Note
Sharp bounds of the zeroth-order general Randić index of bicyclic graphs with given pendent vertices

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A R T I C L E  I N F O

Article history:
Received 6 May 2010
Received in revised form 24 October 2010
Accepted 28 October 2010
Available online 27 November 2010

Keywords:
Bicyclic graph
Zeroth-order general Randić index
Pendent vertex
Sharp bound

A B S T R A C T

Let G be a simple connected graph and $\alpha$ be a given real number. The zeroth-order general Randić index of $^0R_{\alpha}(G)$ is defined as $\sum_{v \in V(G)} [d_G(v)]^\alpha$, where $d_G(v)$ denotes the degree of the vertex $v$ of $G$. In this paper, for any $\alpha(\neq 0, 1)$, we give sharp bounds of the zeroth-order general Randić index $^0R_{\alpha}$ of all bicyclic graphs with $n$ vertices and $k$ pendent vertices.

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1. Introduction

Given a simple connected graph $G = (V(G), E(G))$, where $V(G)$ and $E(G)$ denote the set of vertices and edges of $G$, respectively. The Randić index of $G$ is defined as [12]:

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

where $d_G(u)$ denotes the degree of the vertex $u$ of $G$. Randić himself demonstrated [12] that this index is well correlated with a variety of physico-chemical properties of various classes of organic compounds. The Randić index and some of its variants have received intensive attention and have been generalized in many ways. In particular, the zeroth-order general Randić index is defined in [10] as

$$^0R_{\alpha}(G) = \sum_{v \in V(G)} [d_G(v)]^\alpha,$$

where $\alpha$ is a real number. Until now, many results about the zeroth-order general Randić index can be found in the literature [2–11,13,14]. Among them, Chen et al. [2] and Zhang et al. [14] characterized, for any $\alpha$, the bicyclic graphs with the smallest and greatest $^0R_{\alpha}$. Hu et al. [5] obtained, for any $\alpha$, the molecular $(n, m)$-graphs, i.e., graphs of $n$ vertices,
m edges and vertex degrees not exceeding 4, with smallest and greatest $^0R_n$, whereas Li et al. [7] studied the $(n, m)$-graphs with maximum zeroth-order general Randić index for $\alpha \in (-1, 0)$, and Hu et al. [4] and Pavlović et al. [11] determined the $(n, m)$-graphs with minimum and maximum $^0R_n$ for any $\alpha$. Lin et al. [6] characterized the graphs with the extremal values of $^0R_n$ within two subclasses of connected unicyclic graphs on $n$ vertices, namely, unicyclic graphs with $k$ pendant vertices and unicyclic graphs with a $k$-cycle.

In this paper, we investigate extremal values of general $^0R_n$ for simple connected bicyclic graphs of $n$ vertices and $k$ pendant vertices and give sharp lower bounds and upper bounds for this class of graphs. Since $^0R_0(G) = |V(G)|$ and $^0R_1(G) = |V(G)| + 2$, we only consider $\alpha \neq 0, 1$.

Now we introduce some notations. Undefined graph-theoretical terminology and notation may refer to [1]. A bicyclic graph is a connected simple graph of $n$ vertices and $n + 1$ edges. A pendant vertex of a graph is a vertex with degree 1. $C_n$ is a cycle of length $n$. Let $\mathcal{R}_{n,k}$, where $n - k \geq 4$, denote the set of all bicyclic graphs with order $n$ and $k$ pendant vertices. Denote by $D(G) = (d_1, d_2, \ldots, d_n)$ the degree sequence of the graph $G$, where $d_i$ stands for the degree of the $i$th vertex of $G$ and $d_1 \geq d_2 \geq \ldots \geq d_n$. The zeroth-order general Randić index of a sequence $D = (d_1, d_2, \ldots, d_n)$ of positive integers is defined as

