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On the modified Randić index of trees, unicyclic graphs and bicyclic graphs

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ON THE MODIFIED RANDIĆ INDEX OF TREES, UNICYCLIC GRAPHS AND BICYCLIC GRAPHS

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Abstract. The modified Randić index of a graph G is a graph invariant closely related to the classical Randić index, defined as

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d_G(u), d_G(v)\}},$$

where $E(G)$ is the edge set of G , $d_G(u)$ is the degree of vertex u in G . We obtain best possible lower bounds for the modified Randić index of trees, unicyclic graphs and bicyclic graphs respectively when the number of vertices and matching number are fixed.

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Keywords: Randić index, modified Randić index, tree, unicyclic graph, bicyclic graph, matching number

1. INTRODUCTION

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, $N_G(u)$ denotes the set of neighbors of u in G and the degree of u is $d_G(u) = |N_G(u)|$. The Randić (connectivity) index of G is defined as [12]

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

The Randić index is one of the most successful molecular descriptors in structure–property and structure–activity relationships studies [9, 12]. Its mathematical properties as well as those of its generalizations have been studied extensively as summarized in the books [7, 10].

Various variants of Randić index have been proposed in the literature, see, e.g., [2, 4, 11, 13, 15]. To investigate the relationship between Randić index and radius of a (connected) graph, Dvořák et al. [6] proposed a modified version, which we call the

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modified Randić index, defined as

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d_G(u), d_G(v)\}}.$$

Some basic mathematical properties of the modified Randić index have been established in [1, 3, 6]. Recall that a connected graph on n vertices is known as a tree, a unicyclic graph and a bicyclic graph if it possesses $n - 1$, n and $n + 1$ edges, respectively. Andova et al. [1] obtained best possible lower and upper bounds for the modified Randić index of n -vertex trees and unicyclic graphs, respectively, and determined the corresponding extremal graphs.

In this paper, we obtain best possible lower bounds for the modified Randić index of trees, unicyclic graphs and bicyclic graphs respectively when the number of vertices and matching number are fixed. We also obtain best possible lower and upper bounds for the modified Randić index of n -vertex bicyclic graphs, and determine the corresponding extremal graphs.

2. PRELIMINARIES

A matching M of the graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. The matching number of G is the maximum number of edges of a matching in G . An m -matching is a matching of size m .

If M is a matching of a graph G and vertex $v \in V(G)$ is incident with an edge of M , then v is said to be M -saturated, and if every vertex of G is M -saturated, then M is a perfect matching.

For a graph G with $u, v \in V(G)$, $G - u$ denotes the graph formed from G by deleting vertex u (and its incident edges), $G + uv$ denotes the graph formed from G by adding the edge uv if $uv \notin E(G)$, and $G - uv$ denotes the graph formed from G by deleting the edge uv if $uv \in E(G)$.

First we give some lemmas that will be used.

Lemma 1. [1] *Let G be a connected graph on at least 3 vertices. Let u be a pendent vertex of G and v the unique neighbor of u . Let $a = d_G(v)$ and let l be the number of neighbors of v whose degree is at least a in G . Then*

$$R'(G) - R'(G - u) = \frac{l}{a(a-1)}.$$

Lemma 2. *Let G be a connected graph on at least 5 vertices. Let u be a pendent vertex of G and v the unique neighbor of u . Suppose that $d_G(v) = 2$. Let w be the neighbor of v different from u . Let $a = d_G(w)$ and let l be the number of neighbors of w whose degree is at least a in G . Then*

$$R'(G) - R'(G - u - v) = \begin{cases} 1 & \text{if } a = 2, \\ \frac{1}{2} + \frac{l}{a(a-1)} & \text{if } a \geq 3. \end{cases}$$

Proof. Obviously, $a \geq 2$. Suppose first that $a = 2$. Let w_1 be the neighbor of w different from v . Obviously, $d_{G-u-v}(w_1) = d_G(w_1) \geq 2$. Note that only edges uv and vw affect the difference $R'(G) - R'(G-u-v)$. Thus $R'(G) - R'(G-u-v) = \frac{1}{2} + \frac{1}{2} = 1$. Now suppose that $a \geq 3$. By Lemma 1, $R'(G) - R'(G-u) = \frac{1}{2}$ and $R'(G-u) - R'(G-u-v) = \frac{1}{a(a-1)}$. The result follows easily. \square

Let P_n be the path on n vertices. To attaching a path P at a vertex u of a graph G mean that we add an edge between u and an end vertex of P .

