On the zeroth-order general Randić index of unicycle graphs with k pendant vertices

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Abstract

Let G be a graph. The zeroth-order general Randić index of a graph is defined as $R_\alpha^0(G) = \sum_{v \in V(G)} d^\alpha(v)$, where α is an arbitrary real number and $d(v)$ is the degree of the vertex v in G. In this paper, we give sharp lower and upper bounds for the zeroth-order general Randić index $R_\alpha^0(G)$ among all unicycle graphs G with n vertices and k pendant vertices.

Keywords: Zeroth-order general Randić index; Unicycle graph; Pendant vertex

1. Introduction

Half a century ago, in 1947, Harold Wiener introduced the first chemical index, now called the *Wiener index*. He published papers (see for example [21]) to show that there are excellent correlations between the Wiener index of the molecular graph of an organic compound and a variety of physical and chemical properties of the organic compound. In the past fifty years, a large number of other chemical indices of molecular graphs, including *Merrifield-Simmons index, Hosoya index, Randić index* and *Zagreb indices*,

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have been proposed and widely used in chemistry. In fact, a chemical index is a map from the set of molecular graphs to the real numbers. It has been showed that different indices can indicate different chemical information and describe different properties of chemicals. The chemical indices have been used in the theory of QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship).

The inverse problem for chemical indices is that to find a graph which have some given index value. This problem has been studied by many scholars, for example by Goldman et al. [3] for Wiener index and by Li et al. [13, 15] for Merrifield-Simmons, Zagreb and Zeroth-order general Randić index. All these indices are popular in the study of molecular graphs. In the paper, we are interested in the natural question of finding graphs with minimal or maximal Zeroth-order general Randić index value, given the sizes of the graphs.

Let $G = (V, E)$ be a graph. The Randić index of G defined in [20] is

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-\frac{1}{2}}.$$

Randić showed that the index is well correlated with a variety of Physic-Chemical properties of an alkane. The index $R(G)$ has become one of the most popular molecular descriptors, the interesting reader is referred to [1]-[8], [16]- [20]. The zeroth-order Randić index of G defined by Kier and Hall [11] is $R^0(G) = \sum_{v \in V(G)} d(v)^{-\frac{1}{2}}$. Pavlović [19] determined the unique graph with largest value of $R^0(G)$. In [12], Li et al. investigated the same problem for the topological index $M_1(G)$, also known as Zagreb index, which is defined as $M_1(G) = \sum_{v \in V(G)} d^2(v)$. In 2005, Li et al. [15] defined the zeroth-order general Randić index as $R^0_\alpha(G) = \sum_{v \in V(G)} d^\alpha(v)$, where α is a real number. Then Li and Zhao [14] characterized trees with the first three smallest and largest zeroth-order general Randić index, with the exponent α being equal to k, $-k$, $1/k$ and $-1/k$, where $k \geq 2$ is an integer. In [10], Hua and Deng characterized the unicycle graphs with the maximum and minimum zeroth-order general Randić index. In [9], Hu et al. investigated the molecular graphs having the smallest and largest zeroth-order general Randić index.

Let $G = (V, E)$ be a graph whose vertex set and edge set are $V(G)$ and $E(G)$, respectively. For any $v \in V(G)$, we denote the neighbors of v as $N(v)$, and call $d(v) = |N(v)|$ the degree of v. We call $v \in V(G)$ a pendent vertex if $d(v) = 1$. The graph that arises from G by deleting the edge

$uv \in E$ will be denoted by $G - uv$. Similarly, the graph $G + uv$ arises from G by adding an edge uv between two non-adjacent vertices u and v of G.

Denote, $U(n,k) = \{G \mid G$ is an n-order unicycle graph with k-pendent vertices$\}$. In this paper, we will give sharp lower and upper bounds on the zeroth-order general Randić index of $U(n,k)$.

