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On the sum-connectivity index of unicyclic graphs with k pendent vertices

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Abstract. The sum-connectivity index $R'(G)$ of a graph G is the sum of the weights $(d_u + d_v)^{-\frac{1}{2}}$ of all edges uv of G, where d_u and d_v are the degrees of the vertices u and v in G. This index was recently introduced in [B. Zhou, N. Trinajstić, On a novel connectivity index, J. Math. Chem. **46**(2009), 1252–1270]. In this paper, we give the sharp lower bound of the sum-connectivity index of n-vertex unicyclic graphs with k pendent vertices.

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1. Introduction

All graphs considered in this paper are finite, undirected and simple. For terminology and notation not defined here we follow those in Bondy and Murty [1]. For a graph $G = (V(G), E(G))$, the *weight* of an edge $e = uv \in E(G)$ is defined to be $w_e = (d_u + d_v)^{-\frac{1}{2}}$, where d_u, d_v denote the degree of u, v in G, respectively.

Recall that the Randić connectivity index of a graph G is the sum of the weights w'_e, where $e = uv$ and $w'_e = (d_u d_v)^{-\frac{1}{2}}$. The Randić connectivity index is a graphic invariant much studied in both mathematical and chemical literature; for details see a survey book written by Li and Gutman [8] and the references cited therein. Thus, the graphic invariant studied in this paper can be looked as a novel variant of the Randić index. It is also due to the fact that the two graphic invariants are highly intercorrelated quantities; for example, the value of the correlation coefficient is 0.99088 for 136 trees representing the lower alkanes taken from Ivanciuc et al. [4]. In [12], the Randić connectivity index is called the *product connectivity index*, whereas the sum of edge weights studied in this paper is called the *sum-connectivity index*. However, it is remarkable that until now, the sum-connectivity index eluded the attention of both “pure” and applied graph theoreticians. The aim of the present paper is to contribute towards filling this gap.

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In [12], Zhou and Trinajstić first introduced the sum-connectivity index. They determined the upper and lower bounds of this index for trees in terms of other graph invariants. They determined the unique tree with fixed numbers of vertices and pendent vertices with the minimum value of the sum-connectivity index, and trees with the minimum, second-minimum and third-minimum, and the maximum, second-maximum and third-maximum values of this index. Additionally, they discussed the properties of the sum-connectivity index for a class of trees representing acyclic hydrocarbons. In [7], Lučić, Trinajstić and Zhou report the relationship between the two versions of the connectivity index for a set of lower benzenoid hydrocarbons. They also study the relationship between connectivity indices and π-electronic energy of benzenoids, which implies that the sum-connectivity index even in this case outperforms the product-connectivity index. They finally draw the conclusion that the sum-connectivity index is closely related to molecular descriptors. In [6], we determined the sharp bounds on the sum-connectivity index of trees and unicyclic graphs with a perfect matching in term of vertices, respectively. Additionally, a sharp lower bound on this index of trees and unicyclic graphs with a given size of matching was characterized, respectively. In [5], we determined the n-vertex unicyclic graph of a given girth with the minimum value of this index. We also characterized the unicyclic graphs with the minimum, the second-minimum, the maximum and the second-maximum values of this index. The corresponding extremal graphs were characterized. Some more recent results on the sum-connectivity index can be found in [2, 3, 11, 13].

In this paper, we study an extremal problem on the sum of edge weights of unicyclic graphs: determine the sharp lower bound of the sum-connectivity index of n-vertex unicyclic graphs with the given number of pendent vertices. The extremal graphs with a minimal value of the sum-connectivity index in the set of a unicyclic graph with k pendent vertices are completely characterized.

2. Notations and Lemmas

For a vertex x of the graph G, we denote the neighborhood and the degree of x by $N_G(x)$ and d_x (or $d_G(x)$), respectively. The number $\Delta(G) := \max\{d_v | v \in V(G)\}$ is the *maximum degree* of G. The *Randić connectivity index* [10] $R = R(G)$ of G is defined as

$$R = R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The *sum of edge weights* $R' = R'(G)$ of G, which is called the *sum-connectivity index* [12], is defined as

$$R' = R'(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

We call $R(G)$ and $R'(G)$ the *product-connectivity index* and the *sum-connectivity index*, respectively.