Lemma 3. *Let G be a connected graph with at least two vertices and let $u \in V(G)$. Let G_1 be the graph obtained from G by attaching two paths P_a and P_b to u , G_2 the graph obtained from G by attaching a path P_{a+b} to u , where $a \geq b \geq 1$. Then $R'(G_1) < R'(G_2)$.*

Proof. Let $d = d_G(u)$. Then $d_{G_1}(u) = d + 2$ and $d_{G_2}(u) = d + 1$. Thus

$$\begin{aligned} R'(G_2) - R'(G_1) &= \sum_{v \in N_G(u)} \left(\frac{1}{\max\{d_G(v), d + 1\}} - \frac{1}{\max\{d_G(v), d + 2\}} \right) \\ &\quad + \frac{1}{2} + \frac{1}{d + 1} - \frac{2}{d + 2} \\ &\geq \frac{1}{2} + \frac{1}{d + 1} - \frac{2}{d + 2} \\ &> 0, \end{aligned}$$

implying the result. \square

Lemma 4. *Let G be a connected graph with $u \in V(G)$, where $d_G(u) \geq 2$. Let H be the graph obtained from G by attaching a path P_a to u . Let u_1 be a neighbor of u in G , and u_0 the pendent vertex of the attached path in H . Let $H' = H - uu_1 + u_0u_1$. Then $R'(H') > R'(H)$.*

Proof. Let $d = d_G(u)$. Then $d_H(u) = d + 1$ and $d_{H'}(u) = d$. Note that $d_H(u_0) = 1$, $d_{H'}(u_0) = 2$, and the vertices of $V(H) \setminus \{u, u_0\}$ have the same degree in H' and H . Then

$$\begin{aligned} R'(H') - R'(H) &= \sum_{v \in N_G(u) \setminus \{u_1\}} \left(\frac{1}{\max\{d_G(v), d\}} - \frac{1}{\max\{d_G(v), d + 1\}} \right) \\ &\quad + \frac{1}{d} - \frac{1}{d + 1} \\ &\quad + \frac{1}{\max\{d_G(u_1), 2\}} - \frac{1}{\max\{d_G(u_1), d + 1\}} \\ &\geq \frac{1}{d} - \frac{1}{d + 1} > 0, \end{aligned}$$

implying the result. \square

A vertex $u \in V(G)$ is called a vertex of local maximal degree if $d_G(v) < d_G(u)$ for any $v \in N_G(u)$.

3. MODIFIED RANDIĆ INDEX OF TREES

Let S_n be the star on n vertices. For positive integers n and m with $n \geq 2m$, let $\mathbb{T}_{n,m}$ be the set of trees with n vertices and matching number m , and $T_{n,m}$ the graph obtained from the star S_{n-2m+2} by attaching $m-1$ paths on two vertices to its center.

Lemma 5. [8] *Let G be a n -vertex tree with a perfect matching, where $n \geq 3$. Then G has at least two pendent vertices such that they are adjacent to vertices of degree 2.*

Lemma 6. [8] *Let G be an n -vertex tree with matching number m , where $n > 2m$. Then there is an m -matching M and a pendent vertex v such that v is not M -saturated.*

Theorem 1. *Let $G \in \mathbb{T}_{n,m}$, where $n \geq 2m$. Then $R'(G) \geq \frac{m+1}{2}$ with equality if and only if $G \cong T_{n,m}$.*

Proof. We prove the result by induction on n (for fixed m).

First suppose that $n = 2m$. We prove the result by induction on m . If $m = 1, 2$, then the result follows trivially. If $m = 3$, then $G \cong P_6$ or $T_{6,3}$, and thus the result follows since $R'(T_{6,3}) = 2 = \frac{3+1}{2} < R'(P_6) = \frac{5}{2}$.

Suppose that $m \geq 4$, and the theorem holds for $m-1$. Let $G \in \mathbb{T}_{2m,m}$. Let M be a perfect matching of G . By Lemma 5, G has a pendent vertex u_1 adjacent to a vertex u_2 of degree 2. Let u_3 be the neighbor of u_2 different from u_1 . Let $a = d_G(u_3)$ and l be the number of neighbors of u_3 whose degree is at least a in G . Obviously, $u_1u_2 \in M$. Let $G' = G - u_1 - u_2$. Then $G' \in \mathbb{T}_{2m-2,m-1}$ and $M \setminus \{u_1u_2\}$ is a perfect matching of G' . By Lemma 2 and the induction hypothesis, $R'(G) = R'(G') + 1 \geq \frac{(m-1)+1}{2} + 1 > \frac{m+1}{2}$ if $a = 2$, and $R'(G) = R'(G') + \frac{1}{2} + \frac{l}{a(a-1)} \geq \frac{(m-1)+1}{2} + \frac{1}{2} + \frac{l}{a(a-1)} = \frac{m+1}{2} + \frac{l}{a(a-1)} \geq \frac{m+1}{2}$ with equalities if and only if $G' \cong T_{2m-2,m-1}$ and $l = 0$, i.e., $G' \cong T_{2m-2,m-1}$ and u_3 is a vertex of local maximal degree in G if $a \geq 3$. Thus $R'(G) \geq \frac{m+1}{2}$ with equality if and only if $G \cong T_{2m,m}$.

