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On the Randić Index of Unicyclic Graphs with k Pendant Vertices

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Abstract

The Randić index $R(G)$ of a graph G is the sum of the weights $(d(u)d(v))^{-1/2}$ of all edges uv of G, where $d(u)$ denotes the degree of the vertex u. In this paper, we give sharp lower bounds of Randić index of unicyclic graphs with n vertices and k pendant vertices.

1. Introduction

The Randić index of an organic molecule whose molecular graph is G is defined in [19] as

$$R(G) = \sum_{u,v} (d(u)d(v))^{-1/2},$$

where $d(u)$ denotes the degree of the vertex u of G and the summation goes over all pairs of adjacent vertices of G. The research background of Randić index together with its generalization appears in chemistry or mathematical chemistry and can be found in the literature (see [10, 11]).

Recently, finding bounds for the Randić index or the general Randić index of graphs, as well as related problem of finding the graphs with maximum or minimum value of the

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corresponding index, attracted the attention of many researchers and many results are obtained (see [1,3-9,12-18,20-22]). Among these results, Gao and Lu [6] obtained the sharp bounds on the Randić index of unicyclic graphs; Wu and Zhang [21] gave some results on the unicyclic graphs with minimum general Randić index, and later Li, Wang and Zhang [12] completely solve such a minimum problem; Liu, Lu and Tian [16] gave some bounds on the general Randić index of trees with n vertices and k pendant vertices.

Here, unicyclic graphs with n vertices and k pendant vertices are considered, and the lower bounds of their Randić index are given.

First we introduce some graph notations used in this paper. We only consider finite, undirected and simple graphs. Other undefined terminologies and notations may refer to [2]. For a vertex x of a graph G, we denote the neighborhood and the degree of x by $N(x)$ and $d(x)$, respectively. The maximum degree of a graph G is denoted by $\Delta(G)$. The *star* of order n is denoted by S_n. Let S be a set of vertices of G, we will use $G - S$ to denote the graph that arises from G by deleting the vertices in S together with their incident edges. If $S = \{v\}$, we write $G - v$ for $G - \{v\}$. Unicyclic graphs are connected graphs with n vertices and n edges. A *pendant vertex* is a vertex of degree 1. A *pendant chain* of a graph G is a sequence of vertices $v_0, v_1, \cdots, v_s$ such that v_0 is a pendant vertex of G, $d(v_1) = \cdots = d(v_{s-1}) = 2$ (unless $s = 1$) and $d(v_s) \geq 3$. Let $\mathscr{U}_{n,k} = \{G :\ G$ is a unicyclic graph with n vertices and k pendant vertices$\}$, where $0 \leq k \leq n-3$.

Let U_k^n (see Fig. 1a) be a unicyclic graph with n vertices created from a cycle C_{n-k} of length $n-k$ by attaching k pendant edges to one vertex of C_{n-k}. Let $U(n,k,p)$ (see Fig. 1b) be a unicyclic graph of order n obtained from a path $P_{p+1} = v_0v_1\cdots v_p$ $(p \geq 1)$ by attaching k pendant edges to v_0 and a cycle C_{n-k-p} to v_p, respectively.

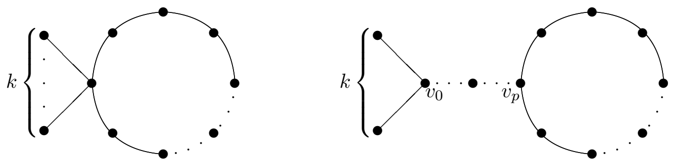

Fig. 1. (a) U_k^n; (b) $U(n,k,p)$

Denote $\varphi(n,k) = \frac{n-k-2}{2} + \frac{k+\sqrt{2}}{\sqrt{k+2}}$. The main result of this paper is stated in the following theorem.

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

$$R(G) \geq \varphi(n,k) \tag{1}$$

and equality in (1) holds if and only if $G \cong U_k^n$.

2. Proof of Theorem 1

We first give some lemmas that will be used in the proof of our result.

