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UNICYCLE GRAPHS WITH THE FIRST THREE EXTREMAL ZEROTH-ORDER GENERAL RANDIĆ INDICES

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Abstract

Let $G = (V, E)$ be a graph and d_v the degree of the vertex v. The zeroth-order general Randić index of G is defined as: $R_{\alpha}^{0}(G) = \sum_{v \in V} d_v^{\alpha}$, where α is an arbitrary real number. In this paper, we characterize the unicycle graphs of order n with the first three largest and the first three smallest zeroth-order general Randić indices.

1. Introduction

Let $G = (V(G), E(G))$ denote a graph with $V(G)$ as the set of vertices and $E(G)$ as the set of edges. $N_G(v_i)$ denotes the neighbors of v_i. The Randić index of G defined in [13] is

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

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where $d_v = d_G(v)$ denotes the degree of the vertex v in G. Randić demonstrated that his 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 [1-3, 11-13]. Eventually, countless research papers are devoted. The zeroth-order Randić index $R^0(G)$ of G defined by Kier and Hall [8] is $R^0(G) = \sum_{v \in V(G)} \frac{1}{\sqrt{d_v}}$. Pavlović [11] gave the unique graph with largest value of $R^0(G)$. In [5], Lielal investigated the same problem for the topological index $M_1(G)$, also known as the first Zagreb index [14], which is defined as $M_1(G) = \sum_{v \in V(G)} d_v{}^2$. Li and Zheng [10] defined the zeroth-order general Randić index of a graph G as :

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

where α is a real number. For α being one of $m, -m, \frac{1}{m}, -\frac{1}{m}$, where $m \geq 2$ is an integer, Li and Zhao [9] characterized the trees with the first three largest and smallest zeroth-order general Randić index; Wang and Deng [15] characterized the unicycle graphs with the maximum zeroth-order General Randić index. Hu et al. [6] characterized the molecular (n, m)-graphs with the smallest and greatest R_α^0. Hua and Deng [7] characterized the unicycle graphs with the smallest and greatest R_α^0.

In this paper, we investigate the zeroth-order general Randić index for the unicycle graphs. All unicycle graphs with the first three largest and the first three smallest zeroth-order general Randić index are characterized.

All graphs considered here are both finite and simple. We denote the star, path and cycle of order n by S_n, P_n and C_n, respectively. Let $G = (V, E)$ be an unicycle graph of order n with its unique cycle $C_r = v_1 v_2$

$\cdots v_r v_1$ of length r, $T_1, T_2, \cdots, T_k (0 \le k \le r)$ are the all nontrivial components (they are all nontrivial trees) of $G - E(C_r)$, u_i is the common vertex of T_i and C_r, $i = 1, 2, \cdots, k$. Such an unicycle graph is denoted by $C_r^{u_1, u_2, \cdots, u_k}(T_1, T_2, \cdots, T_k)$. Let $n(T_i) = l_i + 1$ be the number of vertices in tree T_i, then $l = n - r = l_1 + l_2 + l_3 + \cdots + l_k$.

Specially, $u_1, u_2, \cdots, u_k$ are the centers of $S_{l_1+1}, S_{l_2+1}, \cdots, S_{l_k+1}$, respectively, in

$$G_1 = C_r^{u_1, u_2, \cdots, u_k}(S_{l_1+1}, S_{l_2+1}, \cdots, S_{l_k+1})$$

and $u_1, u_2, \cdots, u_k$ are the end-vertices of $P_{l_1+1}, P_{l_2+1}, \cdots, P_{l_k+1}$, respectively, in

$$G_2 = C_r^{u_1, u_2, \cdots, u_k}(P_{l_1+1}, P_{l_2+1}, \cdots, P_{l_k+1}).$$

We also denote $C_3^{u_1}(S_{n-2})$ by $S_n + e$. $C_3^{u_1}(P_{n-2})$ is simplified by $C_3(P_{n-2})$.

$D(G) = [d_1, d_2, \cdots, d_n]$ denotes the degree sequence of a graph G, and $D(G) = [x_1^{a_1}, x_2^{a_2}, \cdots, x_i^{a_i} \cdots, x_t^{a_t}]$, $x_i^{a_i}$ means that G has a_i vertices of degree x_i, $i = 1, 2, \cdots, t$.