Suppose that $n > 2m$ and the result holds for $n-1$. Let $G \in \mathbb{T}_{n,m}$. By Lemma 6, G has an m -matching M and a pendent u such that M does not saturate u . Then $G-u \in \mathbb{T}_{n-1,m}$. Let v be the unique neighbor of u in G . Let $a = d_G(v)$ and let l be the number of neighbors of v whose degree is at least a in G . By Lemma 1 and the induction hypothesis,

$$R'(G) = R'(G-u) + \frac{l}{a(a-1)} \geq \frac{m+1}{2} + \frac{l}{a(a-1)} \geq \frac{m+1}{2}$$

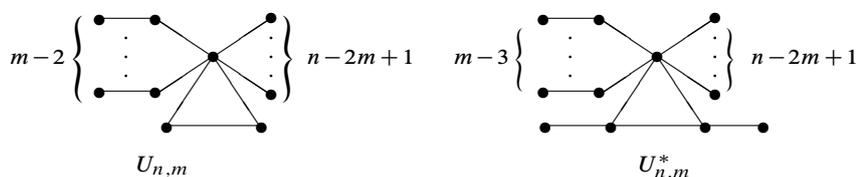


FIGURE 1. The graphs $U_{n,m}$ and $U_{n,m}^*$.

with equalities if and only if $G - u \cong T_{n-1,m}$ and $l = 0$, i.e., $G - u \cong T_{n-1,m}$ and v is a vertex of local maximal degree in G . Thus $R'(G) \geq \frac{m+1}{2}$ with equality if and only if $G \cong T_{n,m}$. \square

Corollary 1. [1] Let G be a tree on $n \geq 2$ vertices. Then $R'(G) \geq 1$ with equality if and only if $G \cong S_n$.

Proof. Let m be the matching number of G . By Theorem 1, $R'(G) \geq \frac{m+1}{2} \geq 1$ with equalities if and only if $G \cong T_{n,1} \cong S_n$. \square

By Lemma 3, we have

Corollary 2. [1] Let G be a tree on at least 2 vertices. Then $R'(G) \leq \frac{n-1}{2}$ with equality if and only if $G \cong P_n$.

4. MODIFIED RANDIĆ INDEX OF UNICYCLIC GRAPHS

Let C_n be a cycle on n vertices. For integers n and m with $n \geq 2m$ and $m \geq 2$, let $\mathbb{U}_{n,m}$ be the set of unicyclic graph with n vertices and matching number m , and $U_{n,m}$ the graph obtained from C_3 by attaching to a vertex $n - 2m + 1$ pendent vertices and $m - 2$ paths on two vertices. For $n \geq 2m$ and $m \geq 3$, let $U_{n,m}^*$ be the graph obtained from C_3 by attaching to a vertex $n - 2m + 1$ pendent vertices and $m - 3$ paths on two vertices and to the other two vertices a pendent vertex each. See Figure 1 for them.

Lemma 7. [14] Let $G \in \mathbb{U}_{n,m}$ and $G \not\cong C_n$, where $n > 2m$. Then there is an m -matching M and a pendent vertex v such that M does not saturate v .

Theorem 2. Let $G \in \mathbb{U}_{n,m}$, where $n \geq 2m$. Then $R'(G) \geq \frac{m+1}{2}$ with equality if and only if $G \cong U_{n,m}$ or $U_{n,m}^*$.

Proof. We prove the result by induction on n (for fixed m).

First suppose that $n = 2m$. We prove the result by induction on m .

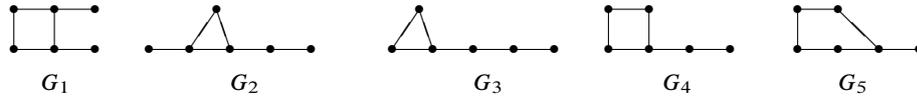


FIGURE 2. Graphs in $\mathbb{U}_{6,3} \setminus \{C_6, U_{6,3}, U_{6,3}^*\}$.

If $m = 2$, then $G \cong U_{4,2}$ or C_4 , and thus the result follows since $R'(U_{4,2}) = \frac{3}{2} < R'(C_4) = 2$. If $m = 3$, then $G \cong C_6, U_{6,3}, U_{6,3}^*$ or G_i for $i = 1, 2, \dots, 5$, see Figure 2, and thus the result follows since

$$R'(G) = \begin{cases} \frac{13}{6} & \text{if } G \cong G_i, i = 1, 2 \\ 3 & \text{if } G \cong C_6, \\ \frac{5}{2} & \text{if } G \cong G_i, i = 3, 4, 5, \\ 2 & \text{if } G \cong U_{6,3} \text{ or } U_{6,3}^*. \end{cases}$$

Suppose that $m \geq 4$ and the result holds for graphs in $\mathbb{U}_{2m-2,m-1}$. Let $G \in \mathbb{U}_{2m,m}$. If $G \cong C_{2m}$, then $R'(G) = m > \frac{m+1}{2}$. Suppose that $G \not\cong C_{2m}$. Let M be a perfect matching of G . There are two cases.

