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Research article

Unicyclic graphs with extremal exponential Randić index

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Abstract: Recently the exponential Randić index e^{χ} was introduced. The exponential Randić index of a graph G is defined as the sum of the weights $e^{\frac{1}{\sqrt{d(u)d(v)}}}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. In this paper, we give sharp lower and upper bounds on the exponential Randić index of unicyclic graphs.

Keywords: exponential Randić index; unicyclic graph; extremal value

1. Introduction

In recent years, graph theory has been widely applied in chemistry. The topological index of a graph is an invariant numerical quantity that can be used to describe some properties of a molecular graph. Topological indices can be divided into several different categories. The indices based on vertex-degree are the most widely studied and applied ones.

In 1975, the famous chemist Milan Randić proposed a structural descriptor called Randić (connectivity) index, which is common used molecular descriptor in the study of structure-activity relations. For a simple connected graph $G = (V, E)$, V and E represent the set of vertices and edges of graph G, respectively. And $d(u)$ refers to the degree of a vertex u in G. The Randić index of the graph G is defined as

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

The Randić index has been shown to be closely related to chemical properities.

Bollobás and Erdös [1] generalized this index by replacing $-\frac{1}{2}$ with any real number α in 1998, which is called the general Randić index and defined as

$$\chi_\alpha(G) = \sum_{uv\in E(G)} (d(u)d(v))^{\alpha}.$$

There are a lot of researches on the mathematical properties of the Randić index and general Randić index of a graph. Du and Zhou [2] gave the extremal values on the Randić indices of trees, unicyclic graphs and bicyclic graphs. Li and Yang [3] obtained the lower and upper bounds for the general Randić index among graphs with n vertices. Hu and Li [4, 5] investigated the trees with the maximum and minimum value of general Randić index among all trees with n vertices. Li and Shi [6] showed that among all unicyclic graphs with n vertices, S_n^+ has the maximum general Randić index for $0 < \alpha < 1$, and $T_{\lceil \frac{n+1}{2} \rceil, \lfloor \frac{n+1}{2} \rfloor}$ has the maximum general Randić index for $\alpha > 2$ and $n \geq 7$. Wu and Zhang [7] showed that among all unicyclic graphs with n vertices, C_n for $\alpha > 0$ and S_n^+ for $-1 \leq \alpha < 0$, respectively, has the minimum general Randić index. See ([8]-[13]) for more information of the Randić index.

In order to study the descrimination properties of Randić index. Rada [14] proposed exponential vertex-degree based topological indices and gave the definition of exponential Randić index

$$e^{\chi}(G) = \sum_{uv\in E(G)} e^{\frac{1}{\sqrt{d(u)d(v)}}}.$$

Cruz, Londoño and Rada [15] gave the definition of general Randić index

$$e^{\chi_\alpha}(G) = \sum_{uv\in E(G)} e^{(d(u)d(v))^\alpha}.$$

They showed that the minimum value of e^{χ_α} is attained in the path P_n when $\alpha > 0$, and in the star S_n when $\alpha < 0$ over the set $\mathcal{T}_n$. Cruz, Monsalve and Rada [16] showed that e^{χ} attains its maximum value in the path P_n.

Theorem 1.1. *([16]) If $T \in \mathcal{T}_n$ and $T \ncong P_n$, then T is not maximal with respect to e^{χ} over $\mathcal{T}_n$.*

This paper discusses the extremal value problems of exponential Randić index of unicyclic graphs. For convenience, there are some notations and terminologies. For integer n, let $\mathcal{U}_n$ as a set of unicyclic graphs with $n \geq 3$ vertices. A vertex of degree one is called a pendent vertex. Let S_n^+ is a unicyclic graphs with n vertices as follows: S_n^+ is obtained from the star graph S_n by connecting two pendent vertices of S_n (see Figure 4). Let $N(u)$ denote the neighborhood of vertex u. We use C_n and P_n to denote the cycle and path with n vertices, respectively. Let $T_{a,b,c}$ is a triangle with leaves, where a, b and c are nonnegative integers that denote the degrees of the vertices on the triangle, respectively. Particularly, if $c = 2$, a triangle with two branches $T_{a,b,2}$ is simply $T_{a,b}$. $T_{a,b}$ is balanced if $|a-b| \geq 1$, i.e., $T_{a,b} = T_{\lceil \frac{n+1}{2}\rceil,\lfloor \frac{n+1}{2}\rfloor}$. A unicyclic graph G is said to be a sun graph [17] if the vertices belonging to the cycle have degree at most three and remaining vertices have degree at most two.

2. Preliminaries

In this section, we will introduce some graph transformations, which increase the exponential Randić index. And we will give some lemmas. These transformations and lemmas will help to prove our main results.

Lemma 2.1. *(i) The function $g_1(x) = \mathrm{e}^{\frac{1}{\sqrt{x}}}$ is monotonously decreasing for $x \geq 2$.*
(ii) The function $g_2(x) = \mathrm{e}^{\frac{1}{\sqrt{2}}} - \mathrm{e}^{\frac{1}{\sqrt{x-1}}}$ is monotonously increasing for $x \geq 2$.
(iii) The function $g_3(x) = (1-\frac{1}{2}x^{-\frac{1}{2}})e^{\frac{1}{\sqrt{x}}}$ is monotonously decreasing for $x \geq 2$.