$$^0R_n(D) = \sum_{i=1}^{n} d_i^\alpha,$$

where $\alpha$ is a real number. Note that $^0R_n(G) = ^0R_n(D(G))$ for any graph $G$. Let $\mathcal{R}_{n,k}(n - k \geq 4)$ denote the following set

$$\{ (d_1, d_2, \ldots, d_n) | d_i \geq d_2 \geq \ldots \geq d_n \text{ are positive integers with}$$

$$d_{n-k} \geq 2, d_{n-k+1} = 1 \text{ and } \sum_{i=1}^{n} d_i = 2n + 2 \}. $$

Let

$$\mathcal{R}_{n,k}^0 = \begin{cases} \mathcal{R}_{n,k} & \text{if } n - k > 4, \\ \mathcal{R}_{n,k} \setminus \{ (n, 2, 2, 1, \ldots, 1) \} & \text{if } n - k = 4. \end{cases}$$

Let $\mathcal{D}(G) = \{ D(G) | G \in \mathcal{R}_{n,k} \}$. Note that for any $D = (d_1, d_2, \ldots, d_n) \in \mathcal{D}_{n,k}$, there are exactly $k$ integers equal to 1 among all $d_1, d_2, \ldots, d_n$, i.e., $d_{n-k+1} = d_{n-k+2} = \ldots = d_n = 1$, and $\mathcal{D}_{n,k} \subseteq \mathcal{D}_{n,k}^0 \subseteq \mathcal{R}_{n,k}$. Let

$$D_1(n, k) = \left( \frac{3 + \mu_{n,k}, \ldots, 3 + \mu_{n,k}, 2 + \mu_{n,k}, \ldots, 2 + \mu_{n,k}, 1, \ldots, 1} {k^{k+2-\lambda_{n,k}}} \right)^{k+2-\lambda_{n,k}} \left( \frac{n-2k-2+\lambda_{n,k}} {n-4} \right)^{n-2k-2+\lambda_{n,k}},$$

where $\mu_{n,k} = \left\lceil \frac{k+1}{n-k} \right\rceil$ and $\lambda_{n,k} = (n-k)\mu_{n,k}$, which are calculated in the proof Lemma 2.5(i), and

$$D_2(n, k) = \begin{cases} (k + 4, 2, \ldots, 2, 1, 1) & \text{if } n - k > 4, \\ (k + 3, 3, 2, 1, 1) & \text{if } n - k = 4. \end{cases}$$

It is not difficult to check that $D_1(n, k), D_2(n, k) \in \mathcal{D}_{n,k}^0$.

The rest of the paper is organized as follows. In Section 2, we determine the sequences of positive integers, i.e., $D_1(n, k)$ and $D_2(n, k)$, with extreme zeroth-order Randić index for $\mathcal{D}_{n,k}^0$, and show that both $D_1(n, k)$ and $D_2(n, k)$ are degree sequences of some bicyclic graphs with order $n$ and $k$ pendant vertices. In Section 3, we show that the sequences with extremum in $\mathcal{D}_{n,k}^0$ are also the degree sequences of extremal graphs in $\mathcal{R}_{n,k}$.

2. Determination of extreme zeroth-order Randić index for $\mathcal{D}_{n,k}^0$

In this section, we give some lemmas that will be used in the proof of our result.

**Lemma 2.1** ([6]). Let $x, y \in \mathbb{N}$ and $\alpha \in \mathbb{R}$. If $x - 2 \geq y \geq 1$, then

$$\begin{cases} (x - 1)^\alpha + (y + 1)^\alpha < x^\alpha + y^\alpha & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ (x - 1)^\alpha + (y + 1)^\alpha > x^\alpha + y^\alpha & \text{if } 0 < \alpha < 1. \end{cases}$$

**Lemma 2.2** ([6]). Let $x, y \in \mathbb{N}$ and $\alpha \in \mathbb{R}$. If $x \geq y \geq 2$, then

$$\begin{cases} (x + 1)^\alpha + (y - 1)^\alpha > x^\alpha + y^\alpha & \text{if } \alpha < 0 \text{ or } \alpha > 1, \\ (x + 1)^\alpha + (y - 1)^\alpha < x^\alpha + y^\alpha & \text{if } 0 < \alpha < 1. \end{cases}$$
By the definition of $^0R_\alpha(D)$ and Lemma 2.1, we have the following lemma.