Lemma 1. *Let* $f(x) := \frac{x+\sqrt{2}-2}{\sqrt{x}}$ *and* $g(x) := \frac{x-1+\frac{1}{\sqrt{2}}}{\sqrt{x}}$, *where* $x \geq 2$. *Then both* $f(x) - f(x+1)$ *and* $g(x-1) - g(x)$ *are strictly monotone increasing.*

Proof. Since

$$\frac{d^2 f(x)}{dx^2} = -\frac{1}{4}x^{-5/2}\left[x + 3(2-\sqrt{2})\right] < 0$$

and

$$\frac{d^2 g(x)}{dx^2} = -\frac{1}{4}x^{-5/2}\left[x + 3(1-\frac{\sqrt{2}}{2})\right] < 0$$

as $x \geq 2$, Lemma 1 follows. ■

Lemma 2. *For* $x \geq 2$, *(i)* $\frac{x+\frac{1}{\sqrt{2}}}{\sqrt{x+1}} - \frac{x+\sqrt{2}}{\sqrt{x+2}} + \frac{\sqrt{6}-2}{2} > 0$;

(ii) $\frac{x}{\sqrt{x+1}} - \frac{x-2+\sqrt{2}}{\sqrt{x}} > 0$.

Proof. (i) Let

$$h(x) = \frac{x+\frac{1}{\sqrt{2}}}{\sqrt{x+1}} - \frac{x+\sqrt{2}}{\sqrt{x+2}} + \frac{\sqrt{6}-2}{2}, \ x \geq 2.$$

Then

$$\begin{aligned}
\frac{dh(x)}{dx} &= \frac{1}{2}\left[(x+1)^{-\frac{1}{2}} - (x+2)^{-\frac{1}{2}}\right] + \frac{2-\sqrt{2}}{4}(x+1)^{-\frac{3}{2}} - \frac{2-\sqrt{2}}{2}(x+2)^{-\frac{3}{2}} \\
&= \frac{1}{4}\zeta^{-\frac{3}{2}} + \frac{2-\sqrt{2}}{4}(x+1)^{-\frac{3}{2}} - \frac{2-\sqrt{2}}{2}(x+2)^{-\frac{3}{2}} \\
&> \frac{1}{4}\zeta^{-\frac{3}{2}} + \frac{2-\sqrt{2}}{4}(x+2)^{-\frac{3}{2}} - \frac{2-\sqrt{2}}{2}(x+2)^{-\frac{3}{2}} \\
&> \frac{1}{4}(x+2)^{-\frac{3}{2}} + \frac{2-\sqrt{2}}{4}(x+2)^{-\frac{3}{2}} - \frac{2-\sqrt{2}}{2}(x+2)^{-\frac{3}{2}} \\
&= \frac{\sqrt{2}-1}{4}(x+2)^{-\frac{3}{2}} \\
&> 0,
\end{aligned}$$

where $\zeta \in (x+1, x+2)$. Thus $h(x) \geq h(2) > 0$.

(ii) Since $\sqrt{x} > 0$ and $\sqrt{x+1} > 0$, to prove Lemma 2 (ii), it just needs to check that

$$x\sqrt{x} > \sqrt{x+1}(x-2+\sqrt{2}),$$

that is,

$$x^3 > (x+1)(x-2+\sqrt{2})^2,$$

i.e.

$$(3-2\sqrt{2})x^2 + 2(\sqrt{2}-1)x - (2-\sqrt{2})^2 > 0.$$

Note that the above inequality holds by $x \geq 2$, and hence $\frac{x}{\sqrt{x+1}} - \frac{x-2+\sqrt{2}}{\sqrt{x}} > 0$ holds. ■

Lemma 3. *Let $G \in \mathscr{U}_{n,k}$, then $\Delta(G) \leq k+2$.*

Proof. Since G is unicyclic graph, we have $|E(G)| = n$. Assume that $\Delta(G) > k+2$. Then

$$2n = 2|E(G)| = \sum_{v \in V(G)} d(v) \geq 2(n-k-1) + k + \Delta > 2(n-k-1) + k + (k+2) = 2n,$$

a contradiction. Thus $\Delta(G) \leq k+2$. ■

Lemma 4. *Let $G \in \mathscr{U}_{n,1}$. Then*

$$R(G) \geq \varphi(n,1). \tag{2}$$

Furthermore, the equality in (2) 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 (2) holds.

Now, we prove that if $G \in \mathscr{U}_{n,1}$, then (2) holds and the equality in (2) holds only if $G \cong U_1^n$. Since $G \in \mathscr{U}_{n,1}$, by Lemma 3, 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

$$R(G) - R(U_1^n) = 1/\sqrt{2} + 1/\sqrt{6} - 1/2 - 1/\sqrt{3} > 0.$$

Thus the lemma follows. ■

Proof of Theorem 1. We apply induction on k. For $k = 0$, $\mathscr{U}_{n,0} = \{C_n\}$ and so the theorem holds obviously. By Lemma 4, Theorem 1 holds for $k = 1$. So in the following proof, we assume $k \geq 2$.