Proof. (i) Let $g(t) = \mathrm{e}^t$, $t(x) = \left(\sqrt{x}\right)^{-1}$. The function $g(t)$ is monotonously increasing for $x \geq 2$. The function $t(x)$ is monotonously decreasing for $x \geq 2$. So that $g(x)$ is monotonously decreasing for $x \geq 2$.
(ii) By applying (i), it is obvious that (ii) holds.
(iii) For $x \geq 2$, we have

$$\begin{aligned}\frac{dg_3(x)}{dx} &= \frac{1}{4}x^{-\frac{3}{2}}e^{\frac{1}{\sqrt{x}}} - \frac{1}{2}x^{-\frac{3}{2}}(1-\frac{1}{2}x^{-\frac{1}{2}})e^{\frac{1}{\sqrt{x}}}\\ &= \frac{1}{4}x^{-\frac{3}{2}}e^{\frac{1}{\sqrt{x}}} - (\frac{1}{2}-\frac{1}{4}x^{-\frac{1}{2}})x^{-\frac{3}{2}}e^{\frac{1}{\sqrt{x}}}\\ &= e^{\frac{1}{\sqrt{x}}}x^{-\frac{3}{2}}(\frac{1}{4}-\frac{1}{2}+\frac{1}{4}x^{-\frac{1}{2}})\\ &= \frac{1}{4}e^{\frac{1}{\sqrt{x}}}x^{-\frac{3}{2}}(\frac{1}{\sqrt{x}}-1)\\ &< 0,\end{aligned}$$

and hence (iii) holds.

Lemma 2.2. *The function $f(x) = \frac{1}{2}e^{\frac{1}{\sqrt{x}}} - \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2x}}}$ is monotonously decreasing for $x \geq 2$.*

Proof. *For $x \geq 2$, we have*

$$\begin{aligned}\frac{df(x)}{dx} &= -\frac{1}{4}e^{\frac{1}{\sqrt{x}}}x^{-\frac{3}{2}} + \frac{\sqrt{2}}{4}(2x)^{-\frac{3}{2}}e^{\frac{1}{\sqrt{2x}}}\\ &= \frac{1}{8}x^{-\frac{3}{2}}e^{\frac{1}{\sqrt{2x}}} - \frac{1}{4}x^{-\frac{3}{2}}e^{\frac{1}{\sqrt{x}}}\\ &< 0.\end{aligned}$$

Lemma 2.3. *For integer $q \geq 2$, the function $f(x) = e^{\frac{1}{\sqrt{qx}}} - e^{\frac{1}{\sqrt{(q-1)x}}}$ is increasing for $x \geq 2$.*

Proof. For $x \geq 2$, we have

$$\begin{aligned}\frac{df(x)}{dx} &= \frac{(q-1)e^{\frac{1}{\sqrt{(q-1)x}}}}{2(x(q-1))^{\frac{3}{2}}} - \frac{qe^{\frac{1}{\sqrt{qx}}}}{2(qx)^{\frac{3}{2}}}\\ &= \frac{1}{2x^{\frac{3}{2}}}\left(\frac{(q-1)e^{\frac{1}{\sqrt{(q-1)x}}}}{(q-1)^{\frac{3}{2}}} - \frac{qe^{\frac{1}{\sqrt{qx}}}}{q^{\frac{3}{2}}}\right)\\ &= \frac{1}{2x^{\frac{3}{2}}}\left(\frac{e^{\frac{1}{\sqrt{(q-1)x}}}}{\sqrt{q-1}} - \frac{e^{\frac{1}{\sqrt{qx}}}}{\sqrt{q}}\right)\\ &> 0,\end{aligned}$$

and hence Lemma 2.3 holds.

Lemma 2.4. *Let x, y be positive integers with $x \geq 1$ and $y \geq 2$. Denote*

$$l(x,y) = e^{\frac{1}{\sqrt{y}}} + x(e^{\frac{1}{\sqrt{y}}} - e^{\frac{1}{\sqrt{y-1}}}) + (y-1-x)(e^{\frac{1}{\sqrt{2y}}} - e^{\frac{1}{\sqrt{2(y-1)}}}),$$

then $l(x,y)$ is monotonously decreasing in x.

Proof. For $x \geq 1$ and $y \geq 2$, we have

$$\frac{\partial l(x,y)}{\partial x} = (e^{\frac{1}{\sqrt{y}}} - e^{\frac{1}{\sqrt{y-1}}}) - (e^{\frac{1}{\sqrt{2y}}} - e^{\frac{1}{\sqrt{2(y-1)}}}).$$

It is easily to know that $e^{\frac{1}{\sqrt{y}}} - e^{\frac{1}{\sqrt{y-1}}} < 0$ and $e^{\frac{1}{\sqrt{2y}}} - e^{\frac{1}{\sqrt{2(y-1)}}} < 0$. By Lemma 2.3, $e^{\frac{1}{\sqrt{2y}}} - e^{\frac{1}{\sqrt{2(y-1)}}} > e^{\frac{1}{\sqrt{y}}} - e^{\frac{1}{\sqrt{y-1}}}$. Hence $l(x,y) < 0$ and $l(x,y)$ is monotonously decreasing in x.