Let $G \in U(n,k)$. Then $|E(G)| = |V(G)| = n$. If $\alpha = 0$ or $\alpha = 1$, then $R_0^0(G) = \sum_{v \in V(G)} d^0(v) = n$ and $R_1^0(G) = \sum_{v \in V(G)} d^1(v) = 2n$, respectively. On the other hand, If $k = 0$, G is just a cycle, and then $R_\alpha^0(G) = 2^\alpha n$. So we always assume that $\alpha \neq 0,\ 1$ and $k \neq 0$ throughout this paper.

2. Lemmas

Let $G \in U(n,k)$. Denote the cycle in G as C, and $Pen(G) = \{v \mid v$ is a pendent vertex in $G\}$. Firstly, we will give some lemmas which will be used in Section 3.

Lemma 2.1 *Let $G \in U(n,k)$ and $A = \{v \in V(C) \mid d(v) \geq 3\}$. If $R_\alpha^0(G)$ is as small as possible for $0 < \alpha < 1$ or $R_\alpha^0(G)$ is as large as possible for $\alpha > 1$ or $\alpha < 0$, then $|A| = 1$.*

Proof. Since $k \neq 0$, $|A| \geq 1$. Suppose $|A| > 1$. Then there exist $u_1, u_2 \in V(C)$ such that $d(u_1) \geq d(u_2) \geq 3$. Assume $N(u_2) - V(C) = \{v_1, v_2, \cdots, v_t\}$. Then $t \geq 1$. Obviously, $u_1 v_1 \notin E(G)$ by $v_1 \notin V(C)$ and $G \in U(n,k)$. Let

$$G' = G - v_1 u_2 + v_1 u_1.$$

Then $G' \in U(n,k)$ and

$$\begin{aligned} R_\alpha^0(G') - R_\alpha^0(G) &= [(d(u_1)+1)^\alpha + (d(u_2)-1)^\alpha] - [d^\alpha(u_1) + d^\alpha(u_2)] \\ &= [(d(u_1)+1)^\alpha - d^\alpha(u_1)] - [d^\alpha(u_2) - (d(u_2)-1)^\alpha] \\ &= \alpha(\zeta^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $d(u_1) < \zeta < d(u_1) + 1$ and $d(u_2) - 1 < \eta < d(u_2)$. Since $d(u_1) \geq d(u_2)$, we have $d(u_2) - 1 < \eta < d(u_2) \leq d(u_1) < \zeta < d(u_1) + 1$. Thus, we have $R_\alpha^0(G') < R_\alpha^0(G)$ for $0 < \alpha < 1$, and $R_\alpha^0(G') > R_\alpha^0(G)$ for $\alpha > 1$ or $\alpha < 0$, a contradiction. ■

Lemma 2.2 *Let $G \in U(n,k)$ and $B = \{v \in V(G) \mid d(v) \geq 3\}$. If $R_\alpha^0(G)$ is as small as possible for $0 < \alpha < 1$ or $R_\alpha^0(G)$ is as large as possible for $\alpha > 1$ or $\alpha < 0$, then $|B| = 1$.*

Proof. Choose $G \in U(n,k)$ such that $R_\alpha^0(G)$ is as small as possible for $0 < \alpha < 1$ or $R_\alpha^0(G)$ is as large as possible for $\alpha > 1$ or $\alpha < 0$.

By Lemma 2.1, we can assume that $V(C) = \{v_1, v_2, \cdots, v_s\}$ with $d(v_1) \geq 3$ and $d(v_2) = \cdots = d(v_s) = 2$.

Suppose $|B| \geq 2$. Then there exists $v_x \in V(G) - V(C)$ such that $d(v_x) \geq 3$. Assume that $N(v_x) = \{u_1, u_2, \cdots, u_t\}$, then $t \geq 3$. Since $G \in U(n,k)$ and $d(v_2) = \cdots = d(v_s) = 2$, there exists an unique path $l(v_1, v_x)$ between v_1 and v_x. Assume, without loss of generality, that $u_t \in l(v_1, v_x)$. Then $u_1, u_2, \cdots, u_{t-1} \notin l(v_1, v_x)$. Since $G \in U(n,k)$, $v_1u_1, v_1u_2, \cdots, v_1u_{t-1} \notin E(G)$. Now we consider the following two cases.