**Lemma 2.3.** If $D = (d_1, d_2, \ldots, d_n) \in \mathcal{D}_{n,k}$ and there are two integers $d_i, d_j$ such that $d_i - 2 \geq d_j \geq 2$, then there exists another sequence of integers $D' \in \mathcal{D}_{n,k}$ satisfying

\[
\begin{cases} 
^{0}R_\alpha(D) > {^{0}R_\alpha(D')} & \text{for } \alpha < 0 \text{ or } \alpha > 1, \\
^{0}R_\alpha(D) < {^{0}R_\alpha(D')} & \text{for } 0 < \alpha < 1.
\end{cases}
\]

**Proof.** Let $d_i' = d_i - 1$, $d_j' = d_j + 1$ and $d_k' = d_k$ for each $k \in \{1, 2, \ldots, n\} \setminus \{i, j\}$. Rearrange $d_i', d_2', \ldots, d_n'$ as $d_i' \geq d_j' \geq \ldots \geq d_n'$. It is not difficult to see that $D' = (d_1', d_2', \ldots, d_n') \in \mathcal{D}_{n,k}$ and, by Lemma 2.1,

\[
^{0}R_\alpha(D) - {^{0}R_\alpha(D')} = d_i'^\alpha + d_j'^\alpha - (d_i - 1)^\alpha - (d_j + 1)^\alpha \begin{cases} > 0 & \text{for } \alpha < 0 \text{ or } \alpha > 1, \\
< 0 & \text{for } 0 < \alpha < 1.
\end{cases}
\]

Then this proof of this lemma is complete. □

By the definition of $^0R_\alpha(D)$ and Lemma 2.2, we have the following lemma.

**Lemma 2.4.** If $D = (d_1, d_2, \ldots, d_n) \in \mathcal{D}_{n,k}$ and there are two integers $d_i, d_j$ such that $d_i \geq d_j \geq 3$, then there exists another sequence of integers $D' \in \mathcal{D}_{n,k}$ satisfying

\[
\begin{cases} 
^{0}R_\alpha(D) < {^{0}R_\alpha(D')} & \text{for } \alpha < 0 \text{ or } \alpha > 1, \\
^{0}R_\alpha(D) > {^{0}R_\alpha(D')} & \text{for } 0 < \alpha < 1.
\end{cases}
\]

**Proof.** The proof of Lemma 2.4 is similar to that of Lemma 2.3, so it is omitted. □

In the following lemma, we determine the sequences of positive integers with the extreme zeroth-order Randić index for $\mathcal{D}_{n,k}^0$.

**Lemma 2.5.** Let $D \in \mathcal{D}_{n,k}^0$.

(i) If $^{0}R_\alpha(D) = \min_{D' \in \mathcal{D}_{n,k}^0}^{0}R_\alpha(D')$ for $0 < \alpha < 1$, then $D = D_1(n, k)$;

(ii) If $^{0}R_\alpha(D) = \max_{D' \in \mathcal{D}_{n,k}^0}^{0}R_\alpha(D')$ for $0 < \alpha < 1$, then $D = D_2(n, k)$.