Lemma 2.5. *For $x \geq 2$, denote*

$$f(x) = e^{\frac{1}{\sqrt{x}}} + (x-2)(e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}}) + (e^{\frac{1}{\sqrt{2x}}} - e^{\frac{1}{\sqrt{2(x-1)}}}).$$

Then $f(x)$ is monotonously decreasing in x.

Proof. For $x \geq 2$, by applying Lemma 2.1(*iii*) and Lemma 2.2, we have

$$\begin{aligned}
\frac{df(x)}{dx} &= e^{\frac{1}{\sqrt{x}}}(-\frac{1}{2}x^{-\frac{3}{2}}) + (e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}}) \\
&\quad + (x-2)[e^{\frac{1}{\sqrt{x}}}(-\frac{1}{2}x^{-\frac{3}{2}}) - e^{\frac{1}{\sqrt{x-1}}}(-\frac{1}{2}(x-1)^{-\frac{3}{2}})] \\
&\quad - e^{\frac{1}{\sqrt{2x}}}(2x)^{-\frac{3}{2}} + e^{\frac{1}{\sqrt{2(x-1)}}}[2(x-1)]^{-\frac{3}{2}} \\
&= -\frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{3}{2}} + (e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}}) \\
&\quad + (x-2)[-\frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{3}{2}} + \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}(x-1)^{-\frac{3}{2}}] \\
&\quad - \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2x}}}x^{-\frac{3}{2}} + \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2(x-1)}}}(x-1)^{-\frac{3}{2}} \\
&= (\frac{1}{2}e^{\frac{1}{\sqrt{x}}} - \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2x}}})x^{-\frac{3}{2}} + (\frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2(x-1)}}} \\
&\quad - e^{\frac{1}{\sqrt{x-1}}})(x-1)^{-\frac{3}{2}} + e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{1}{2}} \\
&\quad + \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}x(x-1)^{-\frac{3}{2}} \\
&\leq (\frac{1}{2}e^{\frac{1}{\sqrt{x}}} - \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2x}}})(x-1)^{-\frac{3}{2}} + (\frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2(x-1)}}} \\
&\quad - e^{\frac{1}{\sqrt{x-1}}})(x-1)^{-\frac{3}{2}} + e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{1}{2}} \\
&\quad + \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}x(x-1)^{-\frac{3}{2}} \\
&= (e^{\frac{1}{\sqrt{x}}} - \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2x}}})(x-1)^{-\frac{3}{2}} + (\frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2(x-1)}}} \\
&\quad - e^{\frac{1}{\sqrt{x-1}}})(x-1)^{-\frac{3}{2}} + e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{1}{2}} \\
&\quad + \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}x(x-1)^{-\frac{3}{2}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}(x-1)^{-\frac{3}{2}} \\
&= (\frac{1}{2}e^{\frac{1}{\sqrt{x}}} - \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2x}}} + \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2(x-1)}}} \\
&\quad - \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}})(x-1)^{-\frac{3}{2}} + e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{1}{2}} \\
&\quad - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}(x-1)^{-\frac{3}{2}} + \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}x(x-1)^{-\frac{3}{2}} \\
&\quad + \frac{1}{2}(e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}})(x-1)^{-\frac{3}{2}} \\
&\leq e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{1}{2}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}(x-1)^{-\frac{3}{2}} \\
&\quad + \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}x(x-1)^{-\frac{3}{2}} + \frac{1}{2}(e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}})(x-1)^{-\frac{3}{2}} \\
&\quad (\text{by } Lemma \text{ } 2.2) \\
&= e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{1}{2}} \\
&\quad + \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}x(x-1)^{-\frac{3}{2}} - \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}(x-1)^{-\frac{3}{2}} \\
&= (1 - \frac{1}{2}x^{-\frac{1}{2}})e^{\frac{1}{\sqrt{x}}} - (1 - \frac{1}{2}(x-1)^{-\frac{1}{2}})e^{\frac{1}{\sqrt{x-1}}} \\
&< 0 \ (\text{by } Lemma \text{ } 2.1 \ (iii)),
\end{aligned}$$

and hence $f(x)$ is monotonously decreasing in x.

Transformation 1. Let H_1 be a cycle subgraph of G_1, which is attached at u in graph G_1. Let v_1 and v_2 be adjacent to u in H_1 with $d(v_1) = 2, 3$ or 4 and $d(v_2) = 2, 3$ or 4. Let K_1 be a graph obtained from G_1 by attaching two paths: $P_1 = uu_1u_2u_3...u_a$ of length a and $P_2 = uw_1w_2w_3...w_b$ of length b. If $K_1 = G_1 - uw_1 + u_aw_1$, we say that K_1 is obtained from G_1 by Transformation 1, as shown in Figure 1.