Case 1. $d(v_1) \geq d(v_x)$.

In the case, let $G' = G - v_xu_1 + v_1u_1$, then $G' \in U(n,k)$, and

$$\begin{aligned} R^0_\alpha(G') - R^0_\alpha(G) &= [(d(v_1)+1)^\alpha + (d(v_x)-1)^\alpha] - [d^\alpha(v_1) + d^\alpha(v_x)] \\ &= \alpha(\zeta^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $d(v_1) < \zeta < d(v_1)+1$ and $d(v_x)-1 < \eta < d(v_x)$. Since $d(v_x) \leq d(v_1)$, we have $d(v_x) - 1 < \eta < d(v_x) \leq d(v_1) < \zeta < d(v_1) + 1$. Thus we have $R^0_\alpha(G') < R^0_\alpha(G)$ for $0 < \alpha < 1$ and $R^0_\alpha(G') > R^0_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$, a contradiction.

Case 2. $d(v_1) < d(v_x) = t$.

Let $G' = G - v_xu_2 - \cdots - v_xu_{t-1} + v_1u_2 + \cdots + v_1u_{t-1}$. Then $G' \in U(n,k)$ and

$$\begin{aligned} & R^0_\alpha(G') - R^0_\alpha(G) \\ = \; & [(d(v_1)+t-2)^\alpha + (d(v_x)-t+2)^\alpha] - [d^\alpha(v_1) + d^\alpha(v_x)] \\ = \; & [(d(v_1)+t-2)^\alpha - t^\alpha] - [d^\alpha(v_1) - 2^\alpha] \\ = \; & \alpha(d(v_1)-2)(\zeta^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $t = d(v_x) < \zeta < d(v_1)+t-2$ and $2 < \eta < d(v_1)$. Since $d(v_1) < d(v_x)$, we have $2 < \eta < d(v_1) < d(v_x) < \zeta < d(v_1) + t - 2$. Thus we have $R^0_\alpha(G') < R^0_\alpha(G)$ for $0 < \alpha < 1$, and $R^0_\alpha(G') > R^0_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$, a contradiction. ∎

Let $G \in U(n,k)$. Set

$$V_1 = \left\{ v \in V(G) \mid d(v) = \left[\frac{2n-k}{n-k}\right] \right\},$$

$$V_2 = \left\{ v \in V(G) \mid d(v) = \left[\frac{2n-k}{n-k}\right] + 1 \right\}.$$

Lemma 2.3 *Let $G \in U(n,k)$. If $R^0_\alpha(G)$ is as large as possible for $0 < \alpha < 1$ or $R^0_\alpha(G)$ is as small as possible for $\alpha > 1$ or $\alpha < 0$, then $|V_1| = (n-k)\left\lceil \frac{2n-k}{n-k} \right\rceil - n$ and $|V_2| = 2n - k - (n-k)\left\lceil \frac{2n-k}{n-k} \right\rceil$.*

Proof. Let $G \in U(n,k)$ such that $R^0_\alpha(G)$ is as large as possible for $0 < \alpha < 1$ or $R^0_\alpha(G)$ is as small as possible for $\alpha > 1$ or $\alpha < 0$. Now we consider two cases.

Case 1. $\frac{2n-k}{n-k}$ is an integer.

In the case, we just need to show $|V_1| = n-k$ and $|V_2| = 0$.

Suppose there exists a vertex $v_1 \in V(G) - Pen(G)$ such that $d(v_1) \neq \frac{2n-k}{n-k}$, say $2 \leq d(v_1) < \frac{2n-k}{n-k}$.

Since $\sum_{v \in V(G)-Pen(G)} d(v) = 2n-k$, there exists a vertex $v_2 \in V(G) - Pen(G)$, such that $d(v_2) \geq \frac{2n-k}{n-k} + 1 > 3$. Set $N(v_2) = \{u_1, u_2, \cdots, u_s\}$. Then $s \geq 4$.