Given a graph G, if $W \subseteq V(G)$, by $G-W$ we denote the subgraph of G obtained by deleting the vertices of W and the edges incident with them; Specially, when $W=\{v\}$, we write $G-v$ instead of $G-\{v\}$. A *pendent vertex* is a vertex of degree one. Let $P=v_0v_1\dots v_s$ be a path of G with $d(v_1)=d(v_2)=\cdots=d(v_s)=2$ (unless $s=1$). If $d(v_0)=1$ and $d(v_s)\geq 3$, then we call P a *pendent path* of G; If $d(v_0)\geq 3$ and $d(v_s)\geq 3$, then we call P an *internal path* of G

Unicyclic graphs are connected graphs with n vertices and n edges. Denote

$$\mathscr{U}_{n,k}=\{G : G \text{ is a unicyclic graph with } n \text{ vertices and } k \text{ pendent vertices}\}.$$

By P_n, C_n and $K_{1,n-1}$ we denote the path, the cycle and the star on n vertices, respectively. Let U_k^n denote the graph obtained by attaching k pendent vertices to exactly one vertex of C_{n-k}; whereas $U(n,k,p)$ denotes the graph obtained by connecting the center of the star graph $K_{1,k}$ and one vertex of C_{n-k-p} by an internal path $P=u_0u_1\dots u_p$. Graphs U_k^n and $U(n,k,p)$ are depicted in Figure 1.

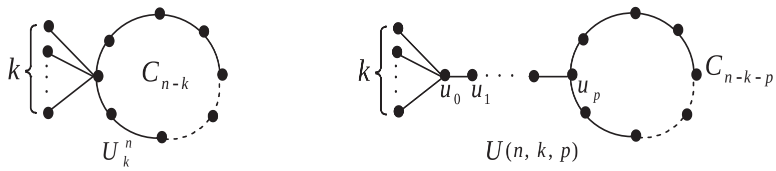

Figure 1: *Graphs U_k^n and $U(n,k,p)$*

In this section, we give some lemmas which will be used in the next section. Let

$$\phi(n,k)=\frac{2}{\sqrt{k+4}}+\frac{k}{\sqrt{k+3}}+\frac{n-k-3}{2}.$$

Lemma 1 (See [9]). *Let $G\in\mathscr{U}_{n,k}$, then $\Delta(G)\leq k+2$.*

Lemma 2. *Let $G\in\mathscr{U}_{n,1}$. Then*

$$R'(G)\geq\phi(n,1). \tag{1}$$

Furthermore, the equality in (1) holds if and only if $G\cong U_1^n$.

Proof. First we note that if $G\cong U_1^n$, then the equality in (1) holds obviously.

Since $G\in\mathscr{U}_{n,1}$, by Lemma 1, it is easy to see that G is isomorphic to the graph obtained from a cycle C_p by attaching a path of length $n-p$ to a vertex of C_p. Then if $G\ncong U_1^n$, we have

$$R'(G)-R'(U_1^n)=\left(\frac{1}{\sqrt{3}}+\frac{3}{\sqrt{5}}+\frac{n-4}{2}\right)-\left(\frac{2}{\sqrt{5}}+\frac{1}{2}+\frac{n-4}{2}\right)=\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{5}}-\frac{1}{2}>0.$$

Thus, the lemma follows. $\square$

Lemma 3. *Let $f(x):=\sqrt{x}-\frac{3}{\sqrt{x}}+\frac{2}{\sqrt{x+1}}$, $g(x):=\sqrt{x+2}-\frac{3}{\sqrt{x+2}}+\frac{2}{\sqrt{x+3}}$ and $h(x):=\sqrt{x+2}-\frac{2}{\sqrt{x+2}}+\frac{2}{\sqrt{x+3}}$, where x is a positive real number. Then $f(x)-f(x+1)$, $g(x)-g(x+1)$ and $h(x)-h(x+1)$ are strictly monotone increasing in x.*

Proof. Note that for $x \geq 0$, we have

$$\frac{\partial^2 f(x)}{\partial x} = -\frac{1}{4} \cdot \frac{1}{x^{\frac{3}{2}}} - \frac{9}{4} \cdot \frac{1}{x^{\frac{5}{2}}} + \frac{3}{2} \cdot \frac{1}{(x+1)^{\frac{5}{2}}} < -\frac{1}{4} \cdot \frac{1}{x^{\frac{3}{2}}} - \frac{9}{4} \cdot \frac{1}{x^{\frac{5}{2}}} + \frac{3}{2} \cdot \frac{1}{x^{\frac{5}{2}}} < 0.$$

Hence, $f'(x)$ is a strict monotone decreasing function for $x > 0$. In order to show that $f(x) - f(x+1)$ is a strict monotone increasing function in x, it suffices to show that $(f(x) - f(x+1))' > 0$. In fact, as $f'(x)$ is a strict monotone decreasing function for $x > 0$, we have $(f(x) - f(x+1))' = f'(x) - f'(x+1) > 0$, as desired.