Lemma 2.6. *If K_1 is obtained from G_1 by Transformation 1 as shown in Figure 1, then*

$$e^{\chi}(G_1) < e^{\chi}(K_1).$$

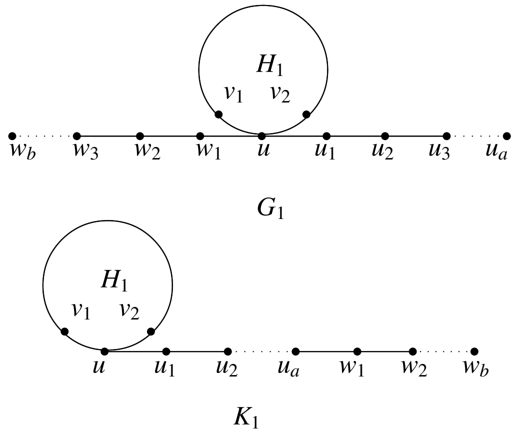
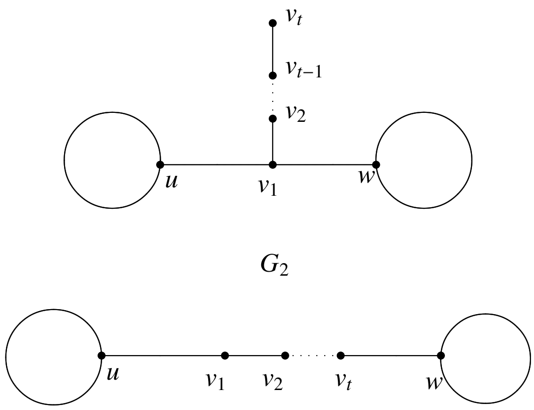


Figure 1. *Transformation* 1.

Proof. Applying Transformation 1, let $d(v_1) = d_1$ and $d(v_2) = d_2$. So

$$\begin{aligned} e^{\chi}(K_1) - e^{\chi}(G_1) &= e^{\frac{1}{\sqrt{3d_1}}} + e^{\frac{1}{\sqrt{3d_2}}} + e^{\frac{1}{\sqrt{6}}} + (a+b-2)e^{\frac{1}{2}} + e^{\frac{1}{\sqrt{2}}} \\ &\quad - e^{\frac{1}{\sqrt{4d_1}}} - e^{\frac{1}{\sqrt{4d_2}}} - 2e^{\frac{1}{\sqrt{8}}} - (a+b-4)e^{\frac{1}{2}} \\ &\quad - 2e^{\frac{1}{\sqrt{2}}} \\ &= e^{\frac{1}{\sqrt{3d_1}}} - e^{\frac{1}{\sqrt{4d_1}}} + e^{\frac{1}{\sqrt{3d_2}}} - e^{\frac{1}{\sqrt{4d_2}}} + e^{\frac{1}{\sqrt{6}}} \\ &\quad - 2e^{\frac{1}{\sqrt{8}}} + 2e^{\frac{1}{2}} - e^{\frac{1}{\sqrt{2}}} \\ &> 0.0265 \ (\textit{by Lemma } 2.3) \\ &> 0. \end{aligned}$$

Transformation 2. $P = v_1v_2...v_{t-1}v_t$ is a pendent path attaching at v_1 in graph G_2. The vertices u and w are two neighbors of v_1 different from v_2 with $d(u) = 2$ or 3 and $d(w) = 2$ or 3, $d(u) \neq d(w)$. If $K_2 = G_2 - wv_1 + v_tw$, we say that K_2 is obtained from G_2 by Transformation 2, as shown in Figure 2.



K_2
Figure 2. Transformation 2.

Lemma 2.7. *If K_2 is obtained from G_2 by Transformation 2 as shown in Figure 2, then*

$$e^{\chi}(G_2) < e^{\chi}(K_2).$$

Proof. By Transformation 2, let $d(u) = d_1$, $d(w) = d_2$ and $d(u) \neq d(w)$, we have

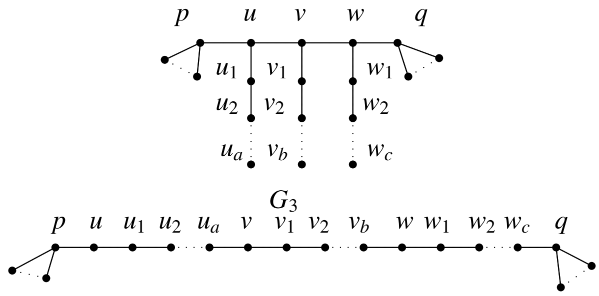
$$\begin{aligned} e^{\chi}(K_2) - e^{\chi}(G_2) &= e^{\frac{1}{\sqrt{2d_1}}} + e^{\frac{1}{\sqrt{2d_2}}} + (t-1)e^{\frac{1}{2}} - e^{\frac{1}{\sqrt{3d_1}}} - e^{\frac{1}{\sqrt{3d_2}}} \\ &\quad - e^{\frac{1}{\sqrt{6}}} - e^{\frac{1}{\sqrt{2}}} - (t-3)e^{\frac{1}{2}} \\ &= e^{\frac{1}{\sqrt{2d_1}}} - e^{\frac{1}{\sqrt{3d_1}}} + e^{\frac{1}{\sqrt{2d_2}}} - e^{\frac{1}{\sqrt{3d_2}}} + 2e^{\frac{1}{2}} \\ &\quad - e^{\frac{1}{\sqrt{6}}} - e^{\frac{1}{\sqrt{2}}} \\ &> 0.0183 \ (\textit{by Lemma } 2.3) \\ &> 0. \end{aligned}$$

Therefore, the proof is complete.