Undefined notations and terminology will conform to those in [9].

2. The Unicycle Graphs with the First Three Largest (Smallest) Zeroth-Order General Randić Indices for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$

We first introduce three transfer operation.

Transfer operation *A*. Let G be an unicycle graph of order n. If there are vertices u and v such that $d_u = p > 1$, $d_v = q > 1$, $p \le q$, and $u_1, u_2, \cdots, u_k$ are the neighbors of u. Then G is changed into G' after the transfer operation A, where $G' = G - \{uu_1, uu_2, \cdots, uu_k\} + \{vu_1, vu_2, \cdots, vu_k\}$, $1 \le k \le p$. As shown in Figure 1.

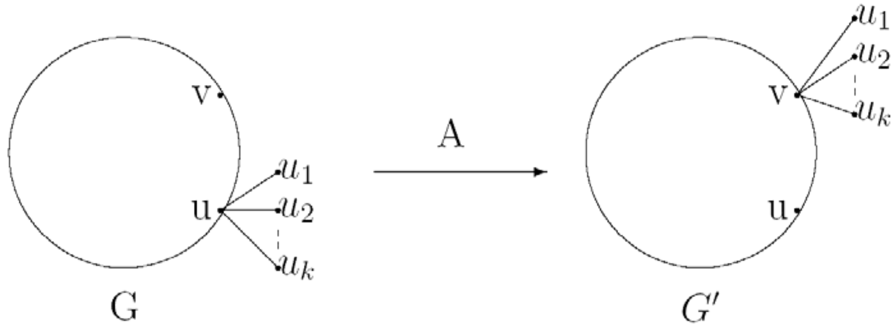

Figure 1. Transfer operation A.

Lemma 2.1. *For the two graphs G and G' above, we have*

(i) $R_\alpha^0(G') > R_\alpha^0(G)$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G') < R_\alpha^0(G)$ for $0 < \alpha < 1$.

Proof. By the definition of $R_\alpha^0(G)$, we have

$$\begin{aligned}\Delta &= R_\alpha^0(G') - R_\alpha^0(G)\\ &= [(p-k)^\alpha + (q+k)^\alpha] - [p^\alpha + q^\alpha]\\ &= [(q+k)^\alpha - q^\alpha] - [p^\alpha - (p-k)^\alpha]\\ &= \alpha \cdot k(\xi^{\alpha-1} - \eta^{\alpha-1}),\end{aligned}$$

where $\eta \in (p-k, p)$, $\xi \in (q, q+k)$. $\xi > \eta$ since $p \le q$. Then $\Delta > 0$ when $\alpha > 1$ or $\alpha < 0$; $\Delta < 0$ when $0 < \alpha < 1$. The proof of Lemma 2.1 is completed.

Remark. Repeating operation A, any unicycle graph of order n can be changed into an unicycle graph which has at most one vertex with degree greater than 2 such as $C_r^{u_1}(T_1)$.

Transfer operation *B*. Let G be an unicycle graph of order n, uv is an edge of G. $d_G(u) = p \geq 3$. $N_G(v)$ is the neighbors of v, and $N_G(v) - \{u\} = \{w_1, w_2, \cdots, w_l\}$. Then G is changed into G'' first and, then into G' after operation B, where $G' = G - \{vw_1, vw_2, \cdots, vw_l\} + \{uw_1, uw_2, \cdots, uw_l\}$, $G'' = G - \{vw_2, vw_3, \cdots, vw_l\} + \{uw_2, uw_3, \cdots, uw_l\}$. As shown in Figure 2.

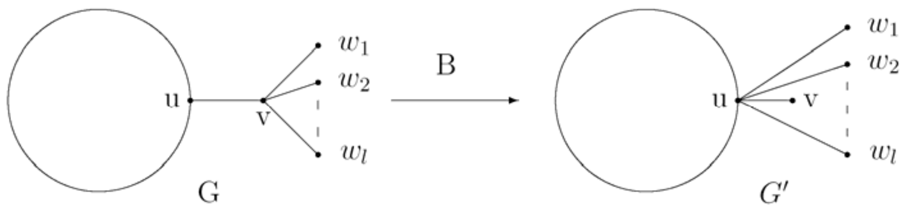

Figure 2. Transfer operation B.

