Maximum zeroth-order general Randić index of orientations of trees, unicyclic and bicyclic graphs with given matching number

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Abstract

The zeroth-order general Randić index \( R_0^a(D) \) of a digraph \( D \) is the sum of \( (d^+_v)^a + (d^-_v)^a \) over all arcs \( uv \) of \( D \), where \( a \) is an arbitrary real number, the out-degree of the vertex \( v \) and the in-degree of the vertex \( v \), respectively. We determine maximum zeroth-order general Randić index of oriented trees, unicyclic and bicyclic graphs in terms of matching number and order in this paper.

Keywords: matching number; oriented bicyclic graph; oriented unicyclic graph; zeroth-order general Randić index.

1 Introduction

Let \( G = (V, E) \) be a simple connected graph with the vertex set \( V(G) \) and the edge set \( E(G) \). We denote by \( d_G(v) \) (\( d_v \) for short) the degree of vertex \( v \) in \( G \), and \( N_G(v) \) the neighbors of vertex \( v \) in \( G \). We denote by \( G - uv \) (resp. \( G + uv \)) the subgraph of \( G \) obtained by deleting (resp. adding) \( uv \) with \( uv \in E(G) \) (resp. \( uv \notin E(G) \)), and \( G - u \) (resp. \( G + u \)) the subgraph of \( G \) obtained by deleting (resp. adding) vertex \( u \) and the edges incident with \( u \), where \( u \in V(G) \) (resp. \( u \notin V(G) \)). A matching \( M \) of the graph \( G \) is a subset of \( E(G) \) in which no two edges share a common vertex. For any matching \( M_1 \) of \( G \), if \( |M_1| \leq |M| \), then the matching \( M \) is maximum in \( G \). The matching number of \( G \) is equal to the number of edges of a maximum matching in \( G \). If vertex \( v \in V(G) \) is incident with an edge of \( M \), then \( v \) is \( M \)-saturated. If \( v \) is \( M \)-saturated for any \( v \in V(G) \), then \( M \) is a perfect matching in \( G \).

Let \( D = (V, A) \) be a digraph with arc set \( A(D) \) and vertex set \( V(D) \), where \( vu \in A(D) \) is an arc that from vertex \( v \) to vertex \( u \) in the graph \( D \) (\( D \) has no loops). \( d^+_u \) (resp. \( d^-_u \)) denotes the out-degree (resp. in-degree) of a vertex \( u \), \( d^+_u = |\{v|uv \in A(D), v \in V(D)\}| \) (resp. \( d^-_u = |\{v|vu \in A(D), v \in V(D)\}| \)). If \( u \in V(D) \) and \( d^+_u = d^-_u = 0 \), then \( u \) is an isolated vertex. If \( d^+_u = 0 \) (resp. \( d^-_u = 0 \)) for \( u \in V(D) \), then \( u \) is a sink vertex (resp. source vertex). We can replace each edge \( uv \) of \( G \) by an arc \( uv \) or \( vu \) and get an oriented graph \( D \) which is also called an orientation of \( G \). Let \( O(G) = \{ D | D \text{ is a orientation of } G \} \), \( D \in O(G) \), if any \( u \in V(D) \), we have \( d^+_u = 0 \) or \( d^-_u = 0 \), then \( D \) is a sink-source orientation of \( G \). Let \( O^0(G) = \{ D | D \text{ is a sink-source orientation of } G \} \).

Topological index has a great influence in QSPR and QSAR [1, 2]. Li and Zheng [3] proposed zeroth-order general Randić index defined as \( R_0^a(G) = \sum_{u \in V(G)} (d_G(u))^a \), where \( a \) is an arbitrary real number.

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It is obvious that the zeroth-order general Randić index is a VDB topological index. The problem that what is extremal graphs over the set of important graphs with respect to zeroth-order general Randić index has been studied by researchers in [4, 5, 6, 7, 8, 9, 10]. Recently, Monsalve and Rada proposed VDB topological indices in digraphs; see [12].

The definition of zeroth-order general Randić index \( R_0^a(D) \) of a digraph is as [17]

\[
R_0^a(D) = \frac{1}{2} \sum_{uv \in A} [(d_u^+)^a + (d_v^-)^a] = \frac{1}{2} \sum_{u \in V} [(d_u^+)^a + (d_u^-)^a + 1].
\]

If \( D \) is obtained by replacing each edge \( uv \in E(G) \) with arcs \( uv \) and \( vu \), then \( d_D^+(u) = d_D^-(u) = d_G(u) \) and

\[
R_0^a(D) = \frac{1}{2} \sum_{uv \in A} [(d_D^+(u))^a + (d_D^-(v))^a] = \frac{1}{2} \sum_{uv \in E} [(d_G(u))^a + (d_G(v))^a] = \frac{1}{2} \sum_{u \in V} [(d_G(u))^a + 1] = R_0^{a+1}(G).
\]

Monsalve and Rada [12] solved the problem on extremal values of the Randić index over an important digraph family, such as oriented paths in terms of the order and cycles in terms of the order, digraphs in terms of the order, oriented hypercubes in terms of the dimension, oriented trees in terms of the order, respectively. Deng et al. [14] solved the problem on extremal values of some VDB topological indices over an important digraph family that is digraphs in terms of the order, such as the harmonic index, the Randić index, the Atom-Bond-Connectivity index, the first and second Zagreb indices, the Geometric-Arithmetic index and the sum-connectivity index. The problem of finding extremal values of VDB topological indices over an important digraph family that are oriented trees in terms of the order and oriented graphs in terms of the order were solved by Monsalve and Rada [11]. The problem of finding extremal values of first Zagreb index over an important digraph family that is oriented unicyclic graphs in terms of matching number and the order was solved by Yang and Deng [13].

In this paper, we discuss orientations of trees, unicyclic and bicyclic graphs in terms of the matching number with maximum value of the zeroth-order general Randić index.

2 Preliminary

We first establish three useful lemmas.

**Lemma 1.** [15] Let \( G \) be a graph. Then \( G \) is a bipartite graph if and only if \( |O'(G)| \geq 1 \). Moreover, If \( G \) is a connected bipartite graph, then \( |O'(G)| = 2 \).

**Lemma 2.** [17] For any simple connected graph \( G, D \in O(G), a \geq 1 \), we have

\[
R_0^a(D) \leq \frac{R_0^{a+1}(G)}{2}
\]

with equality if and only if \( D \in O'(G) \).

**Lemma 3.** Let \( G \) be a graph of order \( n \), \( a \geq 1 \), \( D \in O(G) \).
(1) If $d_G(u) = 1$ and $u \in V(G)$, $G' = G - u$, $D' \in O(G')$ such that $A(D') \cap A(D) = A(D')$, $v \in N_G(u)$. Then

$$R_0^0(D) - R_0^0(D') \leq \frac{1}{2} [1 + (d_G(v))^{a+1} - (d_G(v) - 1)^{a+1}]$$

with equality if and only if $\max\{d_D^+(v), d_D^-(v)\} = d_G(v)$.

(2) If $d_G(w_1) = 1$, $w_2 \in N_G(w_1)$, $d_G(w_2) = 2$ and $w_1, w_2 \in V(G)$, $G' = G - \{w_1, w_2\}$, $D' \in O(G')$ such that $A(D') \cap A(D) = A(D')$, $N_G(w_2) = \{w_1, w_3\}$. Then

$$R_0^0(D) - R_0^0(D') \leq \frac{1}{2} [1 + 2^{a+1} + (d_G(w_3))^{a+1} - (d_G(w_3) - 1)^{a+1}]$$

with equality if and only if $d_D^+(w_3) = d_G(w_3), d_D^-(w_2) = 2$; or $d_D^+(w_3) = d_G(w_3), d_D^+(w_2) = 2$.

(3) If $d_G(w_1) = 2, w_3 \in N_G(w_1), w_1, w_3 \in V(G), G' = G - w_1w_3, D' \in O(G')$ such that $A(D') \cap A(D) = A(D')$. Then

$$R_0^0(D) - R_0^0(D') \leq \frac{1}{2} [2^{a+1} - 1 + (d_G(w_3))^{a+1} - (d_G(w_3) - 1)^{a+1}]$$

with equality if and only if $d_D^+(w_3) = d_G(w_3), d_D^-(w_1) = 2$; or $d_D^+(w_3) = d_G(w_3), d_D^+(w_2) = 2$.