Transformation 3. Let G_3 be a graph as shown in Figure 3. The pendent paths $P_1 = u_1u_2...u_a$, $P_2 = v_1v_2...v_b$, $P_3 = w_1w_2...w_3$ is attached at u, v, w in graph G_3. Let $d(p) = d_1$, $d(q) = d_2$, and $d_1 = 2$ or 3, $d_2 = 2$ or 3. If $K_3 = K_2 - uv - vw - wq + u_av + v_bw + w_cq$, we say that K_3 is obtained from G_3 by Transformation 3, as shown in Figure 3.

Lemma 2.8. *If K_3 is obtained from G_3 by Transformation 3 as shown in Figure 3, then*

$$e^{\chi}(G_3) < e^{\chi}(K_3).$$



K_3

Figure 3. Transformation 3.

Proof. Let $d(p) = d_1$ and $d(q) = d_2$, we have

$$\begin{aligned} e^{\chi}(K_3) - e^{\chi}(G_3) &= e^{\frac{1}{\sqrt{2d_1}}} + (a+b+c+2)e^{\frac{1}{2}} + e^{\frac{1}{\sqrt{2d_2}}} - e^{\frac{1}{\sqrt{3d_1}}} \\ &\quad - e^{\frac{1}{\sqrt{3d_2}}} - 2e^{\frac{1}{3}} - 3e^{\frac{1}{\sqrt{6}}} - 3e^{\frac{1}{\sqrt{2}}} - (a+b+c-6)e^{\frac{1}{2}} \\ &= e^{\frac{1}{\sqrt{2d_1}}} - e^{\frac{1}{\sqrt{3d_1}}} + e^{\frac{1}{\sqrt{2d_2}}} - e^{\frac{1}{\sqrt{3d_2}}} + 8e^{\frac{1}{2}} - 2e^{\frac{1}{3}} \\ &\quad - 3e^{\frac{1}{\sqrt{6}}} - 3e^{\frac{1}{\sqrt{2}}} \\ &> 0.0188 \ (\textit{by Lemma } 2.3) \\ &> 0. \end{aligned}$$

Therefore, the proof is complete.

3. Main results

In this section, we will give the upper and lower bounds on the exponential Randić index of unicyclic graphs.

Theorem 3.1. *Let G be a unicyclic graph on n vertices for* $n \geq 3$. *Then*

$$e^{\chi}(G) \leq e^{\chi}(C_n).$$

The equality holds if and only if $G \cong C_n$.

Proof. By Theorem 1.1, we know that e^{χ} attains its maximum value in the path P_n. For any unicyclic graph G with n vertices, the value of exponential Randić index gets larger when some paths are suspended. By Lemma 2.6, we can find that any unicyclic graph G can be changed into a sun graph with a larger exponential Randić index e^{χ}. We can applying Lemma 2.7 and Lemma 2.8 repeatedly to any sun graph by increasing its exponential Randić index e^{χ} until it is a C_n. So we can prove the theorem.

For a graph $G = S_n^+$, denote

$$e^{\chi}(G) = f(n) = (n-3)e^{\frac{1}{\sqrt{n-1}}} + 2e^{\frac{1}{\sqrt{2(n-1)}}} + e^{\frac{1}{2}}.$$

We have the following result.

Theorem 3.2. *Let G be a unicyclic graph on n vertices for* $n \geq 3$, *then*

$$f(n) \leq e^{\chi}(G).$$

The equality holds if and only if $G = S_n^+$ *(see Figure 4).*

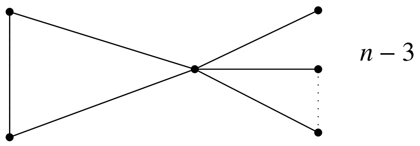


Figure 4. S_n^+

Proof. From the above conclusion, we know the exponential Randić index reaches its maximum value in C_n. In the proof, we assume that G is a unicyclic graph but not a C_n, and just show that $f(n) \leq e^{\chi}(G)$ and equality holds if and only if $G = S_n^+$.

We use induction on the number n. Since G is not a C_n and $G \in \mathcal{U}_n$, we have $n \geq 4$. When $n = 4, 5$, then the theorem holds (see Figure 5). In the following proof, we assume that $G \in \mathcal{U}_n$ with $n \geq 6$. M is the set of vertices with degree one in $V(G)$ (i.e. $M = \{u \in V(G) | d(u) = 1\}$). Since G is not a C_n, $M \neq \emptyset$. Let $u \in M$ and v be the neighbor of u. Then $d(v) \geq 2$. Set $W(u) = \{y | y \in N(v) \setminus \{u\}, d(y) = 1\}$. Choose u_0 such that

(i) the number of the set $W(u_0)$ is as large as possible;

(ii) subject to (i), $d(v)$ is as small as possible.