Lemma 2.2 . *For the three graphs* G, G' *and* G'' *above, we have*

(i) $R_\alpha^0(G') > R_\alpha^0(G'') > R_\alpha^0(G)$ *for* $\alpha > 1$ *or* $\alpha < 0$;

(ii) $R_\alpha^0(G') < R_\alpha^0(G'') < R_\alpha^0(G)$ *for* $0 < \alpha < 1$.

Proof. If $p \geq l + 1$, then

$$\begin{aligned}\Delta &= R_\alpha^0(G'') - R_\alpha^0(G)\\ &= [(p + l - 1)^\alpha + 2^\alpha] - [p^\alpha + (l + 1)^\alpha]\\ &= [(p + l - 1)^\alpha - p^\alpha] - [(l + 1)^\alpha - 2^\alpha]\\ &= \alpha(l - 1)(\xi^{\alpha - 1} - \eta^{\alpha - 1}),\end{aligned}$$

where $\eta \in (2, l + 1)$, $\xi \in (p, p + l - 1)$.

If $p \leq l + 1$, then

$$\begin{aligned}\Delta &= R_\alpha^0(G'') - R_\alpha^0(G)\\ &= [(p + l - 1)^\alpha + 2^\alpha] - [p^\alpha + (l + 1)^\alpha]\end{aligned}$$

$$= [(p + l - 1)^{\alpha} - (l + 1)^{\alpha}] - [p^{\alpha} - 2^{\alpha}]$$

$$= \alpha(p - 2)(\xi^{\alpha-1} - \eta^{\alpha-1}),$$

where $\eta \in (2,\ p)$, $\xi \in (l + 1,\ p + l - 1)$.

And $\xi > \eta$. $\Delta > 0$ when $\alpha > 1$ or $\alpha < 0$; $\Delta < 0$ when $0 < \alpha < 1$. The proof of Lemma 2.2 is completed.

Remark. Repeating the operation B, any unicycle graph $G = C_r^{u_1, u_2, \cdots, u_k}(T_1, T_2, \cdots, T_k)$ can be changed into $C_r^{u_1, u_2, \cdots, u_k}(S_{l_1}, S_{l_2}, \cdots, S_{l_k})$.

So, an unicycle graph $G = C_r^{u_1, u_2, \cdots, u_k}(T_1, T_2, \cdots, T_k)$ can be changed into $G' = C_r^{u_1}(S_{n-r+1})$ after the operations B and A.

Transfer operation *C*. Let G be an unicycle graph of order n. $C_r = u_1 u_2 \cdots u_r u_1$ is the unique cycle of G. $e = xy$ is a pedant edge of G, and $d_y = 1$, $d_x \geq 2$. Then G is changed into G' after the transfer operation C, where $G' = G - \{xy,\ u_i u_{i+1}\} + \{u_i y,\ u_{i+1} y\}$. As shown in Figure 3.

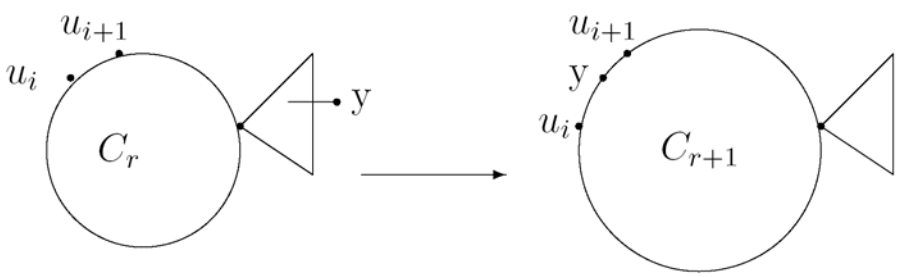

Figure 3. Transfer operation C.