Subcase 1.1 $v_2 \notin V(C)$.

Since $G \in U(n,k)$, there is an unique path $l(v_2, C)$ from v_2 to C. Without loss of generality, we can assume $u_s \in l(v_2, C)$, then $u_1, u_2, \cdots, u_{s-1} \notin l(v_2, C) \cup V(C)$.

If $v_1 = u_s$, then let $G' = G - u_1v_2 + u_1v_1$.

If $v_1 \in N(v_2) - \{u_s\}$, say $v_1 = u_1$, then let $G' = G - u_2v_2 + u_2v_1$.

Suppose $v_1 \in V(G) - N(v_2)$. Since $G \in U(n,k)$ and $v_2 \notin V(C)$, $G - v_2$ is disconnected. Assume, without loss of generality, that v_1 and u_1 are in the different components in $G - v_2$. Then let $G' = G - u_1v_2 + u_1v_1$.

Subcase 1.2 $v_2 \in V(C)$.

In the case, we can assume that $u_1, u_2 \in V(C) \cap N(v_2)$. Then $u_3 \notin V(C)$.

If $v_1 \in V(C)$, then let $G' = G - u_3v_2 + u_3v_1$.

If $v_1 \notin V(C)$, then we can assume $v_1u_1 \notin E(G)$ and let $G' = G - u_1v_2 + u_1v_1$.

In all cases, we have $G' \in U(n,k)$ by $d(v_2) = s \geq 4$ and $d(v_1) \geq 2$. Thus

$$\begin{aligned} R^0_\alpha(G') - R^0_\alpha(G) &= [(d(v_1)+1)^\alpha + (d(v_2)-1)^\alpha] - [d^\alpha(v_1) + d^\alpha(v_2)] \\ &= [(d(v_1)+1)^\alpha - d^\alpha(v_1)] - [d^\alpha(v_2) - (d(v_2)-1)^\alpha] \\ &= \alpha(\zeta^{\alpha-1} - \eta^{\alpha-1}) \end{aligned}$$

where $d(v_1) < \zeta < d(v_1)+1$ and $d(v_2) - 1 < \eta < d(v_2)$. Since $d(v_1) + 1 \leq$

$d(v_2) - 1$, we have $d(v_1) < \zeta < d(v_1) + 1 \leq d(v_2) - 1 < \eta < d(v_2)$. Thus we have $R^0_\alpha(G') > R^0_\alpha(G)$ for $0 < \alpha < 1$, and $R^0_\alpha(G') < R^0_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$, a contradiction.

Case 2. $\frac{2n-k}{n-k}$ is not an integer.

In the case, we just need to show that for every $v \in V(G) - Pen(G)$,

$$\left\lceil \frac{2n-k}{n-k} \right\rceil \leq d(v) \leq \left\lceil \frac{2n-k}{n-k} \right\rceil + 1.$$

Suppose, without loss of generality, that there exists a vertex $v_1 \in V(G) - Pen(G)$ such that $2 \leq d(v_1) < \left\lceil \frac{2n-k}{n-k} \right\rceil$.

By $\sum_{v \in V(G)-Pen(G)} d(v) = 2n - k$, there exists a vertex $v_2 \in V(G) - Pen(G)$ such that $d(v_2) > \left\lceil \frac{2n-k}{n-k} \right\rceil + 1 \geq 3$. Set $N(v_2) = \{u_1, u_2, \cdots, u_s\}$. Then $s \geq 4$.

By the same argument as that of proof in Case 1, we can derive a contradiction.