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

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

Let $d(u) = t$. Then $t = |N(u)| \geq 3$ and by Lemma 3, $t \leq k+2$. Denote $N(u)\cap V_0 = \{v_1, \cdots, v_r\}$ and $N(u)\setminus V_0 = \{x_1, \cdots, x_{t-r}\}$. Then $t - r = |N(u)\setminus V_0| \geq 2$ and all $d(x_i) = d_i \geq 2$. Let $G' = G - v_1$. Then $G' \in \mathscr{U}_{n-1,k-1}$. Thus

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

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

$$\begin{aligned}
R(G) &\geq \varphi(n,k) + [f(k+1) - f(k+2)] - [f(t-1) - f(t)]\\
&\geq \varphi(n,k).
\end{aligned}$$

The last inequality follows by Lemma 1 as $t \leq k+2$.

In order for the equality to hold, all inequalities in the above argument should be equalities. Thus we have

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

By the induction hypothesis, $G' \cong U_{k-1}^{n-1}$. Note that U_{k-1}^{n-1} has a unique vertex of degree greater than 2. Hence $G \cong U_k^n$ and it is easy to check $R(U_k^n) = \varphi(n,k)$.

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

Choose a vertex $u \in V_1$. Let $d(u) = t$. Then $t \leq k+1$ since $G \in \mathscr{U}_{n,k}$. We consider two 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 $1 \leq p \leq n-k-3$.

If $2 \le p \le n-k-3$, by Lemma 2 (i), then

$$R(U(n,k,p)) - \varphi(n,k) = \frac{k+\frac{1}{\sqrt{2}}}{\sqrt{k+1}} - \frac{k+\sqrt{2}}{\sqrt{k+2}} + \frac{\sqrt{6}-2}{2} > 0.$$

If $p = 1$, then

$$R(U(n,k,1)) - R(U(n,k,2)) = \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{k+1}} - \frac{1}{\sqrt{2}}\right) > 0,$$

and hence $R(U(n,k,1)) > R(U(n,k,2)) > \varphi(n,k)$.

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

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

Denote $N(u) \cap V_0 = \{v_1, \cdots, v_{t-1}\}$, $N(u) \setminus V_0 = \{x_1\}$ and $d(x_1) = d_1 \ge 2$.

If $t = 2$, then let $P = u_0u_1 \cdots u_s$ be a pendant chain with $u_0 = v_1$, $u_1 = u$, $u_2 = x_1$, $s \ge 2$ and $d(u_s) \ge 3$. Let $G' = G - \{u_0, u_1, \cdots, u_{s-1}\}$ and $d(u_s) = d$, then $G' \in \mathscr{U}_{n-s,k-1}$ and $d \le k+2$ by Lemma 3. Denote $N(u_s) \setminus \{u_{s-1}\} = \{y_1, y_2, \cdots, y_{d-1}\}$. Then $d(y_i) \ge 2$ for each $i = 1, 2, \cdots, d-1$ (Otherwise, if there exists some i such that $d(y_i) = 1$. If $N(u_s) \cap V_0 = \{y_1, y_2, \cdots, y_{d-1}\}$, then G is isomorphic to a graph obtained from a star S_k and the path $P = u_0u_1 \cdots u_s$ by identify u_s, the terminus of P, with the central vertex of S_k, a contradiction to $G \in \mathscr{U}_{n,k}$. Then $|N(u_s) \cap V_0| \le d-2$. Hence $|N(u_s) \setminus V_0| \ge 2$, again a contradiction to our assumption in Case 2). Thus