**Proof.** (i) Assume that $D_0 \in \mathcal{D}_{n,k}$ and

\[
^{0}R_\alpha(D_0) = \begin{cases} 
\min_{D' \in \mathcal{D}_{n,k}^0}^{0}R_\alpha(D') & \text{for } 0 < \alpha < 1
\end{cases}
\]

By Lemma 2.3, $D_0 = (\Delta, \ldots, \Delta, \Delta - 1, \ldots, \Delta - 1, 1, \ldots, 1)$ for some positive integers $\Delta$ and $x$. Then $1 \leq x \leq n - k - 1$. By considering the total summation of all components of $D_0$, we have

\[
k + x\Delta + (n - k - x)(\Delta - 1) = 2n + 2
\]

\[
x = 3n - 2k + 2 - (n - k)\Delta
\]

\[
1 \leq 3n - 2k + 2 - (n - k)\Delta \leq n - k
\]

\[
\frac{2n - k + 2}{n - k} \leq \Delta \leq \frac{3n - 2k + 1}{n - k}
\]

\[
2 + \frac{k + 2}{n - k} \leq \Delta \leq 3 + \frac{k + 1}{n - k}
\]

\[
2 + \frac{k + 2}{n - k} \leq \Delta \leq 3 + \frac{k + 1}{n - k}.
\]

Since $2 + \frac{k + 2}{n - k} = 3 + \frac{k + 1}{n - k}$. Hence $x = 3n - 2k + 2 - (n - k)\Delta = 3n - 2k + 2 - (n - k)(3 + \mu_{n,k}) = k + 2 + \lambda_{n,k}$ and $n - k - x = n - 2k - 2 + \lambda_{n,k}$.

Thus $D_0 = D_1(n, k)$.

Consequently, $D = D_1(n, k)$, since $D_0 = D_1(n, k) \in \mathcal{D}_{n,k}^0$ and $\mathcal{D}_{n,k}^0 \subseteq \mathcal{D}_{n,k}$. 
Lemma 2.2.

(ii) Assume that $D_3 \in \mathcal{P}_{n,k}$ and

$$0^0 \mathcal{R}_p(D_3) = \begin{cases} \max_{D' \in \mathcal{P}_{n,k}} 0^0 \mathcal{R}_p(D') & \text{for } \alpha < 0 \text{ or } \alpha > 1 \\ \min_{D' \in \mathcal{P}_{n,k}} 0^0 \mathcal{R}_p(D') & \text{for } 0 < \alpha < 1. \end{cases}$$

By Lemma 2.4, $D_3 = (\Delta, 2, \ldots, 2, 1, \ldots, 1)$ for some positive $\Delta$. Since $D_3 \in \mathcal{P}_{n,k}$, $\Delta + 2(n - k - 1) + k = 2n + 2$. Then $\Delta = k + 4$. Thus $D_3 = (k + 4, 2, \ldots, 2, 1, \ldots, 1)$.

If $n - k > 4$, then $D = D_3 = D_2(n,k)$, since $\mathcal{P}_{n,k} = \mathcal{P}_{n,k}$.

If $n - k = 4$, i.e., $k = n - 4$, then $\mathcal{P}_{n,k} = \{(d_1, d_2, d_3, d_4, 1, \ldots, 1) | d_1 \geq d_2 \geq d_3 \geq d_4 \geq 2 $ and $d_1 + d_2 + d_3 + d_4 = k + 10 \}$. By the proof above, $D_3$ has the largest (resp. smallest) zeroth-order Randić index $\mathcal{R}_p(D')$ among all $D' \in \mathcal{P}_{n,k}$ for $\alpha < 0$ or $\alpha > 1$ (resp. $0 < \alpha < 1$). Assume that $D_4 = (x_1, x_2, x_3, x_4, 1, \ldots, 1)$ has the second largest (resp. smallest) zeroth-order Randić index $\mathcal{R}_p(D')$ among all $D' \in \mathcal{P}_{n,k}$ for $\alpha < 0$ or $\alpha > 1$ (resp. $0 < \alpha < 1$). Then we claim that $D_4 = (k + 3, 3, 2, 2, 1, \ldots, 1)$. In fact, we can show $x_4 = 2$, $x_3 = 2$, $x_2 = 3$ and $x_1 = k + 3$ step by step by Lemma 2.2. Firstly, assume that $x_4 \geq 3$, then $x_1 \geq x_4 \geq 3$. Let $\bar{D}_4 = (x_1 + 1, x_2, x_3, x_4 - 1, 1, \ldots, 1)$. Then, by Lemma 2.2,