From the proof above, we know that $|V_1| + |V_2| = n - k$. On the other hand,

$$|V_1| \left\lceil \frac{2n-k}{n-k} \right\rceil + |V_2| \left(\left\lceil \frac{2n-k}{n-k} \right\rceil + 1 \right) = 2n - k$$

Solving the equation, we get

$$|V_1| = (n-k) \left\lceil \frac{2n-k}{n-k} \right\rceil - n \quad and \quad |V_2| = 2n - k - (n-k) \left\lceil \frac{2n-k}{n-k} \right\rceil.$$

Thus the conclusions of our theorem hold. ■

3. Main results

In this section, we use $U(n,k)$ to denote the set of unicycle graphs of order n with k pendent vertices. Let $G \in U(n,k)$ and $d(v_0) = \max\{d(v) | \, v \in V(G)\}$. Denote

$$\Theta = \{G \in U(n,k) | \, d(v_0) = k+2, \; d(v) = 2 \text{ for } v \in V(G) \backslash (Pen(G) \cup \{v_0\})\}.$$

Then we have the following result.

Theorem 3.1 *Let $G \in G(n,k)$. Then*

$$R^0_\alpha(G) \geq (k+2)^\alpha + (n-k-1)2^\alpha + k \qquad for \quad 0 < \alpha < 1$$

and

$$R^0_\alpha(G) \le (k+2)^\alpha + (n-k-1)2^\alpha + k \qquad \textit{for} \quad \alpha > 1 \ \textit{ or } \ \alpha < 0.$$

The equalities hold if and only if $G \in \Theta$.

Proof. Choose $G' \in U(n,k)$ such that $R^0_\alpha(G')$ is as small as possible for $0 < \alpha < 1$ or $R^0_\alpha(G')$ is as large as possible for $\alpha > 1$ or $\alpha < 0$. By Lemma 2.2, there exists unique vertex $v_n \in V(G')$ such that $d(v_n) \ge 3$. Since $G' \in U(n,k)$, we have $G' \in \Theta$. Note that $R^0_\alpha(G') = (k+2)^\alpha + (n-k-1)2^\alpha + k$. Thus the conclusions of our theorem hold. ■

Let $G \in U(n,k)$ and $\gamma = \left[\frac{2n-k}{n-k}\right]$. Set

$$V_1 = \{v \in V(G) \mid d(v) = \gamma\} \quad \textit{and} \quad V_2 = \{v \in V(G) \mid d(v) = \gamma + 1\}.$$

Let $n_1 = (n-k)\gamma - n$ and $n_2 = 2n - k - (n-k)\gamma$. Denote

$$\Omega = \{G \in U(n,k) | V = V_1 \cup V_2 \cup Pen(G) \text{ and } |V_1| = n_1, |V_2| = n_2\}.$$

Theorem 3.2 *Let $G \in U(n,k)$. Denote $\gamma = \left[\frac{2n-k}{n-k}\right]$. Then*

$$R^0_\alpha(G) \le ((n-k)\gamma - n)\gamma^\alpha + (2n-k-(n-k)\gamma)(\gamma+1)^\alpha + k, \textit{for } 0 < \alpha < 1$$

and

$$R^0_\alpha(G) \ge ((n-k)\gamma - n)\gamma^\alpha + (2n-k-(n-k)\gamma)(\gamma+1)^\alpha + k, \textit{for } \alpha > 1 \textit{ or } \alpha < 0.$$

The equalities hold if and only if $G \in \Omega$.

Proof. Choose $G' \in G(n,k)$ such that $R^0_\alpha(G')$ is as large as possible for $0 < \alpha < 1$ or $R^0_\alpha(G')$ is as small as possible for $\alpha > 1$ or $\alpha < 0$. By Lemma 2.3, we have

$$|V_1(G')| = (n-k)\left[\frac{2n-k}{n-k}\right] - n = (n-k)\gamma - n,$$

$$|V_2(G')| = 2n - k - (n-k)\left[\frac{2n-k}{n-k}\right] = 2n - k - (n-k)\gamma.$$

Since $G' \in U(n,r)$, we have $G' \in \Omega$. Note that

$$R^0_\alpha(G') = ((n-k)\gamma - n)\gamma^\alpha + (2n-k-(n-k)\gamma)(\gamma+1)^\alpha + k.$$

Thus the conclusions of our theorem hold. ■

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