$$\begin{aligned}
R(G) &= R(G') + \frac{1}{\sqrt{2}} + \frac{s-2}{2} + \frac{1}{\sqrt{2d}} + \sum_{i=1}^{d-1} \frac{1}{\sqrt{d(y_i)}}\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}\right) \\
&\ge \varphi(n-s,k-1) + \frac{1}{\sqrt{2}} + \frac{s-2}{2} + \frac{1}{\sqrt{2d}} + \sum_{i=1}^{d-1} \frac{1}{\sqrt{d(y_i)}}\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}\right) \\
&= \varphi(n,k) + \frac{1}{\sqrt{2}} - \frac{1}{2} + \frac{1}{\sqrt{2d}} + \sum_{i=1}^{d-1} \frac{1}{\sqrt{d(y_i)}}\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}\right) \\
&\quad + \frac{k-1+\sqrt{2}}{\sqrt{k+1}} - \frac{k+\sqrt{2}}{\sqrt{k+2}} \\
&\ge \varphi(n,k) + \frac{1}{\sqrt{2}} - \frac{1}{2} + \frac{1}{\sqrt{2d}} + \frac{d-1}{\sqrt{2}}\left(\frac{1}{\sqrt{d}} - \frac{1}{\sqrt{d-1}}\right) + \frac{k-1+\sqrt{2}}{\sqrt{k+1}} - \frac{k+\sqrt{2}}{\sqrt{k+2}} \\
&= \varphi(n,k) + \frac{1}{\sqrt{2}} - \frac{1}{2} + \frac{1}{\sqrt{2}}\left(\sqrt{d} - \sqrt{d-1}\right) + \frac{k-1+\sqrt{2}}{\sqrt{k+1}} - \frac{k+\sqrt{2}}{\sqrt{k+2}} \\
&\ge \varphi(n,k) + \frac{1}{\sqrt{2}} - \frac{1}{2} + \frac{1}{\sqrt{2}}\left(\sqrt{k+2} - \sqrt{k+1}\right) + \frac{k-1+\sqrt{2}}{\sqrt{k+1}} - \frac{k+\sqrt{2}}{\sqrt{k+2}}
\end{aligned}$$

$$
\begin{aligned}
&= \varphi(n,k) + \left(\frac{1}{\sqrt{2}} - 1\right)\left(\frac{k}{\sqrt{k+2}} - \frac{k-1}{\sqrt{k+1}} - \frac{1}{\sqrt{2}}\right) \\
&> \varphi(n,k).
\end{aligned}
$$

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

$$
\begin{aligned}
R(G) &= R(G'') + \frac{t-1}{\sqrt{t}} - \frac{t-2}{\sqrt{t-1}} + \frac{1}{\sqrt{d_1}}\left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}\right) \\
&\geq R(G'') + \frac{t-1}{\sqrt{t}} - \frac{t-2}{\sqrt{t-1}} + \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}\right) \\
&\geq \varphi(n-1,k-1) + \frac{t-1}{\sqrt{t}} - \frac{t-2}{\sqrt{t-1}} + \frac{1}{\sqrt{2}}(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}) \\
&= \varphi(n,k) + \frac{k-1+\sqrt{2}}{\sqrt{k+1}} - \frac{k+\sqrt{2}}{\sqrt{k+2}} + \frac{t-1+\frac{1}{\sqrt{2}}}{\sqrt{t}} - \frac{t-2+\frac{1}{\sqrt{2}}}{\sqrt{t-1}} \\
&\geq \varphi(n,k) + \frac{k-1+\sqrt{2}}{\sqrt{k+1}} - \frac{k+\sqrt{2}}{\sqrt{k+2}} + \frac{\frac{k}{2}+\frac{1}{\sqrt{2}}}{\sqrt{\frac{k}{2}+1}} - \frac{\frac{k}{2}-1+\frac{1}{\sqrt{2}}}{\sqrt{\frac{k}{2}}} \\
&= \varphi(n,k) + \left[\left(1+\frac{k}{\sqrt{2}}\right)(\sqrt{2}-1)\right]\left(\frac{1}{\sqrt{k+1}} - \frac{1}{\sqrt{k+2}}\right) \\
&\quad + \frac{1}{\sqrt{2}}\left(\frac{k}{\sqrt{k+1}} - \frac{k-2+\sqrt{2}}{\sqrt{k}}\right) \\
&> \varphi(n,k) + \frac{1}{\sqrt{2}}\left(\frac{k}{\sqrt{k+1}} - \frac{k-2+\sqrt{2}}{\sqrt{k}}\right) \\
&> \varphi(n,k),
\end{aligned}
$$

where the last and last but third inequalities follow by Lemma 2 (ii) and Lemma 1, respectively.

The proof of the theorem is complete. ∎

3. Remarks

It is easy to check that $\varphi(n,k)$ is strictly monotone decreasing in $k \geq 0$. Note that the set of all unicyclic graphs with n vertices is $\bigcup_{k=0}^{n-3} \mathscr{U}_{n,k}$. Then, by Theorem 1, U_{n-3}^n has the minimum Randić index among unicyclic graphs with n vertices, which is the main result in [6].

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