Proof. Let $b_i = d_D^+(w_i), b'_i = d_D^-(w_i), d_i = d_G(w_i), d'_i = d_D^-(w_i), i = 1, 2, 3, d_G(w_3) = t.$

(2) If $w_2w_3 \in A(D)$, then $d_3 = d'_3 + 1, b_3 = b'_3$. Hence,

$$R_0^0(D) - R_0^0(D') = \frac{1}{2} [(b_1)^{a+1} + (d_1)^{a+1} - 0 + (b_2)^{a+1} + (d_2)^{a+1} - 0]$$

$$+ \frac{1}{2} [(b_3)^{a+1} + (d_3)^{a+1} - (b'_3)^{a+1} - (d'_3)^{a+1}]$$

$$\leq \frac{1}{2} [1 + 2^{a+1}] + \frac{1}{2} [(b_3)^{a+1} + (d_3)^{a+1} - (b'_3)^{a+1} - (d'_3)^{a+1}]$$

$$\leq \frac{1}{2} [1 + 2^{a+1} + t^{a+1} - (t - 1)^{a+1}]$$

with equality if and only if $d_3 = t, b_3 = 2$.

Similarly, if $w_3w_2 \in A(D)$, then

$$R_0^0(D) - R_0^0(D') \leq \frac{1}{2} [1 + 2^{a+1} + t^{a+1} - (t - 1)^{a+1}]$$

with equality if and only if $b_3 = t, d_2 = 2$. The lemma holds clearly.

(3) If $w_3w_3 \in A(D)$, then $b_1 = b'_1 + 1, d_1 = d'_1, d_3 = d'_3 + 1, b_3 = b'_3$. Hence,

$$R_0^0(D) - R_0^0(D') = \frac{1}{2} [(b_1)^{a+1} + (d_1)^{a+1} - (b'_1)^{a+1} - (d'_1)^{a+1}]$$

$$+ \frac{1}{2} [(b_3)^{a+1} + (d_3)^{a+1} - (b'_3)^{a+1} - (d'_3)^{a+1}]$$

$$\leq \frac{1}{2} [(b_1)^{a+1} + (d_1)^{a+1} - (b_1 - 1)^{a+1} - (d_1)^{a+1}]$$

$$+ \frac{1}{2} [(b_3)^{a+1} + (d_3)^{a+1} - (b_3)^{a+1} - (d_3 - 1)^{a+1}]$$

$$\leq \frac{1}{2} [2^{a+1} - 1 + t^{a+1} - (t - 1)^{a+1}]$$

with equality if and only if $d_3 = t, b_1 = 2$. 

3
Similarly, if \( w_3w_1 \in A(D) \), then
\[
R^0_a(D) - R^0_a(D') \leq \frac{1}{2}[2^{a+1} - 1 + t^{a+1} - (t-1)^{a+1}]
\]
with equality if and only if \( b_3 = t, d_1 = 2 \). The lemma holds clearly.

3 Maximum zeroth-order general Randić index of orientations of trees, unicyclic graphs with given matching number

In this section, we first determine the maximum zeroth-order general Randić index for oriented trees with given matching number.

Let \( 1 \leq m \leq \left\lfloor \frac{n}{2} \right\rfloor \), where \( n, m \) are integers. Let \( T(n, m) = \{T|T\text{ is a tree of order } n \text{ and matching number } m \} \). Let \( T_{n,m} \) be shown in Figure 1. Obviously, \( T_{n,m} \in T(n,m) \).

![Figure 1: The graph \( T_{n,m} \).](image)

Denote \( h_0(n,m,a) = \frac{1}{2}[n - m + 2^{a+1}(m-1) + (n-m)^{a+1}] \).

**Lemma 4.** [19] Let \( T \in T(n,m) \) with \( 1 \leq m \leq \left\lfloor \frac{n}{2} \right\rfloor \), \( a \geq 1 \). Then
\[
R^0_{a+1}(T) \leq 2h_0(n,m,a)
\]
with equality if and only \( T \cong T_{n,m} \).

We can extend the zeroth-order general Randić index of trees to the oriented trees.

**Theorem 5.** Let \( T \in T(n,m) \) with \( 1 \leq m \leq \left\lfloor \frac{n}{2} \right\rfloor \), \( a \geq 1 \), \( D \in O(T) \). Then
\[
R^0_a(D) \leq h_0(n,m,a)
\]
with equality if and only \( D \in O'(T_{n,m}) \).

**Proof.** From Lemma 2 and Lemma 1, \( R^0_a(D) \leq \frac{1}{2}R^0_{a+1}(T) \) with equality if and only if \( D \in O'(T) \). Then by Lemma 4, we have
\[
\max\{R^0_a(D)|D \in O(T), T \in T(n,m)\} = \max\{\frac{1}{2}R^0_{a+1}(T)|T \in T(n,m)\} = \frac{1}{2}R^0_{a+1}(T_{n,m}).
\]
Consequently, \( R^0_a(D) \leq h_0(n,m,a) \) with equality if and only if \( D \in O'(T_{n,m}) \).

We obtain a oriented tree of matching number \( m \) and order \( n \) with the maximum zeroth-order general Randić index. Now, we will give the maximum zeroth-order general Randić index for oriented unicyclic graphs with given matching number.
Let $2 \leq m \leq \lfloor \frac{n}{2} \rfloor$, $U(n, m) = \{T | T \text{ is a unicyclic graph of order } n \text{ and matching number } m \}$. Let $U_{n,m}, U_{n,m}^{(1)}, U_{n,m}^{(2)}$ be shown in Figure 3. Obviously, $U_{n,m} \in U(n, m)$. Let $C_n$ be the the cycle with $n$ vertices. $	ilde{U}_{n,m} = \{U_{n,m}^{(1)}, U_{n,m}^{(2)}\}$. Let $\mathcal{U}(n, m) = \begin{cases} \tilde{U}(4, 2) \cup \{U^{(3)}(4, 2), U^{(4)}(4, 2)\}, & \text{if } a = 1 \text{ and } (n, m) = (4, 2) \\ \tilde{U}(6, 3) \cup \{U^{(3)}(6, 3), U^{(4)}(6, 3)\}, & \text{if } a = 1 \text{ and } (n, m) = (6, 3) \\ \tilde{U}(n, m), & \text{otherwise} \end{cases}$ where $U^{(3)}_{4,2}, U^{(4)}_{4,2} \in \mathcal{O}(C_4)$ and $U^{(3)}_{6,3}, U^{(4)}_{6,3} \in \mathcal{O}(U_1)$, $U_1$ is shown in Figure 3. Denote $h_1(n, m, a) = \frac{1}{2}((-m + n + 1)^{1+a} + m + 2^{a+1} + n - m - 2^{a+1} + 1]$. The following lemmas are useful to prove main results.

**Lemma 6.** Let $D \in \mathcal{O}(U_{4,2})$, $a \geq 1$. Then

$$R^0_a(D) \leq h_1(4, 2, a)$$

with equality if and only if $D \in \{U^{(1)}_{4,2}, U^{(2)}_{4,2}\}$.

**Lemma 7.** Let $B_0$ be shown in Figure 3. $D \in \mathcal{O}(B_0)$, $a \geq 1$. Then

$$R^0_a(D) < h_1(6, 3, a).$$

![Figure 2](image-url)

Figure 2: $B_0$ and $D_i$, $i = 1, 2, \cdots, 12$ in Lemma 7.

**Proof.** Note that $\mathcal{O}(B_0) = \{D_i | i = 1, 2, \cdots, 12\}$ (see Figure 2). It is easily to obtain that

- $R^0_a(D_1) = R^0_a(D_2) = R^0_a(D_3) = R^0_a(D_4) = R^0_a(D_7) = R^0_a(D_8) = \frac{1}{2}(3 + 2^{a+1} + 6)$,
- $R^0_a(D_5) = R^0_a(D_6) = R^0_a(D_{11}) = R^0_a(D_{12}) = \frac{1}{2}(2^{a+2} + 3^{a+1} + 5)$,
- $R^0_a(D_9) = R^0_a(D_{10}) = \frac{1}{2}(2^{a+1} + 2 \times 3^{a+1} + 4)$.

Since $R^0_a(D_9) - R^0_a(D_1) = \frac{1}{2}(2 \times 3^{a+1} - 2^{a+2} - 2) > 0$ and $R^0_a(D_9) - R^0_a(D_5) = \frac{1}{2}(3^{a+1} - 2^{a+1} - 1) > 0$, $h_1(6, 3, a) - R^0_a(D_9) = \frac{1}{2}(4^{a+1} - 2 \times 3^{a+1} + 2^{a+1}) > 0$, the result follows.

We consider the oriented unicyclic graphs with a perfect matching.
Theorem 8. Let $G \in U(2m, m)$ with $m \geq 2$, $a \geq 1$, $D \in O(G)$. Then

$$R_u^0(D) \leq h_1(2m, m, a)$$

with equality if and only if $D \in U_{2m,m}^*$.