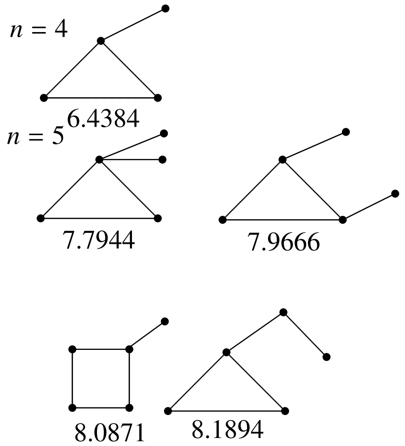


Figure 5. *the value of* e^{χ} *when* $n = 4, 5$.

Let $G^{'} = G - u_0$, then $G^{'} \in \mathcal{U}_{n-1}$, $d(v) = d$ and $N_{G'}(v) = \{y_1, y_2, y_3, ..., y_{d-1}\}$.

Let S be the sum of the weights $e^{\frac{1}{\sqrt{d(u)d(v)}}}$ of the edges incident with v except for the edge $u_0 v$ in G. Then

$$S = \sum_{i=1}^{d-1} \mathrm{e}^{\frac{1}{\sqrt{dd_{y_i}}}}.$$

Let $S^{'}$ be the sum of the weights $e^{\frac{1}{\sqrt{d(u)d(v)}}}$ of the edges incident with v in $G^{'}$. Then

$$S' = \sum_{i=1}^{d-1} e^{\frac{1}{\sqrt{(d-1)d_{y_i}}}}.$$

By induction assumption, we have

$$\begin{aligned}
e^{\chi}(G) &= e^{\chi}(G^{'}) + e^{\frac{1}{\sqrt{d}}} + S - S^{'} \\
&\geq f(n-1) + e^{\frac{1}{\sqrt{d}}} + S - S^{'} \\
&= f(n) - (n-3)e^{\frac{1}{\sqrt{n-1}}} - 2e^{\frac{1}{\sqrt{2(n-1)}}} - e^{\frac{1}{2}} + (n-4)e^{\frac{1}{\sqrt{n-2}}} \\
&\quad + 2e^{\frac{1}{\sqrt{2(n-2)}}} + e^{\frac{1}{2}} + e^{\frac{1}{\sqrt{d}}} + S - S^{'} \\
&= f(n) + (n-4)e^{\frac{1}{\sqrt{n-2}}} + 2e^{\frac{1}{\sqrt{2(n-2)}}} - (n-3)e^{\frac{1}{\sqrt{n-1}}} - 2e^{\frac{1}{\sqrt{2(n-1)}}} \\
&\quad + e^{\frac{1}{\sqrt{d}}} + S - S^{'}.
\end{aligned}$$

Now we consider the following two cases.

Case 1. For $i = 1, 2, 3, ..., d-1$, $d(y_i) \geq 2$.

If $d(v) = 2$, we have

$$\begin{aligned}
e^{\chi}(G) &\geq f(n) + (n-4)e^{\frac{1}{\sqrt{n-2}}} + 2e^{\frac{1}{\sqrt{2((n-2)}}} - (n-3)e^{\frac{1}{\sqrt{n-1}}} - 2e^{\frac{1}{\sqrt{2(n-1)}}} \\
&\quad + e^{\frac{1}{\sqrt{2}}} + e^{\frac{1}{\sqrt{2d_{y_1}}}} - e^{\frac{1}{\sqrt{d_{y_1}}}} \\
&= f(n) + [(n-3)e^{\frac{1}{\sqrt{n-2}}} - (n-3)e^{\frac{1}{\sqrt{n-1}}}] + [2e^{\frac{1}{\sqrt{2(n-2)}}} - 2e^{\frac{1}{\sqrt{2(n-1)}}}] \\
&\quad + [e^{\frac{1}{\sqrt{2}}} - e^{\frac{1}{\sqrt{n-2}}} + e^{\frac{1}{\sqrt{2d_{y_1}}}} - e^{\frac{1}{\sqrt{d_{y_1}}}}].
\end{aligned}$$

By Lemma 2.1(ii) and Lemma 2.3, we have

$$
\begin{aligned}
&e^{\frac{1}{\sqrt{2}}} - e^{\frac{1}{\sqrt{n-2}}} + e^{\frac{1}{\sqrt{2d_{y_1}}}} - e^{\frac{1}{\sqrt{d_{y_1}}}}\\
\geq & e^{\frac{1}{\sqrt{2}}} - e^{\frac{1}{\sqrt{4}}} + e^{\frac{1}{2}} - e^{\frac{1}{\sqrt{2}}}\\
=&0.
\end{aligned}
$$

Then $e^{\chi}(G) > f(n)$ holds.