Lemma 2.3. *For the two graphs G and G' above, we have*

(i) $R_{\alpha}^{0}(G') \leq R_{\alpha}^{0}(G)$ *for* $\alpha > 1$ *or* $\alpha < 0$;

(ii) $R_{\alpha}^{0}(G') \geq R_{\alpha}^{0}(G)$ *for* $0 < \alpha < 1$, with the equality if and only if $d_x = 2$.

Proof. By the definition of $R_\alpha^0(G)$, we have

$$\begin{aligned}\Delta &= R_\alpha^0(G') - R_\alpha^0(G)\\ &= [(d_x - 1)^\alpha + 2^\alpha] - [d_x^\alpha + 1^\alpha]\\ &= [2^\alpha - 1^\alpha] - [d_x^\alpha - (d_x - 1)^\alpha]\\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}),\end{aligned}$$

where $\eta \in (d_x - 1, d_x)$, $\xi \in (1, 2)$. $\xi < \eta$ since $d_x \geq 2$. $\Delta < 0$ when $\alpha > 1$ or $\alpha < 0$; $\Delta > 0$ when $0 < \alpha < 1$. The proof of Lemma 2.3 is completed.

From Lemma 2.3, we know that $R_\alpha^0(C_r^{u_1}(S_{n-r+1}))$, $3 \leq r \leq n$, is the monotone function of r:

If $3 \leq r \leq r' \leq n$, then

(i) $R_\alpha^0(C_r^{u_1}(S_{n-r+1})) > R_\alpha^0(C_r^{u_1}(S_{n-r'+1}))$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(C_r^{u_1}(S_{n-r+1})) < R_\alpha^0(C_{r'}^{u_1}(S_{n-r'+1}))$ for $0 < \alpha < 1$.

The following result is immediate from the Lemmas above.

Theorem 2.4 ([7]). *Among all unicycle graphs of order n,*

(i) $G = C_3(S_{n-2})$ *is the unique unicycle graph with the largest zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$;

(ii) $G = C_3(S_{n-2})$ *is the unique unicycle graph with the smallest zeroth-order general Randić index for* $0 < \alpha < 1$.

In the following, we consider the unicycle graphs with the second and the third largest zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$.

For any unicycle graph $G = C_r^{u_1, u_2, \cdots, u_k}(T_1, T_2, \cdots, T_k)$, by the transfer operation B, there is an unicycle graph $G' = C_r^{u_1, u_2, \cdots, u_k}(S_{l_1+1}, S_{l_2+1}, \cdots, S_{l_k+1})$ such that

(i) $R_\alpha^0(G') \geq R_\alpha^0(G)$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G') \leq R_\alpha^0(G)$ for $0 < \alpha < 1$.

Furthermore, if $k \geq 4$, then, by the transfer operations A and C, there is an unicycle graph $G'' = C_3^{u_1, u_2, u_3}(S_{l'_1+1}, S_{l'_2+1}, S_{l'_3+1})$ such that

(i) $R_\alpha^0(G'') \geq R_\alpha^0(G')$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G'') \leq R_\alpha^0(G')$ for $0 < \alpha < 1$.

Let

$$\mathcal{G}_1 = \{C_3^{u_1, u_2, u_3}(S_{l_1+1}, S_{l_2+1}, S_{l_3+1}) | l_i \geq 1, i = 1, 2, 3, l_1 + l_2 + l_3 = n - 3\},$$

$$\mathcal{G}_2 = \{C_r^{u_1, u_2}(T_1, T_2) | 3 \leq r \leq 4, l_i \geq 1, i = 1, 2, l_1 + l_2 = n - r\},$$

$$\mathcal{G}_3 = \{C_r^{u_1}(T_1) | 3 \leq r \leq 5, l_1 = n - r\}.$$

By the transfer operation A, we know that

(i) the largest value of zeroth-order general Randić indices of the unicycle graphs in $\mathcal{G}_1$ is not more than the third largest value of zeroth-order general Randić indices of all unicycle graphs for $\alpha > 1$ or $\alpha < 0$, and the smallest value of zeroth-order general Randić indices of the unicycle graphs in $\mathcal{G}_1$ is not less than the third smallest value of zeroth-order general Randić indices of all unicycle graphs for $0 < \alpha < 1$;

(ii) the largest value of zeroth-order general Randić indices of the unicycle graphs in $\mathcal{G}_2$ is not more than the second largest value of zeroth-order general Randić indices of all unicycle graphs for $\alpha > 1$ or $\alpha < 0$, and the smallest value of zeroth-order general Randić indices of the unicycle graphs in $\mathcal{G}_2$ is not less than the second smallest value of zeroth-order general Randić indices of all unicycle graphs for $0 < \alpha < 1$.