Proof. Applying induction on $m$.

$U(4, 2) = \{U_{4,2}, C_4\}$ for $m = 2$. It is easily that $D \in O(U_{4,2})$, $R_u^0(D) \leq h_1(4, 2, a)$ with equality if and only if $D \in \{U_{4,2}^{(1)}, U_{4,2}^{(2)}\}$ by Lemma 6. Let $f(a) = h_1(4, 2, a) - 2^{a+2} = \frac{1}{2}[3^{a+1} - 3 \cdot 2^{a+1} + 3] = \frac{1}{2}[27 \cdot 3^{a-2} - 24 \cdot 2^{a-2} + 3] > 0 (a \geq 2)$. As the fact that $f'(a) = \frac{1}{2}[3^{a+1} \cdot \ln 3 - 3 \cdot 2^{a+1} \cdot \ln 2] > 0 (1 \leq a \leq 2)$ (see Figure 10 of the Appendix A) and $f(1) = 0$, $f(a) = \frac{1}{2}[3^{a+1} - 3 \cdot 2^{a+1} + 3] \geq 0 (1 \leq a \leq 2)$ with equality if and only if $a = 1$. By Lemma 3, $D \in O(C_4)$, $R_u^0(D) \leq \frac{1}{2}R_{u+1}^0(C_4) = 2^{a+2} \leq h_1(4, 2, a)$ with equality if and only if $a = 1$ and $D \in O'(C_4)$ which implies that $D \in \{U_{4,2}^{(3)}, U_{4,2}^{(4)}\}$. The result follows.

Suppose that $m \geq 3$ and the result holds for the values smaller than $m$.

Let $G \in U(2m, m)$ with a perfect matching $M$. If $G = C_{2m}$, then $D \in O(C_{2m})$, by Lemma 2 and $h_1(2m, m, a) - 2^{1+a} \cdot m = \frac{1}{2}[(m + 1)^{1+a} - (1 + m) \cdot 2^{a+1} + 1 + m] = \frac{1}{2}[(1 + m)^2 \cdot (1 + m)^{a-1} - 4(1 + m) \cdot 2^{a+1} + 1 + m] > 0$, we have $R_u^0(D) \leq \frac{1}{2}R_{u+1}^0(C_{2m}) = m \cdot 2^{a+1} < h_1(2m, m, a)$. The result follows.

If $G \neq C_{2m}$, let us consider two cases.

Case 1. $|\{v \mid u, v \in V(G), uv \in E(G), d_u = 1, d_v = 2\}| \geq 1$.

Let $d_G(u) = 1$ and $N_G(u) = \{v, u\}$, $d_G(v) = b$.

Since $|E(G)| - |M| = m$ and $|\{v \mid e \in M \text{ is incident with } w\}| = 1$, we have $b - 1 \leq m$ which implies that $b \leq m + 1$. We set $G' = G - \{v, u\}$. Then $G' \in U(2(m-1), m-1)$. Let $D' \in O(G')$ such that $A(D') \cap A(D) = A(D')$.

By the induction hypothesis, $R_u^0(D') \leq h_1(2(m-1), m-1, a)$. By the Lemma 3

$$R_u^0(D) \leq R_u^0(D') + \frac{1}{2}[1 + 2^{a+1} + b^{a+1} - (b-1)^{a+1}]$$

$$\leq h_1(2(m-1), m-1, a) + \frac{1}{2}[1 + 2^{a+1} + (m + 1)^{a+1} - m^{a+1}]$$

$$= h_1(2m, m, a)$$
Lemma 10. Let \( D' \in U_{2(m-1),(m-1)}^* \) and \( \{d_D^-(v) = 2, d_D^+(u) = 1, d_D^+(w) = m+1\} \) or \( \{d_D^+(v) = 2, d_D^-(u) = 1, d_D^-(w) = m+1\} \), which implies that \( D \in U_{2m,m} \). The result follows.

Case 2. \( \{|v|w \in E(G), u, v \in V(G), d_u = 1, d_v = 2\| = 0 \).

\( C = w_1w_2...w_1 \) denotes the unique cycle of \( G \). Since \( |M| = m \), \( G - V(C) \) consists of isolated vertices.

Subcase 2.1. For any \( w_i \in V(C) \), there only exists a pendent vertex which is adjacent to \( w_i \).

When \( m \geq 8 \), by Lemma 2 and \( f(a) = h_1(2m, m, a) - \frac{1}{2}[m + m \cdot 3^{a+1}] = (-1 + m) \cdot 2^a + \frac{1}{2}[(1 + m)^2 \cdot (1 + m)^{a-1} - 9m \cdot 3^{a-1}] + \frac{1}{2} > 0 \), we have \( R^0_a(D) \leq \frac{1}{2}R^0_{a+1}(G) = \frac{1}{2}[m + m \cdot 3^{a+1}] < h_1(2m, m, a) \).

When \( m = 3 \), the result follows from Lemma 7.

When \( m = 4, f(a) = 3 \cdot 2^a + \frac{1}{2}[5^{a+1} - 4 \cdot 3^{a+1}] + \frac{1}{2} = 3 \cdot 2^a + \frac{1}{2}[125 \cdot 5^{a-2} - 108 \cdot 3^{a-2}] + \frac{1}{2} > 0 (a \geq 2) \) and \( f(a) > 0 (1 \leq a \leq 2) \) (see Figure 11 of the Appendix A).

When \( m = 5, 6, 7 \), the proof of the cases is similar to \( m = 4 \). The result follows.

Subcase 2.2. \( \{|u|d_G(u) = 2, u \in V(C)\| \geq 1 \).

We suppose that \( d_{w_3} = 3 \) and \( d_{w_4} = 2 \). Obviously, \( d_{w_1} = 2 \) or 3. Let \( w \in N_G(w_2) \) be a pendent vertex. Since \( w_3 \) is \( M \)-saturated and \( w_2w \in M \), there exists an edge \( w_3w_4 \in M \), where \( d_{w_4} = 2 \). Set \( T' = G - \{w_2, w\} \). Then \( T' \in T(2(m - 1), m - 1) \).

By Lemma 5, we have \( R^0_a(D') \leq h_0(2m - 2, m - 1, a) \). Thus

\[
R^0_a(D) \leq R^0_a(D') + \frac{1}{2}[(d_G(w))^{a+1} - 0 + (d_G(w_2))^{a+1} - 0 + (d_G(w_1))^{a+1} - (d_G(w_1) - 1)^{a+1} + (d_G(w_3))^{a+1} - (d_G(w_3) - 1)^{a+1}]
\]

\[
\leq h_0(2m - 2, m - 1, a) + \frac{1}{2}[1 + 2 \cdot 3^{1+a} - 1]
\]

\[
\leq \frac{1}{2}[m - 1 + 2^{a+1} \cdot (m - 2) + (m - 1)^{1+a} + 6 \cdot 3^a]
\]

Let \( g(x) = h_1(2x, x, a) - \frac{1}{2}[x - 1 + 2^{a+1} \cdot (x - 2) + (x - 1)^{1+a} + 6 \cdot 3^a] = -3^{a+1} + 2^a + \frac{1}{2} \cdot (1 + x)^{a+1} - \frac{1}{2} \cdot (1 + x)^{a-1} + x \geq 3 \).

Since \( g'(x) = \frac{1}{2}(a + 1) \cdot (x + 1)^a - (x - 1)^a > 0 \), we have \( g(x) \geq g(3) \), and \( f(a) = g(3) = -27 \cdot 3^3 + 2^a + \frac{1}{2}(64 \cdot 3^{a-2} - 8 \cdot 2^a) \cdot 1 > 0 (a \geq 2) \).

As the fact that \( f'(a) = -3^{a+1} \cdot ln3 + 2^a \cdot ln2 + \frac{1}{2}(4^{a+1} \cdot ln4 - 2^{a+1} \cdot ln2) \cdot 0 > 0 (1 \leq a \leq 2) \) (see Figure 12 of the Appendix A)

And \( f(1) = 0 \), \( f(a) \geq 0 \) with equality if and only if \( a = 1 \).

Consequently, \( R^0_a(D) \leq h_1(2m, m, a) \) with equality if and only if \( a = 1 \) and \( D \in \{U_{6,3}^{(3)}, U_{6,3}^{(4)}\} \). The result follows.

In order to prove Theorem 11, we need the following lemmas:

Lemma 9. Let \( G \in U(n, m) \), where \( n > 2m, G \neq C_n \). Then there exist a pendent vertex \( v \) and a maximum matching \( M \) of \( G \) such that \( v \) is not \( M \)-saturated.