Case 1. G has a pendent vertex u whose unique neighbor v has degree two. Obviously, $uv \in M$. Let $G_1 = G - u - v$. Then $G_1 \in \mathbb{U}_{2m-2,m-1}$ and $M \setminus \{uv\}$ is a perfect matching of G_1 . Let w be the neighbor of v different from u in G . Let $a = d_G(w)$ and let l be the number of neighbors of w whose degree is at least a in G . By Lemma 2 and the induction hypothesis, $R'(G) = R'(G_1) + 1 \geq \frac{(m-1)+1}{2} + 1 > \frac{m+1}{2}$ if $a = 2$, and $R'(G) = R'(G_1) + \frac{1}{2} + \frac{l}{a(a-1)} \geq \frac{(m-1)+1}{2} + \frac{1}{2} = \frac{m+1}{2}$ with equality if and only if $G_1 = U_{2m-2,m-1}$ or $U_{2m-2,m-1}^*$ and $l = 0$, i.e., $G_1 = U_{2m-2,m-1}$ or $U_{2m-2,m-1}^*$ and w is a vertex of local maximal degree in G if $a \geq 3$. Thus $R'(G) \geq \frac{m+1}{2}$ with equality if and only if $G \cong U_{2m,m}$ or $U_{2m,m}^*$.

Case 2. No neighbor of a pendent vertex has degree two in G . Let $C = u_1 u_2 \dots u_p u_1$ be the unique cycle of G . Since G has a perfect matching, the graph obtained from G by deleting vertices of C consists of isolated vertices. Thus G is obtainable from the cycle C by attaching some pendent vertices and the maximal degree of G is three.

If all vertices on C have degree three, then $R'(G) = \frac{2m}{3} > \frac{m+1}{2}$. Suppose that there is at least one vertex of degree two on C . Since $G \not\cong C_{2m}$, there are adjacent vertices on C , one of degree two and the other of degree three. Assume that $d_G(u_2) = 3$ and $d_G(u_3) = 2$. Let w_2 be the pendent neighbor of u_2 in G . Then $u_2 w_2 \in M$. Since $u_3 u_4 \in M$, we have $d_G(u_4) = 2$. Let $G_2 = G - u_2 - w_2 + u_1 u_3$. Then $G_2 \in \mathbb{U}_{2m-2,m-1}$ and $M \setminus \{u_2 w_2\}$ is a perfect matching of G_2 . If $d_G(u_1) = 3$, then by the induction hypothesis,

$$R'(G) = R'(G_2) + \frac{2}{3} \geq \frac{(m-1)+1}{2} + \frac{2}{3} > \frac{m+1}{2}.$$

If $d_G(u_1) = 2$, then $|V(C)| \geq 5$, and thus $G_2 \not\cong U_{2m-2,m-1}, U_{2m-2,m-1}^*$, implying that

$$R'(G) = R'(G_2) + \frac{1}{2} > \frac{(m-1)+1}{2} + \frac{1}{2} = \frac{m+1}{2}.$$

Thus $R'(G) > \frac{m+1}{2}$.

By combining Cases 1 and 2, the result follows for $n = 2m$.

Suppose that $n > 2m$ and the result holds for $n - 1$. Let $G \in \mathbb{U}_{n,m}$. If $G \cong C_n$, then $n = 2m + 1$, and thus $R'(G) = \frac{2m+1}{2} > \frac{m+1}{2}$. Suppose that $G \not\cong C_n$. By Lemma 7, G has an m -matching M and a pendent u such that M does not saturate u . Let $G_3 = G - u$. Then $G_3 \in \mathbb{U}_{n-1,m}$. Let v be the unique neighbor of u in G . Let $a = d_G(v)$ and let l be the number of neighbors of v whose degree is at least a in G . By Lemma 1 and the induction hypothesis,

$$R'(G) = R'(G_3) + \frac{l}{a(a-1)} \geq \frac{m+1}{2} + \frac{l}{a(a-1)} \geq \frac{m+1}{2}$$

with equalities if and only if $G_3 \cong U_{n-1,m}$ or $U_{n-1,m}^*$ and $l = 0$, i.e., $G_3 \cong U_{n-1,m}$ or $U_{n-1,m}^*$, and v is a vertex of local maximal degree in G . Thus $R'(G) \geq \frac{m+1}{2}$ with equality if and only if $G \cong U_{n,m}$ or $U_{n,m}^*$. \square