On the other hand,

$$\begin{aligned} \frac{\partial^2 g(x)}{\partial x} &= -\frac{1}{4(x+2)^{\frac{3}{2}}} - \frac{9}{4(x+2)^{\frac{5}{2}}} + \frac{3}{2(x+3)^{\frac{5}{2}}} \\ &< -\frac{1}{4(x+2)^{\frac{3}{2}}} - \frac{9}{4(x+2)^{\frac{5}{2}}} + \frac{3}{2(x+2)^{\frac{5}{2}}} < 0. \end{aligned}$$

Hence, $g'(x)$ is a strict monotone decreasing function for $x > 0$. Hence, $(g(x) - g(x+1))' = g'(x) - g'(x+1) > 0$, which implies that $g(x) - g(x+1)$ is a strict monotone increasing function in x.

By a similar discussion as above, we can also show that $h(x) - h(x+1)$ is strictly monotone increasing in x. We omit the procedure here.

This completes the proof. □

It is straightforward to check that the following lemma is true.

Lemma 4. *Let* $t(x) = \frac{x}{\sqrt{x+2}} - \frac{x-1}{\sqrt{x+1}}$ *and* $p(x) = \frac{1}{\sqrt{x+3}} - \frac{1}{\sqrt{x+2}}$, *where* $x \geq 0$. *Then both* $t(x)$ *and* $p(x)$ *are monotone increasing.*

Lemma 5. *For* $x > 0$, *the function* $q(x) = \frac{x-2}{\sqrt{x+1}} + \frac{1}{\sqrt{x+2}} - \frac{x-2}{\sqrt{x}}$ *is monotone decreasing in* x.

Proof. Let $l(x) = \sqrt{x} - \frac{2}{\sqrt{x}} + \frac{1}{\sqrt{x+1}}$. Note that

$$\begin{aligned} q(x) &= \frac{x-2}{\sqrt{x+1}} + \frac{1}{\sqrt{x+2}} - \frac{x-2}{\sqrt{x}} \\ &= \sqrt{x+1} - \sqrt{x} - \frac{3}{\sqrt{x+1}} + \frac{2}{\sqrt{x}} + \frac{1}{\sqrt{x+2}} = l(x+1) - l(x). \end{aligned}$$

As

$$l''(x) = -\frac{1}{4x^{\frac{3}{2}}} - \frac{3}{2x^{\frac{5}{2}}} + \frac{3}{4(x+1)^{\frac{5}{2}}} < -\frac{1}{4x^{\frac{3}{2}}} - \frac{3}{2x^{\frac{5}{2}}} + \frac{3}{4(x)^{\frac{5}{2}}} < 0,$$

we obtain $l(x+1) - l(x)$ is monotone decreasing, i.e., $q(x)$ is monotone decreasing. □

3. Minimum $R'(G)$-value of graphs in $\mathscr{U}_{n,k}$

In this section, mathematical properties of the sum $R'(G)$ of edge weights of unicyclic graphs are studied. We determine the unique n-vertex unicyclic graph with k pendent vertices having the minimum R'-value. The product-connectivity index for unicyclic graphs with k pendent vertices has been studied in [9].

Theorem 1. *Let $G \in \mathscr{U}_{n,k}$. Then*

$$R'(G) \geq \phi(n,k) \tag{2}$$

and the equality in (2) holds if and only if $G \cong U_k^n$.

Proof. Note that if $G \cong U_k^n$, then by an elementary calculation the equality in (2) holds. Now we proceed by induction on k to show that if $G \in \mathscr{U}_{n,k}$, then (2) holds and the equality in (2) holds only if $G \cong U_k^n$.

For $k = 0$, $\mathscr{U}_{n,0} = \{C_n\}$, whence the theorem holds obviously. By Lemma 1, Theorem 1 holds for $k = 1$. So in what follows, we assume that $k \geq 2$.