Lemma 10. Let \( n > 2m \) and \( 2 \leq m \leq \lfloor \frac{n}{4} \rfloor \), where \( n, m \) are integers.

(1) If \( a = 1 \), then

\[
h_1(n, m, 1) > 2n.
\]
(2) If \( a \geq 1 \), then
\[ h_1(n, m, a) > 2^n \ast n. \]

Proof. (2) Let \( f(a) = h_1(n, m, a) - 2^n \ast n = \frac{1}{2}[(1 - m + n)^{a+1} + (m - 1) \ast 2^{a+1} + 1 - n - m] > 2^n \ast n \), we have \( f'(a) = \frac{1}{2}[(n - m + 1)^{a+1} \ast \ln(1 - m + n) + (n - 1 + m) \ast 2^{a+1} \ast \ln 2] > 0 \), by (1), \( f(a) \geq f(1) > 0 \).

Now, we consider oriented unicyclic graphs with given matching number.

**Theorem 11.** Let \( G \in U(n, m) \) with \( 2 \leq m \leq \lfloor \frac{n}{2} \rfloor \), \( D \in \mathcal{O}(G) \), \( a \geq 1 \). Then
\[ R^0_u(D) \leq h_1(n, m, a) \]
with equality if and only if \( D \in U_{n, m}^* \).

Proof. Applying induction on \( n \).

The result follows for \( n = 2m \) by Theorem 8.

Suppose that \( n > 2m \) and the result holds for the values smaller than \( n \).

From Lemma 2 and Lemma 10, if \( D \in \mathcal{O}(G) \) and \( G = C_n \), then \( R^0_u(D) \leq \frac{R^0_u(C_n)}{2} = n \ast 2^n < h_1(n, m, a) \). The result follows.

If \( G \neq C_n \), by Lemma 9, there exists a pendent vertex \( u \) such that \( G' = G - \{u\} \in U(n - 1, m) \). Let \( N_G(u) = \{v\} \), \( d_G(v) = b, D' \in \mathcal{O}(G') \) such that \( A(D') \cap A(D) = A(D') \).

Since \( |E(G)| - |M| = n - m \) and \( |\{v \in M \text{ is incident with } v\}| = 1 \), we have \( b - 1 \leq n - m \) which implies that \( b \leq n - m + 1 \).

By the induction hypothesis,
\[ R^0_u(D') \leq h_1(n - 1, m, a). \]

By Lemma 3, we have
\[
R^0_u(D) \leq R^0_u(D') + \frac{1}{2}(1 + b^{a+1} - (b - 1)^{a+1})
\leq h_1(n - 1, m, a) + \frac{1}{2}(1 + (1 - m + n)^{a+1} - (-m + n)^{a+1})
= h_1(n, m, a)
\]
with equality if and only if \( R^0_u(D') = h_1(n - 1, m, a) \), \( D' \in U_{n-1, m}^* \) and \( \{d_D^-(v) = n - m + 1, d_D^+(u) = 1\} \) or \( \{d_D^-(v) = n - m + 1, d_D^+(u) = 1\} \), which implies that \( D \in U_{n, m}^* \). The result follows.

### 4 Maximum zeroth-order general Randić index of orientations of bicyclic graphs with given matching number

In this section, Let \( B_n = \{G|G \text{ is a bicyclic graph of order } n \geq 4\}; B(n, m) = \{G|G \text{ is a bicyclic graph of order } n \text{ and matching number } m \} \), where \( 3 \leq m \leq \lfloor \frac{n}{2} \rfloor \). Let \( B^0_n = \{G|G \text{ is a bicyclic graph of order } n \geq 4 \text{ and } d_u \neq 1 \text{ for any vertex } u \in V(G)\} \). \( B^0_n \) contains five cases according to the arrangement of cycles, which are \( B^0_n, i = 1, 2, 3, 4, 5 \) (see Figure 4). We denote by \( C_1 \) and \( C_2 \) two independent cycles in...
It is obvious that $B_0^*(n,m) = \bigcup_{i=1}^{5} B_i^*(n,m)$.

For $3 \leq m \leq \lfloor \frac{n}{2} \rfloor$, $B_n^{(1)}, B_n^{(2)}$ are shown in Figure 5. Obviously, $B(n,m) \in B(n,m)$. Let $B_{n,m}^* = \{B_{n,m}^{(1)}, B_{n,m}^{(2)}\}$.

Figure 5: $B_{n,m}$ and its two orientations : $B_{n,m}^{(1)}, B_{n,m}^{(2)}$.

Denote $h_2(n,m,a) = \frac{1}{2} [m * 2^{a+1} - 2^{a+1} - m + 2 + n - (m + 2)^{a+1}]$.

**Lemma 12.** Let $G$ be a connected graph, and $w_1 \in V(G)$ with $d_G(w_1) = 2$, $N_G(w_1) = \{w_2, w_3\}$, $d_G(w_2) \geq 2$ and $w_2 w_3 \notin E(G)$, $a \geq 1$. Let $G' = G - w_1 w_3 + w_2 w_3$, then $R^0_{a+1}(G') > R^0_{a+1}(G)$.

**Proof.** Let $d_G(w_i) = b_i$, $d_{G'}(w_i) = b'_i$, $i = 1, 2, 3$. Obviously, $b_3 = b'_3$, $b_1 = b'_1 + 1$, $b_2 = b'_2 - 1$, $b_2 \geq 2$. Let $f(x) = (x+1)^{a+1} - x^{a+1}$ ($x \geq 2$), then $f'(x) = (a+1)(x+1)^a - x^a > 0$ ($x \geq 2$). Hence,

$$R^0_{a+1}(G') - R^0_{a+1}(G) = (b_3)^{a+1} + (b_2)^{a+1} + (b_1)^{a+1} - (b'_3)^{a+1} - (b'_2)^{a+1} - (b'_1)^{a+1}$$

$$= (b_2)^{a+1} - (b_2 - 1)^{a+1} + (b_1)^{a+1} - (b_1 - 1)^{a+1}$$

$$= 2^{a+1} - 1 - [(b_2 - 1)^{a+1} - (b_2)^{a+1}] < 0$$

The result follows.

If $m = 3$, then $B(6,3) = \{G_i | i = 1, 2, \cdots, 17\}$ (see Figure 6). We give the maximum zeroth-order general Randić index for orientations of $G_1 = B_{6,3}$ and $G_4$, which will be used in the proof of Theorem 10.
Lemma 13. Let $G_4$ be the bicyclic graph in Figure 7, $D \in O(G_4)$, $a \geq 1$. Then

$$R_a^0(D) < h_2(6, 3, a).$$

Proof. Let $B_1$ be the bicyclic graph in Figure 6, $D \in O(G_4)$, $D' \in O(B_1)$. $V(G_4) = \{v_4, v_3, v_2, v_1, u_2, u_1\}$, $V(B_1) = \{v_1, v_3, v_2, v_1\}$, and $d_{G_4}(u_i) = 1$, where $i = 1, 2$. $u_i$ has unique neighbor $v_i$ for $i = 1, 2$ and $d_{G_4}(v_1) = 3$, $d_{G_4}(v_2) = 4$. $d_{G_4}(v_3) = 3$, $d_{G_4}(v_4) = 2$. $d_{B_1}(v_1) = 2$, $d_{B_1}(v_2) = 3$, $d_{B_1}(v_3) = 3$, $d_{B_1}(v_4) = 2$.

Case 1. $D \in \{D | A(D) \cap A(D_1) = A(D_1), D \in O(G_4)\}$.

By $1 + 3^{1+a} - 2^{1+a} \ast 2 = 9 \ast 3^{1+a} + 1 - 8 \ast 2^{1+a} > 0$, we have $\Sigma_{i=1}^a[(d^+_D(v_i))^{a+1} + (d^-_D(v_i))^{a+1} + (d^+_D(u_i))^{a+1} + (d^-_D(u_i))^{a+1}] \leq \frac{1}{2}[4 + 2^{a+1} + 3^{a+1}]$. Hence, $R_a^0(D) = \frac{1}{2} \Sigma_{i=1}^a[(d^+_D(v_i))^{a+1} + (d^-_D(v_i))^{a+1} + (d^+_D(u_i))^{a+1} + (d^-_D(u_i))^{a+1}] + \frac{1}{2} \Sigma_{i=1}^a[(d^+_D(v_i))^{a+1} + (d^-_D(v_i))^{a+1}] \leq \frac{1}{2}[4 + 3^{1+a} + 2^{1+a}] + \frac{1}{2}[3 + 2^{1+a}] = \frac{1}{2}[7 + 2^{a+2} + 3^{a+1}].$

Case 2. $D \in \{D | A(D) \cap A(D_2) = A(D_2), D \in O(G_4)\}$.