Corollary 3. [1] *Let G be a unicyclic graph G on $n \geq 3$ vertices. Then $R'(G) \geq \frac{3}{2}$ with equality if and only if $G \cong C_3$ or $U_{n,2}$.*

Proof. Let m be the matching number of G . If $m = 1$, then $G \cong C_3$ and $R'(G) = \frac{3}{2}$. If $m \geq 2$, then by Theorem 2, $R'(G) \geq \frac{m+1}{2} \geq \frac{3}{2}$ with equalities if and only if $G \cong U_{n,2}$. \square

By Lemmas 3 and 4, we have

Corollary 4. [1] *Let G be a unicyclic graph on at least 3 vertices. Then $R'(G) \leq \frac{n}{2}$ with equality if and only if $G \cong C_n$.*

5. MODIFIED RANDIĆ INDEX OF BICYCLIC GRAPHS

In this section, we use techniques developed from [5].

For integers n and m with $n \geq 2m$ and $m \geq 2$, let $\mathbb{B}_{n,m}$ be the set of bicyclic graphs with n vertices and matching number m . Let $B_{n,3}^1$ be the graph obtained by identifying a vertex of two triangles, and attaching to this common vertex of the two triangles $n - 5$ pendent vertices. Let $B_{n,3}^2$ be the graph obtained from the unique bicyclic graph on four vertices by attaching to a vertex of degree three $n - 5$ pendent vertices and to a vertex of degree two a pendent vertex. For $n \geq 2m$ and $m \geq 4$, let $B_{n,m}$ be the graph obtained from the unique bicyclic graph on four vertices by attaching to a vertex of degree three $n - 2m + 1$ pendent vertices and $m - 4$ paths on two vertices to the three other vertices a pendent vertex each, see Figure 3.

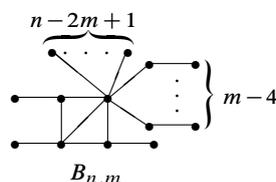


FIGURE 3. The graph $B_{n,m}$.

Lemma 8. *Let G be a connected graph with $uv \in E(G)$, where $d_G(u), d_G(v) \geq 2$, and u and v have no common neighbor in G . Let G_1 be the graph obtained from G by deleting the edge uv , identifying u and v , which is denoted by w , and adding a vertex w_1 and the edge w_1w . Then $R'(G) > R'(G_1)$.*

Proof. Note that $d_{G_1}(w) = d_G(u) + d_G(v) - 1$, and the vertices of $V(G) \setminus \{u, v\}$ have the same degree in G_1 and G . Obviously, $d_{G_1}(w) > \max\{d_G(u), d_G(v)\}$ since $d_G(u), d_G(v) \geq 2$, and for any $u' \in N_G(u) \cup N_G(v) \setminus \{u, v\}$, $u' \in N_{G_1}(w)$. Thus

$$\begin{aligned}
 & R'(G_1) - R'(G) \\
 &= \sum_{u' \in N_G(u) \setminus \{v\}} \left(\frac{1}{\max\{d_{G_1}(w), d_G(u')\}} - \frac{1}{\max\{d_G(u), d_G(u')\}} \right) \\
 &+ \sum_{u' \in N_G(v) \setminus \{u\}} \left(\frac{1}{\max\{d_{G_1}(w), d_G(u')\}} - \frac{1}{\max\{d_G(v), d_G(u')\}} \right) \\
 &+ \frac{1}{d_{G_1}(w)} - \frac{1}{\max\{d_G(u), d_G(v)\}} \\
 &\leq \frac{1}{d_{G_1}(w)} - \frac{1}{\max\{d_G(u), d_G(v)\}} \\
 &< 0,
 \end{aligned}$$

as desired. □

Lemma 9. *Let $G \in \mathbb{B}_{6,3}$. Then $R'(G) \geq 2$ with equality if and only if $G \cong B_{6,3}^1$ or $B_{6,3}^2$.*

Proof. If G has a pendent vertex with a neighbor of degree two, then G is the graph obtained from the unique bicyclic graph on four vertices by attaching to a vertex (of degree two or three) a path on two vertices, and thus it is easily seen that $R'(G) = \frac{13}{6}$ or $\frac{5}{2}$, implying that $R'(G) > 2$. Suppose that there is no pendent vertex

with a neighbor of degree two. If there is no vertex of degree two in G , then G is obtained by attaching a pendent vertex to every vertex of degree two of the unique bicyclic graph on four vertices, and thus $R'(G) = \frac{7}{3} > 2$. Suppose that there is a vertex, say u , of degree two in G . Let v and w be the two neighbors of u in G . Then one of the two edges incident with u , say $uv \in M$, where M is a perfect matching of G . Then u lies on some cycle of G , and thus $G' = G - uw$ is a unicyclic graph with a perfect matching. Let $a = d_G(w)$ and let l be the number of neighbors of w whose degree is at least a in G . Note that $a \geq 2$. Then by Theorem 2, $R'(G) = R'(G') + \frac{1}{2} \geq \frac{3+1}{2} + \frac{1}{2} = \frac{5}{2} > 2$ if $a = 2$, and $R'(G) = R'(G') + \frac{a-l}{a} - \frac{a-l-1}{a-1} = R'(G') + \frac{l}{a(a-1)} \geq \frac{3+1}{2} = 2$ with equality if and only if $G' \cong U_{6,3}$ or $U_{6,3}^*$ and $l = 0$, i.e., $G' \cong U_{6,3}$ or $U_{6,3}^*$ and w is a vertex of local maximal degree if $a \geq 3$. The result follows. \square