Let $V_0 = \{u : u \text{ is a pendent vertex of } G\}$, $V_1 = \bigcup_{u \in V_0} N(u)$ and $V_2 = V(G) \backslash (V_0 \cup V_1)$.

Case 1. There exists some $v \in V_1$ such that $|N(v) \backslash V_0| \geq 2$.

In this case, let $d_v = t$. Then $t = |N(v)| \geq 3$ and by Lemma 1, $t \leq k + 2$. Denote $N(v) \cap V_0 = \{v_1, v_2, \ldots, v_r\}$ and $N(v) \backslash V_0 = \{x_1, x_2, \ldots, x_{t-r}\}$. Then $t - r = |N(v) \backslash V_0| \geq 2$ and all $d(x_i) = d_i \geq 2$. Let $G' = G - v_1$. Then $G' \in \mathscr{U}_{n-1,k-1}$. Thus, by the definition of the sum-connectivity index, we have

$$\begin{aligned}
R'(G) &= R'(G') + \frac{r}{\sqrt{t+1}} - \frac{r-1}{\sqrt{t}} - \sum_{i=1}^{t-r} \left(\frac{1}{\sqrt{t+d_i-1}} - \frac{1}{\sqrt{t+d_i}} \right) \\
&\geq R'(G') + \frac{r}{\sqrt{t+1}} - \frac{r-1}{\sqrt{t}} - (t-r) \left(\frac{1}{\sqrt{t+1}} - \frac{1}{\sqrt{t+2}} \right) & (3) \\
&= R'(G') + \sqrt{t+1} - \sqrt{t} + \frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t+1}} + (t-r) \left(\frac{1}{\sqrt{t}} - \frac{2}{\sqrt{t+1}} + \frac{1}{\sqrt{t+2}} \right) \\
&\geq \phi(n-1,k-1) + \sqrt{t+1} - \sqrt{t} + \frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t+1}} & (4) \\
&\quad + 2 \left(\frac{1}{\sqrt{t}} - \frac{2}{\sqrt{t+1}} + \frac{1}{\sqrt{t+2}} \right) \\
&= \phi(n,k) - \left(\frac{2}{\sqrt{k+4}} + \frac{k}{\sqrt{k+3}} + \frac{n-k-2}{2} \right) \\
&\quad + \left(\frac{2}{\sqrt{k+3}} + \frac{k-1}{\sqrt{k+2}} + \frac{n-k-2}{2} \right) \\
&\quad + \frac{t}{\sqrt{t+1}} - \frac{t-1}{\sqrt{t}} + 2 \left(\frac{1}{\sqrt{t}} - \frac{2}{\sqrt{t+1}} + \frac{1}{\sqrt{t+2}} \right) \\
&= \phi(n,k) + \left(\frac{k-1}{\sqrt{k+2}} - \frac{k-2}{\sqrt{k+3}} - \frac{2}{\sqrt{k+4}} \right) - \left(\frac{t-3}{\sqrt{t}} - \frac{t-4}{\sqrt{t+1}} - \frac{2}{\sqrt{t+2}} \right). & (5)
\end{aligned}$$

Equality in (4) holds if and only if $d_i = 2, i = 1, 2, \ldots, t-r$, whereas equality in (5) holds if and only if $R'(G') = \phi(n-1, k-1)$ and $t - r = 2$.

Let $f(x) = \sqrt{x} - \frac{3}{\sqrt{x}} + \frac{2}{\sqrt{x+1}}$. Then, by (5), we have

$$\begin{aligned} R'(G) &\geq \phi(n,k) + (f(k+2) - f(k+3)) - (f(t) - f(t+1)) \\ &\geq \phi(n,k). \end{aligned} \tag{6}$$

The last inequality follows from Lemma 3 as $t \leq k+2$. The equality in (6) holds if and only if $t = k+2$.

Hence, $R'(G) = \phi(n,k)$ holds if and only if equalities in (3), (4) and (6) hold, i.e.,

$$R'(G') = \phi(n-1, k-1),\ t = k+2,\, t - r = 2 \text{ and } d_1 = d_2 = 2.$$

By the induction hypothesis, $G' \cong U_{k-1}^{n-1}$. Notice that U_{k-1}^{n-1} has a unique vertex of a degree greater than 2. Hence, $G \cong U_k^n$.