$R_a^0(D) \leq \frac{1}{2}[5 + 3 \ast 2^{a+1} + 3^{a+1}].$

Case 3. $D \in \{D | A(D) \cap A(D_3) = A(D_3), D \in O(G_4)\}$.

$R_a^0(D) \leq \frac{1}{2}[5 + 3 \ast 2^{a+1} + 3^{a+1}].$

Case 4. $D \in \{D | A(D) \cap A(D_4) = A(D_4), D \in O(G_4)\}$.

$R_a^0(D) \leq \frac{1}{2}[7 + 2^{a+2} + 3^{a+1}].$

Case 5. $D \in \{D | A(D) \cap A(D_5) = A(D_5), D \in O(G_4)\}$.
Case 1. \( R_0(D) \leq \frac{1}{2}[3 + 2a^2 + 3a^1 + 4a^1]. \)

Case 6. \( D \in \{ D | A(D) \cap A(D_6) = A(D_6), D \in O(G_4) \}. \)

Case 11. \( D \in \{ D | A(D) \cap A(D_{11}) = A(D_{11}), D \in O(G_4) \}. \)

So

\[
\frac{1}{2}[3 + 2a^2 + 4a^1 + 3a^1] - \frac{1}{2}[3 + 2a^2 + 3a^1 + 2a^1] = \frac{1}{2}[2a^1 + 4a^1 - 2a^1] > 0;
\]

\[
h_2(6, 3, a) - \frac{1}{2}[3 + 2a^2 + 4a^1 + 3a^1] = \frac{1}{2}[2 + 5a^1 + 3a^1 - 4a^1] = \frac{1}{2}[2 + 25 + 9 - 9 + 16 - 3 + 4a^1] > 0;
\]

\[
\frac{1}{2}[3 + 2a^2 + 3a^1 + 2a^1] - \frac{1}{2}[4 + 2a^2 + 3a^1] = \frac{1}{2}[-1 + 3 + 2a^1] > 0;
\]

\[
\frac{1}{2}[4 + 2a^2 + 3a^1] - \frac{1}{2}[3 + 2a^1 + 2a^1] = \frac{1}{2}[-2 + 2a^1] > 0,
\]
\[
\frac{1}{2}[6 + 2a + 1 + 2 \times 3a + 1] - \frac{1}{2}[5 + 3 \times 2(1+a) + 3a + 1] = \frac{1}{2}[1 - 2^{a+2} + 3^{1+a}] = \frac{1}{2}[1 - 8 \times 2^{a-1} + 9 \times 3^{a-1}] > 0,
\]
\[
\frac{1}{2}[5 + 3 \times 2^{1+a} + 3^{1+a}] - (8[7 + 2^{4+a} + 3^{1+a}] = \frac{1}{2}[-2 + 2^{1+a}] > 0,
\]
we have \( h_2(6,3,a) > \frac{1}{2}(3 + 2^{3+a} + 4^{1+a} + a + 3^{1+a}) > \frac{1}{2}(3 + 2^{3+a} + 3^{2+a}) > \frac{1}{2}(4 + 2^{3+a} + 2 \times 3^{1+a}) > \frac{1}{2}(6 + 2^{3+a} + 2 \times 3^{1+a}) > \frac{1}{2}(5 + 3 \times 2^{3+a} + 3^{1+a}) > \frac{1}{2}(7 + 2^{3+a} + 2 + 3^{1+a}). \]

It is easy to get that
\[
R_0(D) \leq h_2(6,3,a)
\]
with equality if and only if \( D \in \{B_{6,3}(1), B_{6,3}(2)\} \) (see Figure 5).

**Lemma 14.** Let \( D \in O(B_{6,3}) = O(G_1) \), where \( G_1 = B_{6,3} \) is shown in Figure 6, \( a \geq 1 \). Then

\[
R_0(D) \leq h_2(6,3,a)
\]

with equality if and only if \( D \in \{B_{6,3}(1), B_{6,3}(2)\} \) (see Figure 5).

**Proof.** Let \( O(G_1) = \{D_1, D_2, \cdots, D_{26}\} \). By directly calculation, we have

\[
R_0(D_1) = R_0(D_{11}) = \frac{1}{2}(9 + 2^{a+1} + 3^{a+1}),
\]
\[
R_0(D_2) = R_0(D_{14}) = \frac{1}{2}(8 + 2^{a+1} + 4^{a+1}),
\]
\[
R_0(D_3) = R_0(D_9) = R_0(D_{13}) = R_0(D_{19}) = \frac{1}{2}(5 + 3 \times 2^{a+1} + 3^{a+1}),
\]
\[
R_0(D_4) = R_0(D_{12}) = \frac{1}{2}(7 + 2^{a+2} + 3^{a+1}),
\]
\[
R_0(D_5) = R_0(D_{17}) = \frac{1}{2}(4 + 3 \times 2^{a+1} + 4^{a+1}),
\]
\[
R_0(D_6) = R_0(D_{16}) = \frac{1}{2}(1 + 5 \times 2^{a+1} + 3^{a+1}),
\]

Figure 8: \( G_1 \) and its orientations.
Lemma 15. Let \( G \in \mathcal{B}(2m, m) \) \( (m \geq 3), a \geq 1, D \in \mathcal{O}(G) \) and no pendent vertex has neighbor of degree 2 in \( G \). Then

\[
R^0_a(D) \leq h_2(2m, m, a)
\]

with equality if and only if \( G \in \mathcal{B}^*_a(m, 3) \).

Proof. Suppose that \( M \) is a maximum matching in \( G \). Since \( |M| = m \), we have that every vertex in \( G \) is adjacent to at most one pendent vertex. Since \( G \in \mathcal{B}(2m, m) \) and no pendent vertex has neighbor of degree 2, we can attach pendent vertices to \( G' \in \mathcal{B}^0_a(m \leq k \leq 2m) \) and get \( G \). We take two cases into consideration according to that \( G \) has vertices of degree 2 or not.

**Case 1.** \( \{|v|v \in V(G), d_G(v) = 2\| = 0 \).

Then either \( k = m \) or \( k = m+1 \). If \( k = m \), then we can get \( G \) by attaching a pendent vertex to every vertex of \( G' \in \mathcal{B}^0_a(m) \). If \( k = m+1 \), then we can get \( G \) by attaching a pendent vertex to every vertex of degree 2 of \( G' \in \mathcal{B}^1_{m+1} \cup \mathcal{B}^2_{m+1} \cup \mathcal{B}^3_{m+1} \).

If \( m = 3 \), then \( G \cong Q_1 \) (see Figure 9). Let \( f(a) = h_2(6, 3, a) - \frac{1}{2}[3a^2 + 4 + 2] = \frac{1}{2}[2a^2 + 5 + 5a^2 - 2 - 12 * 3^a] \), then \( f(a) = \frac{1}{2}[2a^2 + 5 + 125 * 5a^2 - 2 - 108 * 3a^2] > 0(a \geq 2), f'(a) = \frac{1}{2}[2a^2 + 5a + 12 * 3^a] > 0 (1 \leq a \leq 2) \) (see Figure 13 of the Appendix A) and \( f(1) = 0 \), hence \( f(a) \geq 0 (1 \leq a \leq 2) \) with equality if and only if \( a = 1 \). By Lemma 2, \( D \in \mathcal{O}(Q_1) \), \( R^0_a(D) \leq \frac{1}{2}R^0_{a+1}(Q_1) = \frac{1}{2}[3a^2 + 4 + 2] = h_2(6, 3, a) \) with equality if and only if \( a = 1 \) and \( D \in \mathcal{O}'(Q_1) \), but by Lemma 1 and \( Q_1 \) is not a bipartite graph, \( |\mathcal{O}'(Q_1)| = 0 \) and \( R^0_a(D) < h_2(6, 3, a) \). The result follows.