Lemma 10. [16] *Let $G \in \mathbb{B}_{n,m}$ with $n > 2m \geq 6$, and G has at least one pendent vertex. Then there is an m -matching M and a pendent vertex u such that u is not M -saturated.*

$$\text{Let } g(m) = \frac{m+1}{2} - \frac{1}{12}.$$

Let $\tilde{\mathbb{B}}(n)$ be the set of bicyclic graphs on n vertices without pendent vertices, where $n \geq 4$. Let $\mathbb{B}_n^1(t)$ be the bicyclic graph with n vertices containing two edge-disjoint cycles C_a and C_b that are joined by a path of length $t = n - a - b + 1$ (C_a and C_b has a common vertex and $a + b = n + 1$ if $t = 0$). Let $\mathbb{B}_n^2(s)$ be the set of bicyclic graphs obtained by joining two non-adjacent vertices of C_a with $4 \leq a \leq n$ by a path of length $s = n - a + 1$, where $n \geq 4$ and $s \geq 1$. Obviously, $\tilde{\mathbb{B}}(n) = \mathbb{B}_n^1(t) \cup \mathbb{B}_n^2(s)$.

Lemma 11. *Let $G \in \mathbb{B}_{2m,m}$ and no pendent vertex has neighbor of degree two, where $m \geq 4$. Then $R'(G) \geq g(m)$ with equality if and only if $m = 4$ and $G \cong B_{8,4}$.*

Proof. Since $G \in \mathbb{B}_{2m,m}$ and no pendent vertex has neighbor of degree two, G is obtainable by attaching some pendent vertices to a graph in $\tilde{\mathbb{B}}(k)$, where $m \leq k \leq 2m$, and any two pendent vertices have no common neighbor (if $k = 2m$, then no pendent vertex is attached).

Case 1. There is no vertex of degree two in G . Then either $k = m$, G is obtainable by attaching a pendent vertex to every vertex of a graph G_1 in $\tilde{\mathbb{B}}(k)$, or $k = m + 1$, G is obtainable by attaching a pendent vertex to every vertex with degree two of a graph $G_1 \in \mathbb{B}_{m+1}^1(1) \cup \mathbb{B}_{m+1}^2(1)$. By direct calculation, we have

$$R'(G) = \begin{cases} \frac{2}{3}m - \frac{1}{4} & \text{if } G_1 \in \mathbb{B}_m^1(1) \cup \mathbb{B}_m^2(1), \\ \frac{2}{3}m - \frac{1}{3} & \text{if } G_1 \in \mathbb{B}_m^1(t) \cup \mathbb{B}_m^1(0) \cup \mathbb{B}_m^2(t) \text{ with } t \geq 2, \\ \frac{2}{3}m + \frac{1}{3} & \text{if } G_1 \in \mathbb{B}_{m+1}^1(1) \cup \mathbb{B}_{m+1}^2(1). \end{cases}$$

Then $R'(G) \geq g(m)$ with equality if and only if $m = 4$ and $G \cong B_{8,4}$.

Case 2. There is a vertex, say u , of degree two in G . Denote by v and w the two neighbors of u in G . Then one of the two edges incident with u , say $uv \in M$, where

M is a perfect matching of G . Suppose that there is no vertex of degree two in any cycle of G . Since no pendent vertex has neighbor of degree two in G , u lies on the path joining the two disjoint cycles of G . For $G_1 = G - uw + vw \in \mathbb{B}_{2m,m}$, the difference of the numbers of vertices of degree two outside any cycle of G and G_1 is equal to one, and thus by Lemma 8, $R'(G_1) < R'(G)$. Repeating the operation from G to G_1 , we finally get a graph $G' \in \mathbb{B}_{2m,m}$, which has no vertex of degree two, such that $R'(G) > R'(G')$, and thus the result follows from Case 1. Now suppose that u lies on some cycle of G . Consider $G' = G - uw$, which is a unicyclic graph with perfect matching. Let $a = d_G(w)$ and let k be the number of neighbors of w whose degree is at least a in G . Then by Theorem 2, $R'(G) = R'(G') + \frac{1}{2} \geq \frac{m+1}{2} + \frac{1}{2} > g(m)$ if $a = 2$, and $R'(G) = R'(G') + \frac{k}{a(a-1)} \geq \frac{m+1}{2} > g(m)$ if $a \geq 3$. \square