If $d(v) = 3$ and $n \geq 9$, applying Lemma 2.3, then we have

$$
\begin{aligned}
e^{\chi}(G) \geq\ & f(n) + [(n-3)e^{\frac{1}{\sqrt{n-2}}} - (n-3)e^{\frac{1}{\sqrt{n-1}}}]\\
&+ [2e^{\frac{1}{\sqrt{2(n-2)}}} - 2e^{\frac{1}{\sqrt{2(n-1)}}}] - e^{\frac{1}{\sqrt{n-2}}} + e^{\frac{1}{\sqrt{3}}} + e^{\frac{1}{\sqrt{3d_{y_1}}}}\\
&- e^{\frac{1}{\sqrt{2d_{y_1}}}} + e^{\frac{1}{\sqrt{3d_{y_2}}}} - e^{\frac{1}{\sqrt{2d_{y_2}}}}\\
=\ & f(n) + [(n-3)e^{\frac{1}{\sqrt{n-2}}} - (n-3)e^{\frac{1}{\sqrt{n-1}}}] + [2e^{\frac{1}{\sqrt{2(n-2)}}}\\
&- 2e^{\frac{1}{\sqrt{2(n-1)}}}] + e^{\frac{1}{\sqrt{3}}} - e^{\frac{1}{\sqrt{n-2}}} + e^{\frac{1}{\sqrt{3d_{y_1}}}} - e^{\frac{1}{\sqrt{2d_{y_1}}}}\\
&+ e^{\frac{1}{\sqrt{3d_{y_2}}}} - e^{\frac{1}{\sqrt{2d_{y_2}}}}\\
\geq\ & f(n) + [(n-3)e^{\frac{1}{\sqrt{n-2}}} - (n-3)e^{\frac{1}{\sqrt{n-1}}}] + [2e^{\frac{1}{\sqrt{2(n-2)}}}\\
&- 2e^{\frac{1}{\sqrt{2(n-1)}}}] + 0.0329\\
>\ & f(n).
\end{aligned}
$$

If $d(v) = 3$ and $n = 6, 7, 8$, it's not difficult to check that

$$
\begin{aligned}
&[(n-3)e^{\frac{1}{\sqrt{n-2}}} - (n-3)e^{\frac{1}{\sqrt{n-1}}}] + [2e^{\frac{1}{\sqrt{2(n-2)}}} - 2e^{\frac{1}{\sqrt{2(n-1)}}}] + e^{\frac{1}{\sqrt{3}}}\\
&- e^{\frac{1}{\sqrt{n-2}}} + e^{\frac{1}{\sqrt{3d_{y_1}}}} - e^{\frac{1}{\sqrt{2d_{y_1}}}} + e^{\frac{1}{\sqrt{3d_{y_2}}}} - e^{\frac{1}{\sqrt{2d_{y_2}}}} > 0.
\end{aligned}
$$

We have proved that the theorem holds when $d(v) = 2$ and $d(v) = 3$. If $d(v) \geq 4$, then there is at least one vertex in $\{y_1, y_2, y_3, ..., y_{d-1}\}$ such that the subgraph H of $G - v$ which including the vertex is a tree and $|V(H)| \geq 2$. Because $W(u) = \Phi$ for all $u \in M$, there exists $u' \in V(H) \bigcap M$ and $u'v' \in E(G)$ such that $d(v') = 2$, which is a contradiction. So $d(v) = d \leq 3$.

Case 2. There exists some $i (1 \leq i \leq d-1)$ such that $d(y_i) = 1$.

Without loss of generality, $d(y_1) = d(y_2) = ... = d(y_k) = 1$ and $d(y_i) \geq 2$ for $k+1 \leq i \leq d-1$, where $k \geq 1$.

By applying Lemma 2.3, we have

$$
\begin{aligned}
S - S' &= k\mathrm{e}^{\frac{1}{\sqrt{d}}} + \sum_{i=k+1}^{d-1} \mathrm{e}^{\frac{1}{\sqrt{dd_{y_i}}}} - k\mathrm{e}^{\frac{1}{\sqrt{d-1}}} + \sum_{i=k+1}^{d-1} \mathrm{e}^{\frac{1}{\sqrt{(d-1)d_{y_i}}}}\\
&= k(e^{\frac{1}{\sqrt{d}}} - e^{\frac{1}{\sqrt{d-1}}}) + \sum_{i=k+1}^{d-1} \mathrm{e}^{\frac{1}{\sqrt{dd_{y_i}}}} - \sum_{i=k+1}^{d-1} \mathrm{e}^{\frac{1}{\sqrt{(d-1)d_{y_i}}}}\\
&\geq k(e^{\frac{1}{\sqrt{d}}} - e^{\frac{1}{\sqrt{d-1}}}) + (d-1-k)(e^{\frac{1}{\sqrt{2d}}} - e^{\frac{1}{\sqrt{2(d-1)}}}).
\end{aligned}
$$