Case 2. For every $u \in V_1, |N(u) \backslash V_0| = 1$.

Choose a vertex $u \in V_1$. Let $d_u = t$. Note that $G \in \mathscr{U}_{n,k}$, hence we get that $t \leq k+1$. We consider the following two possible subcases.

Subcase 2.1. $t = k+1$.

In this subcase, it is not difficult to see that $G \cong U(n,k,p)$ for some $1 \leq p \leq n-k-3$. Let $f(n,k) := R'(U(n,k,p)) - R'(U_k^n)$. Then by the definition of the sum-connectivity index, we have

$$\begin{aligned} f(n,k) &= \frac{k}{\sqrt{k+2}} + \frac{1}{\sqrt{k+3}} + \frac{3}{\sqrt{5}} + \frac{n-k-4}{2} - \phi(n,k) \\ &= \sqrt{k+2} - \sqrt{k+3} + \frac{4}{\sqrt{k+3}} - \frac{2}{\sqrt{k+2}} - \frac{3}{\sqrt{k+4}} + \frac{3}{\sqrt{5}} - \frac{1}{2} \\ &= \left(\sqrt{k+2} - \frac{2}{\sqrt{k+2}} + \frac{2}{\sqrt{k+3}}\right) \\ &\quad - \left(\sqrt{k+3} - \frac{2}{\sqrt{k+3}} + \frac{2}{\sqrt{k+4}}\right) + \frac{3}{\sqrt{5}} - \frac{1}{2}. \end{aligned} \tag{7}$$

Let $h(x) = \sqrt{x+2} - \frac{2}{\sqrt{x+2}} + \frac{2}{\sqrt{x+3}}$, then in view of equation (7), we have

$$\begin{aligned} f(n,k) &= h(k) - h(k+1) + \frac{3}{\sqrt{5}} - \frac{1}{2} \\ &> (\sqrt{3} - \frac{2}{\sqrt{3}} + 1) - (\sqrt{4} - 1 + \frac{2}{\sqrt{5}}) + 0.8416 = 0.5246 > 0. \end{aligned}$$

The last second inequality follows by Lemma 3.

Subcase 2.2. $t \neq k+1$.

In this subcase, $|V_1| \geq 2$. Then there exists some $v \in V_1$ such that $|N(v) \cap V_0| \leq \frac{k}{2}$. Without loss of generality, assume that $|N(u) \cap V_0| \leq \frac{k}{2}$. Then $t = |N(u)| \leq \frac{k}{2} + 1$.

Denote $N(u) \cap V_0 = \{v_1, v_2, \dots, v_{t-1}\}$, $N(u) \backslash V_0 = \{x_1\}$ and $d(x_1) = d_1 \geq 2$.

If $t = 2$, then let $P = u_0 u_1 \cdots u_s$ be a pendent path with $u_0 = v_1, u_1 = u, u_2 = x_1, s \geq 2$ and $d(u_s) \geq 3$. Let $G' = G - \{u_0, u_1, \dots, u_{s-1}\}$ and $d(u_s) = d$, then $G' \in \mathscr{U}_{n-s,k-1}$ and $d \leq k+1$ by Lemma 1. Denote $N(u_s) \backslash \{u_{s-1}\} = \{y_1, y_2, \dots, y_{d-1}\}$. Then $d(y_i) \geq 2$ for each $i = 1, 2 \dots, d-1$ (otherwise, there exists some y_i such that $d(y_i) = 1$. If $N(u_s) \cap V_0 = \{y_1, y_2, \dots, y_{d-1}\}$, then G is isomorphic to a graph obtained from a star S_k and the path $P = u_0 u_1 \cdots u_s$ by identifying u_s with the central vertex of S_k, a contradiction to $G \in \mathscr{U}_{n,k}$. Then, $|N(u) \cap V_0| \leq d - 2$, hence $|N(u) \backslash V_0| \geq 2$, once again a contradiction to our assumption in Case 2). Thus,