Lemma 12. *Let $G \in \mathbb{B}_{8,4}$. Then $R'(G) \geq \frac{29}{12}$ with equality if and only if $G \cong B_{8,4}$.*

Proof. If there is no pendent vertex with neighbor of degree two in G , then by Lemma 11, $R'(G) \geq g(4) = \frac{29}{12}$ with equality if and only if $G \cong B_{8,4}$. Suppose that G has a pendent vertex u whose neighbor v is of degree two. Then $uv \in M$ and $G - u - v \in \mathbb{B}_{6,3}$. Let w be the neighbor v different from u . Let $a = d_G(w)$ and let k the number of neighbors of w whose degree is at least a . By Lemmas 2 and 9, $R'(G) = R'(G - u - v) + 1 \geq 2 + 1 = 3 > \frac{29}{12}$ if $a = 2$, and $R'(G) = R'(G - u - v) + \frac{1}{2} + \frac{k}{a(a-1)} \geq 2 + \frac{1}{2} + \frac{k}{a(a-1)} \geq \frac{5}{2} > \frac{29}{12}$ if $a \geq 3$. \square

Let $B_n(a, b)$ be the graph obtained from the unique bicyclic graph on four vertices by attaching to the two vertices of degree three $a - 3$ and $b - 3$ pendent vertices, respectively, where $a \geq b \geq 3$, $a + b = n + 2$ and $n \geq 4$.

Theorem 3. *Among the graphs in $\mathbb{B}_{n,2}$ with $n \geq 6$,*

$$R' \left(B_n \left(\left\lceil \frac{n}{2} \right\rceil + 1, \left\lfloor \frac{n}{2} \right\rfloor + 1 \right) \right) > R' \left(B_n \left(\left\lceil \frac{n}{2} \right\rceil + 2, \left\lfloor \frac{n}{2} \right\rfloor \right) \right) > \dots > R' (B_n(n - 1, 3)) = \frac{5}{3},$$

and for $G \in \mathbb{B}_{n,2}$ not appearing in the above inequalities, $R'(G) = 2$.

Proof. Let $G \in \mathbb{B}_{n,2}$. Then G is of three types:

(1) $G = B_n(a, b)$ with $a \geq b \geq 3$. Then $R'(G) = 2 - \frac{1}{b}$. It follows that

$$R' \left(B_n \left(\left\lceil \frac{n}{2} \right\rceil + 1, \left\lfloor \frac{n}{2} \right\rfloor + 1 \right) \right) > R' \left(B_n \left(\left\lceil \frac{n}{2} \right\rceil + 2, \left\lfloor \frac{n}{2} \right\rfloor \right) \right) > \dots > R' (B_n(n - 1, 3)) = \frac{5}{3}.$$

(2) G is the graph obtained from the unique bicyclic graph on four vertices by attaching to a vertex of degree two $n - 4$ pendent vertices. Then $R'(G) = 2$.

(3) G is the graph obtained from the unique bicyclic graph on five vertices in $\mathbb{B}_5^2(2)$ by attaching to one or two vertices of degree three some pendent vertices. Then $R'(G) = 2$.

Now the result follows easily. □

Theorem 4. *Let $G \in \mathbb{B}_{n,3}$. Then $R'(G) \geq 2$ with equality if and only if $G \cong B_{n,3}^1$ or $G \cong B_{n,3}^2$.*

Proof. We prove the result by induction on n . If $n = 6$, then the result follows from Lemma 9.

Suppose that $n \geq 7$ and the result holds for graphs in $\mathbb{B}_{n-1,3}$. Let $G \in \mathbb{B}_{n,3}$. If there is no pendent vertex in G , then $G \in \tilde{\mathbb{B}}(n)$, $n = 7$, and thus

$$R'(G) = \begin{cases} 3 + \frac{1}{6} & \text{if } G \in \mathbb{B}_7^1(1) \cup \mathbb{B}_7^2(1), \\ 3 & \text{otherwise,} \end{cases} > 2.$$

Suppose that there is at least one pendent vertex in G . By Lemma 10, there is a 3-matching M and a pendent vertex u of G such that u is not M -saturated. Then $G - u \in \mathbb{B}_{n-1,3}$. Let v be the unique neighbor of u . Let $a = d_G(v)$ and let l be the number of neighbors of v whose degree is at least a in G . By Lemma 1, we have

$$R'(G) = R'(G - u) + \frac{l}{a(a-1)} \geq 2 + \frac{l}{a(a-1)} \geq 2$$

with equalities if and only if $G - u \cong B_{n-1,3}^1$ or $B_{n-1,3}^2$ and $l = 0$, i.e., $G - u \cong B_{n-1,3}^1$ or $B_{n-1,3}^2$ and v is a vertex of local maximal degree. Thus $R'(G) \geq 2$ with equality if and only if $G \cong B_{n,3}^1$ or $G \cong B_{n,3}^2$ □

Theorem 5. *Let $G \in \mathbb{B}_{n,m}$, where $n \geq 2m$ and $m \geq 4$. Then $R'(G) \geq g(m)$ with equality if and only if $G \cong B_{n,m}$.*

Proof. We prove the result by induction on n (for fixed m).