Since $G \in \mathcal{U}_n$, $k \leq d-2$, and $d(v) = d \leq n-2$. By Lemma 2.4 and Lemma 2.5, we have that

$$
\begin{aligned}
e^{\chi}(G) \geq\ & f(n) + (n-4)e^{\frac{1}{\sqrt{n-2}}} + 2e^{\frac{1}{\sqrt{2(n-2)}}} - (n-3)e^{\frac{1}{\sqrt{n-1}}}\\
&- 2e^{\frac{1}{\sqrt{2(n-1)}}} + e^{\frac{1}{\sqrt{d}}} + k(e^{\frac{1}{\sqrt{d}}} - e^{\frac{1}{\sqrt{d-1}}})\\
&+ (d-1-k)(e^{\frac{1}{\sqrt{2d}}} - e^{\frac{1}{\sqrt{2(d-1)}}})\\
\geq\ & f(n) + (n-4)e^{\frac{1}{\sqrt{n-2}}} + 2e^{\frac{1}{\sqrt{2(n-2)}}} - (n-3)e^{\frac{1}{\sqrt{n-1}}}\\
&- 2e^{\frac{1}{\sqrt{2(n-1)}}} + e^{\frac{1}{\sqrt{d}}} + (d-2)(e^{\frac{1}{\sqrt{d}}} - e^{\frac{1}{\sqrt{d-1}}})\\
&+ (e^{\frac{1}{\sqrt{2d}}} - e^{\frac{1}{\sqrt{2(d-1)}}})\ (by\ Lemma\ 2.4)\\
\geq\ & f(n) + (n-4)e^{\frac{1}{\sqrt{n-2}}} + 2e^{\frac{1}{\sqrt{2(n-2)}}} - (n-3)e^{\frac{1}{\sqrt{n-1}}}\\
&- 2e^{\frac{1}{\sqrt{2(n-1)}}} + e^{\frac{1}{\sqrt{n-2}}} + (n-4)(e^{\frac{1}{\sqrt{n-2}}} - e^{\frac{1}{\sqrt{n-3}}})\\
&+ (e^{\frac{1}{\sqrt{2(n-2)}}} - e^{\frac{1}{\sqrt{2(n-3)}}})\ (by\ Lemma\ 2.5)\\
=\ & f(n) + (n-3)(e^{\frac{1}{\sqrt{n-2}}} - e^{\frac{1}{\sqrt{n-1}}}) + (n-4)(e^{\frac{1}{\sqrt{n-2}}} - e^{\frac{1}{\sqrt{n-3}}})\\
&+ 2(e^{\frac{1}{\sqrt{2(n-2)}}} - e^{\frac{1}{\sqrt{2(n-1)}}}) + (e^{\frac{1}{\sqrt{2(n-2)}}} - e^{\frac{1}{\sqrt{2(n-3)}}})\\
>\ & f(n).
\end{aligned}
$$

We put the proof of the last inequality in the appendix, and the proof is complete.

4. Conclusions

In this paper, we give the extremal value on exponential Randić index of unicyclic graphs, and the corresponding extremal graph is characterized. However, determining the extremal value with respect to exponential Randić index of bicyclic graphs still remains an open and challenging problem.

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Conflict of interest

The authors declare that they have no conflicts of interest to this work.

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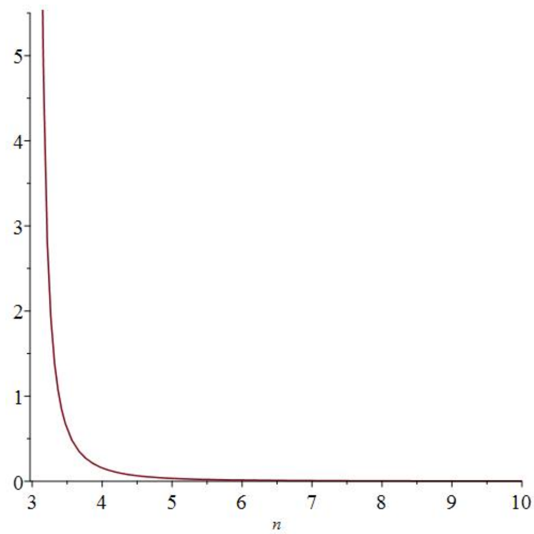
Appendix

Proposition 4.1. *Let n be a positive integer with* $n \geq 6$*, we will show that*

$$(n-3)(e^{\frac{1}{\sqrt{n-2}}} - e^{\frac{1}{\sqrt{n-1}}}) + (n-4)(e^{\frac{1}{\sqrt{n-2}}} - e^{\frac{1}{\sqrt{n-3}}}) + 2(e^{\frac{1}{\sqrt{2(n-2)}}} - e^{\frac{1}{\sqrt{2(n-1)}}}) + (e^{\frac{1}{\sqrt{2(n-2)}}} - e^{\frac{1}{\sqrt{2(n-3)}}}) > 0.$$

Proof. Let $g(n) = (n-3)(e^{\frac{1}{\sqrt{n-2}}} - e^{\frac{1}{\sqrt{n-1}}}) + (n-4)(e^{\frac{1}{\sqrt{n-2}}} - e^{\frac{1}{\sqrt{n-3}}}) + 2(e^{\frac{1}{\sqrt{2(n-2)}}} - e^{\frac{1}{\sqrt{2(n-1)}}}) + (e^{\frac{1}{\sqrt{2(n-2)}}} - e^{\frac{1}{\sqrt{2(n-3)}}})$, the image of function $g(n)$ is shown in the following figure.



It can be seen from the function image that $g(n)$ is above the horizontal axis. Calculated by MATLAB, the point of intersection of $g(n)$ and the horizontal axis is $(0, -27852563104487148.539894396758705 - 23751291381668762.757332046522084 * i)$. So $g(n) > 0$ is always established when $n \geq 6$.