$$\begin{cases} 0^0 \mathcal{R}_p(\bar{D}_4) > 0^0 \mathcal{R}_p(D_4) & \text{for } \alpha < 0 \text{ or } \alpha > 1 \\ 0^0 \mathcal{R}_p(\bar{D}_4) < 0^0 \mathcal{R}_p(D_4) & \text{for } 0 < \alpha < 1. \end{cases}$$

and $\bar{D}_4 \neq D_3$, a contradiction to the choice of $D_4$. Thus $x_4 = 2$. Similarly, we can prove $x_3 = 2$ and $x_2 = 3$ one by one.

Therefore $D = D_4 = D_2(n, n - 4)$ for this case, since $\mathcal{P}_{n,n-4} = \mathcal{P}_{n,n-4} \setminus \{(n, 2, 2, 1, \ldots, 1)\}$. □

In the following lemma, we show that both $D_1(n,k)$ and $D_2(n,k)$ are degree sequences of some bicyclic graphs with order $n$ and $k$ pendant vertices.

Lemma 2.6. $D_1(n,k), D_2(n,k) \in \mathcal{P}_{n,k}$.

Proof. Firstly, we show $D_1(n,k) \in \mathcal{P}_{n,k}$.

Let $H_{n-k}$ (shown in Fig. 1) denote the graph of order $n-k$ obtained from $C_3$ and $C_{n-k-1}$ by identifying an edge on $C_3$ with another edge on $C_{n-k-1}$. If $k < n - k - 1$, i.e., $k < \frac{1}{2} (n - 1)$, choose any $k$ vertices, say $v_1, v_2, \ldots, v_k$, from $n - k - 2$ vertices of degree 2 in $H_{n-k}$ and let $B'_{n,k}$ denote the graph obtained from $H_{n-k}$ by attaching a pendant vertex $v_i$ to $v_i$ for each $i = 1, 2, \ldots, k$.

If $k \geq n - k - 1$, i.e., $k \geq \frac{1}{2} (n - 1)$, denote by $F_{2n-2k-2}$ the graph obtained from $H_{n-k}$ by attaching one pendant vertex to each vertex of degree 2 in $H_{n-k}$. Then each non-pendant vertex of $F_{2n-2k-2}$ is of degree 3. Let $B'_{n,k}$ denote the graph obtained from $F_{2n-2k-2}$ by attaching $\mu_{n,k}$ - 1 pendant vertices to each of $n - 2k - 2 + \lambda_{n,k}$ vertices with degree 3 in $F_{2n-2k-2}$ and attaching $\mu_{n,k}$ pendant vertices to each of the other vertices with degree 3 in $F_{2n-2k-2}$.

It is not difficult to check that $B'_{n,k} \in \mathcal{P}_{n,k}$ and $D(B'_{n,k}) = D_1(n,k)$.

Thus $D_1(n,k) \in \mathcal{P}_{n,k}$.

Secondly, we show $D_2(n,k) \in \mathcal{P}_{n,k}$.

When $n - k > 4$, let $B'_{n,k}$ (shown in Fig. 1) denote the graph obtained from $C_3$ and $C_{n-k-2}$ by identifying one vertex of $C_3$ with another vertex of $C_{n-k-2}$ and attaching $k$ pendant vertices to the common vertex of $C_3$ and $C_{n-k-2}$.
When \( n - k = 4 \), let \( B''_{n,n-4} \) denote the graph shown in Fig. 1. Obviously, \( B''_{n,k} \in \mathcal{P}_{n,k} \) and \( D(B''_{n,k}) = D_2(n, k) \) for all \( n - k \geq 4 \).
Hence \( D_2(n, k) \in \mathcal{D}_{n,k} \). □

### 3. Determination of extreme zeroth-order Randić index for bicyclic graphs with order \( n \) and \( k \) pendant vertices

