^{\alpha}+(x+3)^{\alpha}]\\ &+ \alpha^2(y+2)^{\alpha-1}(n-x-y-1)^{\alpha-1}\\ &< \alpha(n-x-y-1)^{\alpha-2}[\alpha(y+2)^{\alpha}-2(\alpha-1)(y+2)^{\alpha}] < 0.\end{aligned}$$

So $\frac{\partial f(x,\ y,\ n)}{\partial y}$ is decreasing function of n, and furthermore $\frac{\partial f(x,\ y,\ n)}{\partial y} < \frac{\partial f(x,\ y,\ 6)}{\partial y} = \frac{\partial f(1,\ 1,\ 6)}{\partial y} = \alpha(1-2^{\alpha})\cdot 3^{\alpha-1} < 0$.

Hence, $f(x,y,n)$ is monotonously decreasing in y.

Case 3. $n-4-x-y < x < y$.

Now we will prove that $f(x,y,n)$ is monotonously increasing in x for $\alpha \geq 2$. Set $A = n-4-y$, we have

$$\begin{aligned}\frac{\partial f(x,\ y,\ n)}{\partial x} &= (x+3)^{\alpha}-(A-x+3)^{\alpha}+\alpha x(x+3)^{\alpha-1}\\ &- \alpha(A-x)(A-x+3)^{\alpha-1}+\alpha[2^{\alpha}+(y+2)^{\alpha}][(x+3)^{\alpha-1}\\ &- (A-x+3)^{\alpha-1}]-\alpha(2x-A)(x+3)^{\alpha-1}(A-x+3)^{\alpha-1}\\ &> \alpha(2x-A)[(\alpha-1)(y+2)^{\alpha}\xi_1^{\alpha-2}\\ &- (x+3)^{\alpha-1}(A-x+3)^{\alpha-1}],\end{aligned}$$

where $\xi_1 \in (A-x+3, x+3)$. Since $\alpha \geq 2$ and $A-x < x < y$,

$$\begin{aligned}\frac{\partial f(x,\ y,\ n)}{\partial x} &> (x+3)^{\alpha}(A-x+3)^{\alpha-2} - (x+3)^{\alpha-1}(A-x+3)^{\alpha-1} \\ &= (x+3)^{\alpha-1}(A-x+3)^{\alpha-2}(2x-A) > 0.\end{aligned}$$

This means that $R_\alpha(\mathcal{F}_{x,\ y,\ n-4-x-y}) < R_\alpha(\mathcal{F}_{x+1,\ y,\ n-5-x-y}) < \cdots$ $< R_\alpha(\mathcal{F}_{n-4-y,\ y,\ 0})$ for $n-4-x-y < x < y$. And by Lemma 3.5 we have $R_\alpha(\mathcal{F}_{n-4-y,\ y,\ 0}) < R_\alpha(\mathcal{F}_{n-4-y,\ y})$, which is desired.

The proof of the theorem is now complete. □

4 Concluding remarks

In this paper, we study bicyclic graphs with the maximum general Randić index for $\alpha \geq 1$. We use the following table to summarize our main results.

α	$\alpha = 1$	$1 < \alpha < 2$	$\alpha \geq 2$
extremal bicyclic graph	S_n^{++}	in $\mathcal{F}$	for $n \geq 7, \mathcal{F}_{\lceil \frac{n-4}{2} \rceil,\ \lfloor \frac{n-4}{2} \rfloor}$

For $n = 6$, $\mathcal{F}_{1,\ 1}$ has the maximum general Randić index when $\alpha \geq \alpha'$, S_6^{++} has the maximum general Randić index when $2 \leq \alpha < \alpha'$, where α' is the root of the equation $R_\alpha(\mathcal{F}_{1,\ 1}) = R_\alpha(S_6^{++})$; for $n = 5$, S_5^{++} has the maximum general Randić index. The case for $\alpha < 1$ seems much more complicated and left for further study.

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