$$\begin{aligned}
R'(G) &= R'(G') + \frac{1}{\sqrt{3}} + \frac{s-2}{2} + \frac{1}{\sqrt{d+2}} - \sum_{i=1}^{d-1} \left(\frac{1}{\sqrt{d+d(y_i)-1}} - \frac{1}{\sqrt{d+d(y_i)}} \right) \\
&\geq \phi(n-s, k-1) + \frac{1}{\sqrt{3}} + \frac{s-2}{2} + \frac{1}{\sqrt{d+2}} \\
&\quad - \sum_{i=1}^{d-1} \left(\frac{1}{\sqrt{d+d(y_i)-1}} - \frac{1}{\sqrt{d+d(y_i)}} \right) \\
&= \phi(n,k) + \frac{1}{\sqrt{d+2}} - (d-1) \left(\frac{1}{\sqrt{d+1}} - \frac{1}{\sqrt{d+2}} \right) \\
&\quad + \frac{k-1}{\sqrt{k+2}} - \frac{k-2}{\sqrt{k+3}} - \frac{2}{\sqrt{k+4}} + \frac{1}{\sqrt{3}} - \frac{1}{2} \\
&= \phi(n,k) + \frac{d}{\sqrt{d+2}} - \frac{d-1}{\sqrt{d+1}} + \frac{k-1}{\sqrt{k+2}} - \frac{k-2}{\sqrt{k+3}} - \frac{2}{\sqrt{k+4}} + \frac{1}{\sqrt{3}} - \frac{1}{2} \\
&\geq \phi(n,k) + \frac{k+1}{\sqrt{k+3}} - \frac{k}{\sqrt{k+2}} + \frac{k-1}{\sqrt{k+2}} - \frac{k-2}{\sqrt{k+3}} - \frac{2}{\sqrt{k+4}} + \frac{1}{\sqrt{3}} - \frac{1}{2} \qquad (8) \\
&\geq \phi(n,k) + \frac{3}{\sqrt{k+3}} - \frac{1}{\sqrt{k+2}} - \frac{2}{\sqrt{k+4}} + \frac{1}{\sqrt{3}} - \frac{1}{2} \\
&\geq \phi(n,k) + \frac{1}{\sqrt{k+3}} - \frac{1}{\sqrt{k+2}} + \frac{1}{\sqrt{3}} - \frac{1}{2} \qquad (9) \\
&\geq \phi(n,k) + \frac{1}{\sqrt{5}} - \frac{1}{2} + \frac{1}{\sqrt{3}} - \frac{1}{2} \\
&\geq \phi(n,k) + 0.0246 > \phi(n,k).
\end{aligned}$$

Inequalities in (8) and (9) follow from Lemma 4.

Otherwise, $t \geq 3$. Let $G'' = G - v_1$. Then $G'' \in \mathscr{U}_{n-1,k-1}$. Thus,

$$\begin{aligned}
R'(G) &= R'(G'') + \frac{t-1}{\sqrt{t+1}} - \frac{t-2}{\sqrt{t}} + \frac{1}{\sqrt{d_1+t}} - \frac{1}{\sqrt{d_1+t-1}} \\
&\geq \phi(n-1, k-1) + \frac{t-1}{\sqrt{t+1}} - \frac{t-2}{\sqrt{t}} + \frac{1}{\sqrt{t+2}} - \frac{1}{\sqrt{t+1}} \\
&\geq \phi(n,k) + \frac{k-1}{\sqrt{k+2}} - \frac{k-2}{\sqrt{k+3}} - \frac{2}{\sqrt{k+4}} + \frac{t-2}{\sqrt{t+1}} + \frac{1}{\sqrt{t+2}} - \frac{t-2}{\sqrt{t}}
\end{aligned}$$