If \( m = 4 \), we have \( G' \cong Q_2, G \cong Q_3 \) or \( G \cong Q_4 \) or \( G' \cong Q_6 \). \( G \cong Q_5 \). (see Figure 9). Let \( f(a) = h_2(8, 4, a) - \frac{1}{2}[3 + 3^a + 3 * 5] = \frac{1}{2}[3 * 2a^2 + 3 + 6a^2 - 5 * 3a^2 + 1] \), then \( f(a) = \frac{1}{2}[3 * 2a^2 + 3 + 216 *}
\[6^{a-2} - 135 \cdot 3^{a-2}] > 0 \ (a \geq 2) \text{ and } f(a) > 0 \ (1 \leq a \leq 2) \] (see Figure 14 of the Appendix A). By Lemma 2, \(D \in \mathcal{O}(Q_2), R^0_0(D) \leq \frac{1}{2} R^0_0(Q_2) = \frac{1}{2} [3 + 3^{a+1} \cdot 5] < h_2(8, 4, a).\)

Let \( f(a) = h_2(8, 4, a) - \frac{1}{2} [3 + 2^{a+1} + 3 + 6^{a+1} - 3^{a+1} - 125 - 5^{a+1} - 2 + 2^{a+1} + 3^{a+1}] > 0 (a \geq 2), \) then \( f(a) = 3 + 2^{a+1} + 106 + 3^{a+1} - 128 > 0 (a \geq 2), \) (see Figure 15 of the Appendix A) and \( f(1) = 0, \) hence \( f(a) \geq 0 \ (1 \leq a \leq 2) \) with equality if and only if \( a = 1. \) By Lemma 2, \( D \in \mathcal{O}(Q_4), R^0_0(D) \leq \frac{1}{2} R^0_0(Q_4) = \frac{1}{4} \) (see Figure 22 of the Appendix A). Hence, \( D \in \mathcal{O}(Q_5), R^0_0(D) \leq \frac{1}{2} R^0_0(Q_5) = \frac{1}{4} [3 + 5 \cdot 3^{a+1}] < h_2(8, 4, a). \) The result follows.

Now if \( m \geq 5, \) then

\[
R^0_{a+1}(G) = \begin{cases} 
(\text{if } G' \in B^1_m \cup B^1_m \cup B^2_m \cup B^5_m) \\
(\text{if } G' \in B^3_m) \\
n + (m - 1) + 3^{a+1} + 5^{a+1} \\
n + (m - 1) + 3^{a+1} + 5^{a+1} \\
\end{cases}
\]

Since \( m + (m - 1) + 3^{a+1} + 5^{a+1} > 0, \) we have \( R^0_{a+1}(G) \leq m + (m - 1) + 3^{a+1} + 5^{a+1}. \)

Let \( f(x) = h_2(2x, x, a) - \frac{1}{2} [x + (x - 1) + 3^{a+1} + 5^{a+1}] = \frac{1}{2} [2 + (x - 1) + (2 \cdot 3^{a+1} + (x + 2) \cdot 5^{a+1})] \) \((x \geq 5), \) then \( f'(x) = \frac{1}{2} [2^{1+a} - 3^{a+1} + (a + 1) + 3^{a+1}] > 0, \) hence \( f(x) \geq f(5) = \frac{1}{2} [2 + 4(2^{a+1} - 3^{a+1}) + 7^{a+1} - 125 - 5^{a+1}] \) \( (1 \leq a \leq 2) \) (see Figure 16 of the Appendix A), we have \( f(m), \) \( f(5) > 0. \) Thus by Lemma 2, \( D \in \mathcal{O}(G), R^0_0(D) \leq \frac{1}{2} R^0_{a+1}(G) \leq \frac{1}{2} [m + (m - 1) + 3^{a+1} + 5^{a+1}] < h_2(2m, m, a). \) The result follows.

As the fact that \( m = 3, \) \( \frac{1}{2} R^0_{a+1}(G) \leq h_2(6, 3, a); m = 4, \) \( \frac{1}{2} R^0_{a+1}(G) \leq h_2(8, 4, a); m \geq 5, \) \( \frac{1}{2} R^0_{a+1}(G) \leq h_2(2m, m, a) \) in Case 1.

**Case 2.** \( |\{v \in V(G), d_G(v) = 2\}| \geq 1. \)

Let \( u \in V(G) \) and \( d_G(u) = 2, v, w \in N_G(u) \) with \( d_G(v) = s \geq 2 \) and \( d_G(w) = t \geq 2. \) Since \( v \) and \( w \)
are symmetric, without lost of generality, suppose that \( uv \in M \).

**Subcase 2.1.** If the cycles of \( G \) have no vertex of degree 2.

Since \( G \) has no pendent vertex which has neighbor of degree 2, we have \( G' \in \mathcal{B}^2_2 \) and \( u \) lies on the path which is connecting two vertex-disjoint cycles of \( G \). So \( uv \notin E(G) \). Since \( uv \in M \) and \( |M| = m \), we have

\[
d_G(v) = \begin{cases} 
2, & \text{if } v \text{ lies on the path which is connecting two vertex-disjoint cycles of } G. \\
\infty, & \text{if } v \text{ lies on cycles of } G.
\end{cases}
\]

Let \( G'' = G + vw - uw \), we have \( G'' \in \mathcal{B}(2m, m) \). By Lemma 12 we have \( R^0_{a+1}(G'') > R^0_{a+1}(G) \). Obviously,

\[
|V'(G)| = \begin{cases} 
|V'_1(G'')| + 2, & \text{if } v \text{ lies on the path which is connecting two vertex-disjoint cycles of } G, \\
|V'_1(G'')| + 1, & \text{if } v \text{ lies on cycles of } G,
\end{cases}
\]

where \( V'(G) \) is set of vertices of degree two in \( G \) and \( V'(G'') \) is set of vertices of degree two in \( G'' \). Repeating this operation from \( G \) to \( G'' \), and we can get a bicyclic graph described in Case 1, say \( H \). By Lemma 12 and \( \frac{1}{2}R^0_{a+1}(G) \leq h_2(2m, m, a) \) in Case 1, we have \( R^0_{a+1}(G) < R^0_{a+1}(G'') < R^0_{a+1}(H) \leq 2h_2(2m, m, a) \). Hence, \( D \in \mathcal{O}(G) \), \( R^0_{0}(D) < h_2(2m, m, a) \) the result follows.

**Subcase 2.2.** We can suppose that it exists a vertex of degree 2 on some cycle of \( G \), without lost of generality, say \( u \).

Let \( N_G(u) = \{u = w_0, w_1, \ldots, w_{t-1}\} \), and \( G'' = G - uw \), we have \( G'' \in \mathcal{B}(2m, m) \). Note that \( 2 \leq s, t \leq 5 \) and \( w \) is adjacent to at most one pendant vertex. Let \( D' \in \mathcal{O}(G'') \) such that \( A(D) \cap A(D') = A(D') \).

By Theorem 8, \( R^0_{a}(D') \leq h_1(2m, m, a) \).

Let \( f(x) = h_2(2x, x, a) - \frac{1}{2}[2(x+1)^{a+1} + x^{2a+1} - x^{a+1} + x] = \frac{1}{2}[2 - 2^{a+1} + (x+2)^{a+1} - 2(x+1)^{a+1} + x^{a+1}] \) \((x \geq 4)\), then \( f'(x) = \frac{1}{2}[(a+1)(x+2)^a - 2(a+1)(x+1)^a + (a+1)x^a] > 0 \), \( f(x) \geq f(4) = \frac{1}{2}[2 - 2^{a+1} + 6^{a+1} - 2 \ast 5^{a+1} + 4^{a+1}] \). Let \( g(a) = f(4) \), then \( g(a) = \frac{1}{2}[2 - 2^{a+1} + 1296 + 6^{a+3} - 1250 \ast 5^{a-3} + 4^{a+1}] > 0(a \geq 3) \).

\( g'(a) = \frac{1}{2}[-2^{a+1} \ast ln2 + 6^{a+1} \ast ln6 - 2 \ast 5^{a+1} \ast ln5 + 4^{a+1} \ast ln4] > 0 \) (1 \( \leq a \leq 3 \)) (see Figure 23 of the Appendix A) and \( g(1) = 0 \), hence \( g(a) \geq 0 \) (1 \( \leq a \leq 3 \)) with equality if and only if \( a = 1 \). From Lemma 3 when \( m \geq 4 \), we have

\[
R^0_{a}(D) \leq R^0_{a}(D') + \frac{1}{2}[(d_G(u)]^{a+1} - (d_G(u) - 1)^{a+1} + t^{a+1} - (t-1)^{a+1}]
\leq h_1(2m, m, a) + \frac{1}{2}[2^{a+1} - 1 + (m+1)^{a+1} - m^{a+1}]
\leq \frac{1}{2}[2(m+1)^{a+1} + m \ast 2^{a+1} + m - m^{a+1}]
\leq h_2(2m, m, a)
\]

with equality if and only if \( a = 1 \) and \( R^0_{a}(D') = h_1(2m, m, a) \), \( d_D'(u) = 2, d_D'(w) = d_G(w) = 5 \); or \( d_D'(u) = 2, d_D'(w) = d_G(w) = 5 \). If \( D \) is satisfied with that \( D' \in U_{2m,m} \), \( d_D'(u) = 2, d_D'(w) = 5 \); or \( d_D'(u) = 2, d_D'(w) = 5 \), then \( D \) is conflicted with that no pendent vertex has neighbor of degree 2 in \( G \), we have \( R^0_{a}(D) < h_2(2m, m, a) \). The result follows.