First suppose that $n = 2m$. We prove the result by induction on m .

If $m = 4$, then from Lemma 12, $R'(G) \geq g(4)$ with equality if and only if $G \cong B_{8,4}$.

Suppose that $m \geq 5$ and the result holds for graphs in $\mathbb{B}_{2m-2,m-1}$. Let $G \in \mathbb{B}_{2m,m}$ with a perfect matching M . If there is no pendent vertex with neighbor of degree two in G , then by Lemma 11, $R'(G) > g(m)$. Suppose that G has a pendent vertex u whose neighbor v is of degree two. Then $uv \in M$ and $G - u - v \in \mathbb{B}_{2m-2,m-1}$. Let w be the neighbor of v different from u . Let $a = d_G(w)$ and let l be the number of neighbors of w whose degree is at least a . By Lemma 2 and the induction hypothesis, $R'(G) = R'(G - u - v) + 1 \geq g(m-1) + 1 > g(m)$ if $a = 2$, and $R'(G) = R'(G - u - v) + \frac{1}{2} + \frac{l}{a(a-1)} \geq g(m-1) + \frac{1}{2} + \frac{l}{a(a-1)} \geq g(m)$ with equalities if and only if $G - u - v \cong B_{2m-2,m-1}$ and $l = 0$, i.e., $G - u - v \cong B_{2m-2,m-1}$ and w is a vertex

of local maximal degree if $a \geq 3$. Thus $R'(G) \geq g(m)$ with equality if and only if $G \cong B_{2m,m}$.

Suppose that $n > 2m$ and the result holds for graphs in $\mathbb{B}_{n-1,m}$. Let $G \in \mathbb{B}_{n,m}$. If there is no pendent vertex in G , then $G \in \tilde{\mathbb{B}}(2m+1)$, and thus

$$R'(G) = \begin{cases} m + \frac{1}{6} & \text{if } G \in \mathbb{B}_n^1(1) \cup \mathbb{B}_n^2(1) \\ m & \text{otherwise} \end{cases} > g(m).$$

Suppose that there is at least one pendent vertex in G . By Lemma 10, there is an m -matching M and a pendent vertex u of G such that u is not M -saturated. Then $G - u \in \mathbb{B}_{n-1,m}$. Let v be the unique neighbor of u . Let $a = d_G(v)$ and let l be the number of neighbors of v whose degree is at least a . By Lemma 1, we have

$$R'(G) = R'(G - u) + \frac{l}{a(a-1)} \geq g(m) + \frac{l}{a(a-1)} \geq g(m)$$

with equalities if and only if $G - u \cong B_{n-1,m}$ and $l = 0$, i.e., $G - u \cong B_{n-1,m}$ and v is a vertex of local maximal degree. Thus $R'(G) \geq g(m)$ with equality if and only if $G \cong B_{n,m}$. \square

Corollary 5. *Let G be a bicyclic graph on $n \geq 6$ vertices. $R'(G) \geq \frac{5}{3}$ with equality if and only if $G \cong B_n(n-1, 3)$.*

Proof. Let m be the matching number of G . If $m \geq 4$, then by Theorem 5, $R'(G) \geq g(m) \geq \frac{5}{2} - \frac{1}{12} > \frac{5}{3}$. If $m = 3$, then by Theorem 4, $R'(G) \geq 2 > \frac{5}{3}$. Thus the result follows from Theorem 3. \square

Theorem 6. *Let G be a bicyclic graph on at least 5 vertices. Then $R'(G) \leq \frac{n}{2} - \frac{1}{3}$ with equality if and only if $G \in \mathbb{B}_n^1(1) \cup \mathbb{B}_n^2(1)$.*

Proof. Let G be a graph with the maximum modified Randić index among the bicyclic graphs on n vertices. By Lemmas 3 and 4, $G \in \tilde{\mathbb{B}}(n)$. By direct calculation, we have

$$R'(G) = \begin{cases} \frac{n}{2} - \frac{1}{3} & \text{if } G \in \mathbb{B}_n^1(1) \cup \mathbb{B}_n^2(1), \\ \frac{n}{2} - \frac{1}{2} & \text{if } G \in \mathbb{B}_n^1(t) \cup \mathbb{B}_n^2(t) \cup \mathbb{B}_n^1(0) \text{ with } t \geq 2. \end{cases}$$

The result follows. \square

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