$$
\begin{aligned}
&\geq \phi(n,k) + \frac{k-1}{\sqrt{k+2}} - \frac{k-2}{\sqrt{k+3}} - \frac{2}{\sqrt{k+4}} + \frac{\frac{k}{2}-1}{\sqrt{\frac{k}{2}+2}} + \frac{1}{\sqrt{\frac{k}{2}+3}} - \frac{\frac{k}{2}-1}{\sqrt{\frac{k}{2}+1}} \qquad (10)\\
&= \phi(n,k) + \frac{k-1}{\sqrt{k+2}} - \frac{k-2}{\sqrt{k+3}} - \frac{2}{\sqrt{k+4}} + \frac{k-2}{\sqrt{2k+8}} + \frac{\sqrt{2}}{\sqrt{k+6}} + \frac{k-2}{\sqrt{2k+4}}\\
&> \phi(n,k) + \frac{k-1}{\sqrt{k+3}} - \frac{k-2}{\sqrt{k+3}} - \frac{2}{\sqrt{k+4}} + \frac{k-2}{\sqrt{2k+8}} + \frac{\sqrt{2}}{\sqrt{k+6}} + \frac{k-2}{\sqrt{2k+4}}\\
&= \phi(n,k) + \frac{1}{\sqrt{k+3}} - \frac{2}{\sqrt{k+4}} + \frac{k-2}{\sqrt{2k+8}} + \frac{\sqrt{2}}{\sqrt{k+6}} + \frac{k-2}{\sqrt{2k+4}}\\
&> \phi(n,k) + \frac{1}{\sqrt{k+4}} - \frac{2}{\sqrt{k+4}} + \frac{k-2}{\sqrt{2k+8}} + \frac{\sqrt{2}}{\sqrt{k+6}} + \frac{k-2}{\sqrt{2k+4}}\\
&= \phi(n,k) + \frac{k-2-\sqrt{2}}{\sqrt{2}\sqrt{k+4}} + \frac{\sqrt{2}}{\sqrt{k+6}} + \frac{k-2}{\sqrt{2k+4}}\\
&> \phi(n,k) + \frac{k-2-\sqrt{2}}{\sqrt{2}\sqrt{k+6}} + \frac{2}{\sqrt{2}\sqrt{k+6}} + \frac{k-2}{\sqrt{2k+4}}\\
&= \phi(n,k) + \frac{k-\sqrt{2}}{\sqrt{2}\sqrt{k+6}} + \frac{k-2}{\sqrt{2k+4}}\\
&> \phi(n,k),
\end{aligned}
$$

where the inequality in (10) follows from Lemma 5 and the last inequality follows for $k \geq 2$.

By Cases 1 and 2, we complete the proof of Theorem 1. $\square$

4. Final remark

Note that the set of all n-vertex unicyclic graphs is $\bigcup_{k=0}^{n-3} \mathscr{U}_{n,k}$. So by Theorem 1 we can determine sharp upper and lower bounds on $R'(G)$-values for $G \in \bigcup_{k=0}^{n-3} \mathscr{U}_{n,k}$. In fact, let

$$\phi(n,x) = \frac{2}{\sqrt{x+4}} + \frac{x}{\sqrt{x+3}} + \frac{n-x-3}{2},$$

where $x \geq 0$. Then,

$$\frac{\partial \phi(n,x)}{\partial x} = -\frac{1}{(x+4)^{\frac{3}{2}}} + \frac{1}{(x+3)^{\frac{1}{2}}} - \frac{x}{(x+3)^{\frac{3}{2}}} - \frac{1}{2} \leq -\frac{1}{(x+4)^{\frac{3}{2}}} - \frac{x}{(x+3)^{\frac{3}{2}}} < 0,$$

where the last second inequality holds for $x \geq 1$. That is to say, $\phi(n,x)$ is a strict decreasing function for $x \geq 1$. Hence, we have

$$\phi(n,n-3) < \phi(n,n-4) < \cdots < \phi(n,3) < \phi(n,2) < \phi(n,1),$$

i.e.,

$$R'(U_{n-3}^n) < R'(U_{n-4}^n) < \cdots < R'(U_3^n) < R'(U_2^n) < R'(U_1^n).$$

On the other hand,

$$R'(U_1^n) = \frac{n-2}{2} + \frac{2}{\sqrt{5}}, \quad R'(U_0^n) = \frac{n}{2},$$

which gives

$$R'(U_0^n) - R'(U_1^n) = 1 - \frac{2}{\sqrt{5}} > 0.$$

Hence, together with (11), we get

$$R'(U_{n-3}^n) < R'(U_{n-4}^n) < \cdots < R'(U_3^n) < R'(U_2^n) < R'(U_1^n) < R'(U_0^n).$$

Hence, in view of Theorem 1, we obtain the following result, in which the upper bound is proven in [5].

Theorem 2. *Let $G \in \bigcup_{k=0}^{n-3} \mathscr{U}_{n,k}$, then*

(i) ([5]) $R'(G) \leq \phi(n,0)$, the equality holds if and only if $G \cong C_n$.

(ii) $R'(G) \geq \phi(n,n-3)$, the equality holds if and only if $G \cong U_{n-3}^n$.

Finally, the maximum value of $R'(G)$ among unicyclic graphs with a given number of pendent vertices is left for future research.

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