When \( m = 3 \), \( \mathcal{B}(6,3)/\{G_6, G_7, G_{15}\} \) is the set of bicyclic graphs in which no pendent vertex has neighbor of degree 2 and cycles contain vertex of degree 2 (see Figure 23). Let \( G \in \mathcal{B}(6,3)/\{G_6, G_7, G_{15}\} \).

If \( G = G_1 \), \( D \in \mathcal{O}(G_1) \), by Lemma 14 we have \( R^0_{a}(D) \leq h_2(6,3, a) \) with equality if and only if \( D \in \{B_{6,3}^{(1)}, B_{6,3}^{(2)}\} \).
Let \( f(a) = h_2(6,3,a) - \frac{1}{2}[1 + 3 \cdot 2^{a+1} + 3^{a+1} + 4^{a+1}] = \frac{1}{2}[4^{a+1} + 2 - 2 \cdot 3^{a+1}] \), then \( f(a) = \frac{1}{2}[64 \cdot 4^{a-2} + 2 - 54 \cdot 3^{a-2}] > 0 (a \geq 2) \), \( f'(a) = \frac{1}{2}[4^{a+1} \cdot ln4 - 2 \cdot 3^{a+1} \cdot ln3] > 0 (1 \leq a \leq 2) \) (see Figure 17 of the Appendix A) and \( f(1) = 0 \), hence \( f(a) \geq 0 (1 \leq a \leq 2) \) with equality if and only if \( a = 1 \).

If \( G \in \{G_2,G_9\} \) and \( \frac{1}{2}R_{a+1}^0(G_2) = \frac{1}{2}R_{a+1}^0(G_9) = \frac{1}{2}[1 + 4^{a+1} + 3^{a+1} + 2 \cdot 1^{a+1}] \), then by Lemma 2 we have \( D \in \mathcal{O}(G) \), \( R_0^0(D) \leq \frac{1}{2}R_{a+1}^0(G) = \frac{1}{2}[1 + 4^{a+1} + 3^{a+1} + 3 \cdot 2^{a+1}] \leq h_2(6,3,a) \) with equality if and only if \( a = 1 \) and \( D \in \mathcal{O}'(G) \), but by Lemma 1 and \( G_2, G_9 \) are not bipartite graph, \( |\mathcal{O}'(G_2)| = 0 \) and \( |\mathcal{O}'(G_9)| = 0 \), hence \( R_0^0(D) < h_2(6,3,a) \). The result follows.

Let \( f_1(a) = h_2(6,3,a) - \frac{1}{2}[4 \cdot 2^{a+1} + 3^{a+1} \cdot 2] = \frac{1}{2}[2 \cdot 4^{a+1} - 2^{a+1} + 3 - 3^{a+2}] \), then \( f_1(a) = \frac{1}{2}[32 \cdot 4^{a-1} - 4 \cdot 2^{a-1} + 3 - 27 \cdot 3^{a-1}] > 0 \).

Let \( f_2(a) = h_2(6,3,a) - \frac{1}{2}[1 + 2 \cdot 4^{a+1} + 3^{a+1}] = \frac{1}{2}[2 \cdot 4^{a+1} + 2^{a+1} + 2 - 4 \cdot 3^{a+1}] \), then \( f_2(a) > \frac{1}{2}[128 \cdot 4^{a-2} - 108 \cdot 3^{a-2}] > 0 (a \geq 2) \) and \( f_2(a) > 0 (1 \leq a \leq 2) \) (see Figure 18 of the Appendix A).

Let \( f_3(a) = h_2(6,3,a) - \frac{1}{2}[5 \cdot 2^{a+1} + 4^{a+1}] = \frac{1}{2}[4^{a+1} - 2^{a+2} + 3 - 3^{a+1}] \), then \( f_3(a) = \frac{1}{2}[64 \cdot 4^{a-2} - 16 \cdot 2^{a-2} + 3 - 27 \cdot 3^{a-2}] > 0 (a \geq 2) \) and \( f_3(a) > 0 (1 \leq a \leq 2) \) (see Figure 19 of the Appendix A).

If \( G \in \{B(6,3)/\{G_1,G_2,G_4,G_5,G_7,G_9,G_{15}\}, \) by Lemma 2 and \( \frac{1}{2}R_{a+1}^0(G_5) = \frac{1}{2}R_{a+1}^0(G_{11}) = \frac{1}{2}R_{a+1}^0(G_{12}) = \frac{1}{2}R_{a+1}^0(G_{13}) = \frac{1}{2}R_{a+1}^0(G_{14}) = \frac{1}{2}[2^{a+1} + 4 \cdot 2 + 3 \cdot 3^{a+1}] < h_2(6,3,a) \),

\[
\frac{1}{2}R_{a+1}^0(G_3) = \frac{1}{2}[5 \cdot 2^{a+1} + 4^{a+1}] < h_2(6,3,a).
\]

\[
\frac{1}{2}R_{a+1}^0(G_8) = \frac{1}{2}R_{a+1}^0(G_{16}) = \frac{1}{2}R_{a+1}^0(G_{17}) = \frac{1}{2}R_{a+1}^0(G_{10}) = \frac{1}{2}[1 + 2^{a+2} + 3 \cdot 3^{a+2}] < h_2(6,3,a) \), we have \( D \in \mathcal{O}(G) \), \( R_0^0(D) \leq \frac{1}{2}R_{a+1}^0(G) < h_2(6,3,a) \). The result follows.

If \( G = G_1 \), by Lemma 13 we have \( D \in \mathcal{O}(G_1) \), \( R_0^0(D) < h_2(6,3,a) \). The result follows.

Consequently, \( G \in \{B(6,3)/\{G_6,G_7,G_{15}\}, \) \( D \in \mathcal{O}(G) \), we have \( R_0^0(D) \leq h_2(6,3,a) \) with equality if and only if \( D \in \{B(6,3)/\{G_6,G_7,G_{15}\}. \)

Now, we are ready to obtain the maximum zeroth-order general Randić index of orientations of bicyclic graphs with a perfect matching.

**Theorem 16.** Let \( G \in \mathcal{B}(2m,m), a \geq 1, D \in \mathcal{O}(G) \), where \( m \geq 3 \). Then

\[
R_0^0(D) \leq h_2(2m,m,a)
\]

with equality if and only if \( D \in \mathcal{B}_2^{2m,m} \).

**Proof.** Applying induction on \( m \).

If \( m = 3 \), then by Lemma 15 we can suppose that it exists a pendent vertex whose neighbor degree is 2 in \( G \). So we get the bicyclic graphs \( Q_7 \) and \( Q_8 \) (see Figure 20). It is easy to get that \( G \in \{Q_7,Q_8\} \), \( R_{a+1}^0(G) \leq 1 + 2^{a+1} + 4^{a+1} + 2^{a+1} + 2 + 3^{a+1} = 1 + 3 \cdot 2^{a+1} + 3^{a+1} + 4^{a+1} \).

Let \( f(a) = h_2(6,3,a) - \frac{1}{2}[1 + 3 \cdot 2^{a+1} + 4^{a+1} + 3^{a+1}] = \frac{1}{2}[1 - 2^{a+1} + 4 + 5^{1+a} - 4^{a+1} - 3^{a+1}] \), then \( f(a) = \frac{1}{2}[-2^{a+1} + 4 + 5^{1+a} - 4^{a+1} - 3^{a+1}] > 0 (a \geq 2) \), \( f'(a) = \frac{1}{2}[-2^{a+1} \cdot ln2 + 5^{1+a} \cdot ln5 - 4^{a+1} \cdot ln4 - 3^{a+1} \cdot ln3] > 0 (1 \leq a \leq 2) \) (see Figure 20 of the Appendix A) and \( f(1) = 0 \), hence \( f(a) \geq 0 \) with equality if and only if \( a = 1 \). Then by Lemma 2 we have \( D \in \mathcal{O}(G) \), \( R_0^0(D) \leq \frac{1}{2}R_{a+1}^0(G) \leq \frac{1}{2} \).
Let $G$ be a maximum matching in $G$, we have $|M| = m$. If $G$ has no pendent vertex which has neighbor of degree 2, then by Lemma 15 the result follows.