Let
\[
\beta(n, k) = k + (n - 2k - 2 + \lambda_{n,k})(2 + \mu_{n,k})^\alpha + (k + 2 - \lambda_{n,k})(3 + \mu_{n,k})^\alpha
\]
and
\[
\phi(n, k) = \begin{cases} 
  k + (n - k - 1)2^\alpha + (k + 4)^\alpha & \text{if } n - k > 4 \\
  k + 3^\alpha + 2(2^\alpha) + (k + 3)^\alpha & \text{if } n - k = 4.
\end{cases}
\]

Now we determine the extreme zeroth-order Randić index for \( \mathcal{P}_{n,k} \) and give the degree sequences with extremum.

**Theorem 3.1.** Let \( G \in \mathcal{P}_{n,k} \).

(i) If \( \alpha < 0 \) or \( \alpha > 1 \), then
\[
\beta(n, k) \leq 0^{R_n}(G) \leq \phi(n, k),
\]
with \( 0^{R_n}(G) = \beta(n, k) \) (resp. \( \phi(n, k) \)) if and only if \( D(G) = D_1(n, k) \) (resp. \( D(G) = D_2(n, k) \));

(ii) If \( 0 < \alpha < 1 \), then
\[
\phi(n, k) \leq 0^{R_n}(G) \leq \beta(n, k),
\]
with \( 0^{R_n}(G) = \phi(n, k) \) (resp. \( \beta(n, k) \)) if and only if \( D(G) = D_2(n, k) \) (resp. \( D(G) = D_1(n, k) \)).

**Proof.** We only show Theorem 3.1(i), while the proof of Theorem 3.1(ii) is similar and thus omitted.
Assume \( \alpha < 0 \) or \( \alpha > 1 \) in the following.
Firstly, it is easy to check that if \( D(G) = D_1(n, k) \) (resp. \( D_2(n, k) \)), then \( 0^{R_n}(G) = \beta(n, k) \) (resp. \( \phi(n, k) \)).
Secondly, by Lemma 2.5, we have
\[
\beta(n, k) = 0^{R_n}(D_1(n, k)) = \min_{D' \in \mathcal{D}_{n,k}} 0^{R_n}(D')
\]
\[
\leq \min_{D' \in \mathcal{D}_{n,k}} 0^{R_n}(D')
\]
\[
= 0^{R_n}(G)
\]
\[
\leq \max_{D' \in \mathcal{D}_{n,k}} 0^{R_n}(D')
\]
\[
= 0^{R_n}(D_2(n, k)) = \phi(n, k).
\]

In order for \( 0^{R_n}(G) = \beta(n, k) \),
\[
\beta(n, k) = 0^{R_n}(D_1(n, k)) = \min_{D' \in \mathcal{D}_{n,k}} 0^{R_n}(D') = \min_{D' \in \mathcal{D}_{n,k}} 0^{R_n}(D') = 0^{R_n}(G).
\]

Then, by Lemmas 2.5 and 2.6, \( D(G) = D_1(n, k) \). Similarly, we can show that if \( 0^{R_n}(G) = \phi(n, k) \), then \( D(G) = D_2(n, k) \).
So Theorem 3.1(i) is true. □

### 4. Remark

In this paper, we give a definition of the zeroth-order general Randić index of a sequence of positive integers. It may be a very useful method for dealing with the zeroth-order general Randić index of graphs, that is to say, given a class of graphs \( \mathcal{G} \), if we can obtain a suitable set \( \mathcal{D} \) of sequences of positive integers, which contains the set \( \mathcal{D} \) of all degree sequences of graphs in \( \mathcal{G} \), and the sequence with extremal zeroth-order general Randić index in \( \mathcal{D} \) can be a degree sequence of some graph in \( \mathcal{G} \), then we can get the sharp bounds of the zeroth-order general Randić index of graphs in \( \mathcal{G} \).

### Acknowledgements

The authors would like to express their sincere gratitude to the referees for their valuable suggestions, which led to great deal of improvement in this paper.

### References