If $G$ has a pendent vertex $u$ whose neighbor $v$ has degree 2. Let $N_G(v) = \{u, w\}$ with $d_G(w) = t \geq 2$, $N_G(u) = \{w_0 = v, w_1, \ldots, w_{t-1}\}$, and $G' = G - u - v$. By $uv \in M$, we have $G' \in \mathcal{B}(2(m-1), (m-1))$.

Since $|E(G)| - |M| = m + 1$ and $|\{e \in M \text{ is incident with } w\}| = 1$, we have $t − 1 \leq m + 1$ which implies that $t \leq m + 2$. $D' \in \mathcal{O}(G')$ such that $A(D) \cap A(D') = A(D')$. Note that $w$ is adjacent to at most one pendent vertex in $G$.

By the induction hypothesis, $R^0_a(D') \leq h_2(2m - 2, m - 1, a)$.

From Lemma 3 we have

\[
R^0_a(D) \leq R^0_a(D') + \frac{1}{2} [1 + 2^{a+1} + t^{a+1} - (t - 1)^{a+1}]
\]

\[
\leq h_2(2m - 2, m - 1, a) + \frac{1}{2} [1 - (1 + m)^{1+a} + (m + 2)^{1+a} + 2^{1+a}]
\]

\[
= h_2(2m, m, a)
\]

with equality if and only if $R^0_a(D') = h_2(2m - 2, m - 1, a)$, $d_D^+(v) = 2, d_D^-(w) = m + 2; d_D^+(v) = 2, d_D^-(w) = m + 2$, which implies that $D \in \mathcal{B}_{2m, m}$. The result follows.

We will give the maximum zeroth-order general Randić index of orientations of bicyclic graphs with given matching number. For this we need the following result:

**Lemma 17.** [13] Let $G \in \mathcal{B}(n, m)$ and $G$ contains at least one pendent vertex, where $6 \leq 2m < n$. Then there exists a pendent vertex $v$ and a maximum matching $M$ in $G$ such that $v$ is not $M$-saturated.

**Theorem 18.** Let $G \in \mathcal{B}(n, m)$, $a \geq 1$, $D \in \mathcal{O}(G)$, where $3 \leq m \leq \lfloor \frac{n}{2} \rfloor$. Then

\[
R^0_a(D) \leq h_2(n, m, a)
\]

with equality if and only if $D \in \mathcal{B}_{n, m}^*$.

**Proof.** Applying induction on $n$.

If $n = 2m$, then by Theorem 16 the result follows.

So we will suppose that if $n > 2m$ and the result holds for the values smaller than $n$.

If any $u \in V(G)$ and $d_G(u) \neq 1$, then $G \in \mathcal{B}_{n}^*$ and $n = 2m + 1$.

Since $2m \ast 2^{a+1} + 4^{a+1} - [(2m - 1) \ast 2^{a+1} + 2 \ast 3^{a+1}] = 4^{a+1} - 2 \ast 3^{a+1} + 2^{a+1} > 0$, we have $2m \ast 2^{a+1} + 4^{a+1} > (2m - 1) \ast 2^{a+1} + 2 \ast 3^{a+1}$. Let $f(x) = h_2(n, x, a) - \frac{1}{2} [2x \ast 2^{a+1} + 4^{a+1}] = \frac{1}{2} [-1 + x] \ast 2^{a+1} + 3 + x + (x + 3)^{a+1} - 4^{a+1}] (x \geq 3)$, then $f'(x) = \frac{1}{2} [-2^{2a+2} + 1 + (a + 1) \ast (x + 3)^a] > 0$ and $f(x) \geq f(3)$. $f(3) = \frac{1}{2} [-4 \ast 2^{a+1} + 6 + 6^{a+1} - 4^{a+1}] = \frac{1}{2} [-32 \ast 2^{a-2} + 2 + 216 \ast 6^{a-2} - 64 \ast 4^{a-2}] > 0$ ($a \geq 2$) and $f(3) > 0$ ($1 \leq a \leq 2$) (see Figure 21 of the Appendix A). Since
\[ R^0_{u+1}(G) = \begin{cases} 
(2m - 1) \ast 2^{a+1} + 2 \ast 3^{a+1}, & \text{if } G \in B_2^{m+1} \cup B_4^{m+1} \cup B_5^{m+1} \cup B_5^{m+1}, \\
2m \ast 2^{a+1} + 4^{a+1}, & \text{if } G \in B_3^{m+1} 
\end{cases} \]

we have \( D \in O(G) \), \( R^0_a(D) \leq \frac{1}{2} R^0_{u+1}(G) \leq \frac{1}{2} [2m \ast 2^{a+1} + 4^{a+1}] < h_2(n, m, a) \). The result follows.

We can suppose that \( G \) contains at least one pendent vertex. Then by Lemma 17, there exists a maximum matching \( M \) and a pendent vertex \( u \in V(G) \) such that \( u \) is not \( M \)-saturated. Let \( v \in N_G(u) \) and \( d_G(v) = s \geq 2 \), \( G' = G - u \), we have \( G' \in B(n-1, m) \).

Since \( |E(G)| - |M| = n + 1 - m \) and \( |\{e \in M \text{ is incident with } v\}| = 1 \), we have \( s - 1 \leq n + 1 - m \) which implies that \( s \leq n - m + 2 \).

Let \( D' \in O(G') \) such that \( A(D) \cap A(D') = A(D') \).

By the induction hypothesis, \( R^0_u(D') \leq h_2(n - 1, m, a) \).

From Lemma 3, we have

\[
R^0_u(D) \leq R^0_u(D') + \frac{1}{2} [1 + s^{a+1} - (s - 1)^{a+1}]
\leq h_2(n - 1, m, a) + \frac{1}{2} [1 + (n - m + 2)^{a+1} - (n - m + 1)^{a+1}]
= h_2(n, m, a)
\]

with equality if and only if \( R^0_u(D') = h_2(n - 1, m, a) \), \( \max\{d^+_D(v), d^-_D(v)\} = n - m + 2 \) which implies that \( D \in B^*_n,m \). The result follows.

\[ \Box \]

**Acknowledgment.** This work is supported by the Hunan Provincial Natural Science Foundation of China (2020JJ4423), the Department of Education of Hunan Province (19A318) and the National Natural Science Foundation of China (11971164).

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Appendix A

Figure 10: $h(a) = 2f'(a) = 3^{a+1} * ln 3 - 3 * 2^{a+1} * ln 2$  
Figure 11: $h(a) = 2f(a) = 3 * 2^{a+1} + 5^{a+1} - 4 * 3^{a+1} + 1$
Figure 12: $h(a) = 2f'(a) = -2 * 3^{a+1} * \ln(3) + 4^{a+1} * \ln(4)$

Figure 13: $h(a) = 2f'(a) = 2^{a+2} * \ln(2) + 5^{a+1} * \ln(5) - 12 * 3^{a} * \ln(3)$

Figure 14: $h(a) = 2f(a) = 3 * 2^{a+1} + 3 + 6^{a+1} - 5 * 3^{a+1}$

Figure 15: $h(a) = f'(a) = 3 * 2^{a} * \ln(2) + 3 * 6^{a} * \ln(6) - 3^{a+1} * \ln(3) - 2 * 2^{2a+2} * \ln(2)$

Figure 16: $h(a) = 2f(5) = 2 + 4 * [2^{a+1} - 3^{a+1}] + 7^{a+1} - 5^{a+1}$

Figure 17: $h(a) = 2f'(a) = 4^{a+1} * \ln(4) - 2 * 3^{a+1} * \ln(3)$
Figure 18: \( h(a) = 2f_2(a) = 2 \times 4^{a+1} + 2^{a+1} + 2 - \frac{4}{3} \)

Figure 19: \( h(a) = 2f_3(a) = 4^{a+1} - 2^{a+2} + 3 - 3^{a+1} \)

Figure 20: \( h(a) = 2f'(a) = -2^{a+1} \ln(2) + 5^{a+1} - 4^{a+1} \ln(4) - 3^{a+1} \ln(3) \)

Figure 21: \( h(a) = 2f(3) = -4 \times 2^{a+1} + 6 + 6^{a+1} - \frac{ln(5) - 4^{a+1} \ln(4) - 3^{a+1} \ln(3)}{4^{a+1}} \)

Figure 22: \( h(a) = 2f(a) = 3 \times 2^{a+1} + 3 + 6^{a+1} - \frac{5}{3} \)

Figure 23: \( h(a) = 2g'(a) = -2^{a+1} \ln(2) + 6^{a+1} - \frac{ln(6) - 2 \times 5^{a+1} \ln(5) + 4^{a+1} \ln(4)}{ln(6)} \)