Therefore, in order to find the unicycle graph with the second and the third largest (smallest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$, we only need to find

(i) the unicycle graph with the largest (smallest) zeroth-order general Randić index in $\mathcal{G}_1$ for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$; and

(ii) the unicycle graphs with the first two largest (smallest) zeroth-order general Randić index in $\mathcal{G}_2$ for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$; and

(iii) the unicycle graph with the first three largest (smallest) zeroth-order general Randić index in $\mathcal{G}_3$ for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ and, then compare them in turn.

From the transfer operation *A*, it is immediate that

Lemma 2.5. (i) *The unicycle graph in* $\mathcal{G}_1$ *with the largest* (*smallest*) *zeroth-order general Randić index for* $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ is $G_1 = C_3^{u_1, u_2, u_3}(S_2, S_2, S_{n-4})$.

(ii) *The unicycle graph in* $\mathcal{G}_2$ *with the largest* (*smallest*) *zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$ $(0 < \alpha < 1)$ *is* $G_{10} = C_3^{u_1, u_2}(S_2, S_{n-3})$.

(iii) *The unicycle graph in* $\mathcal{G}_3$ *with the largest* (*smallest*) *zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$ $(0 < \alpha < 1)$ *is* $G_2 = C_3(S_{n-2})$, *it is also the unicycle graph with the largest* (*smallest*) *zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$ $(0 < \alpha < 1)$ *among all unicycle graphs of order n*.

Lemma 2.6. *The unicycle graph* $\mathcal{G}_2$ *with the second largest* (*smallest*) *zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$ $(0 < \alpha < 1)$ *is* $G_{11} = C_3^{u_1, u_2}(S_3, S_{n-4})$.

Proof. Let $G = C_r^{u_1, u_2}(T_1, T_2) \in \mathcal{G}_2$, $3 \leq r \leq 4$, $G \neq C_3^{u_1, u_2}(S_2, S_{n-3})$.

Case 1. If $r = 3$, then $\{T_1, T_2\} \neq \{S_2, S_{n-3}\}$.

(1) $\{T_1, T_2\} = \{S_{l_1+1}, S_{l_2+1}\}$, where $l_1 \geq 2$, $l_2 \geq 2$, $l_1 + l_2 = n - 2$, and u_1, u_2 are the centers of T_1 and T_2, respectively. By the transfer operation A, we have

(1) $R_\alpha^0(G) \leq R_\alpha^0(G_{11})$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G) \geq R_\alpha^0(G_{11})$ for $0 < \alpha < 1$,

where $G_{11} = C_3^{u_1, u_2}(S_3, S_{n-4})$, as shown in Figure 4.

(2) Otherwise, by the transfer operations A and B, we have

(i) $R_\alpha^0(G) \leq R_\alpha^0(G')$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G) \geq R_\alpha^0(G')$ for $0 < \alpha < 1$,

where $G' = G_{11}$ or G_{12}, as shown in Figure 4.

Case 2. If $r = 4$, then by the transfer operations A and B, we have

(i) $R_\alpha^0(G) \leq R_\alpha^0(G')$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G) \geq R_\alpha^0(G')$ for $0 < \alpha < 1$,

where $G' = G_{13}$ or G_{14}, as shown in Figure 4. Continuing the transfer operation C, we have

(i) $R_\alpha^0(G') \leq R_\alpha^0(G_{11})$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G') \geq R_\alpha^0(G_{11})$ for $0 < \alpha < 1$.

Finally, comparing the zeroth-order general Randić indices of G_{11}, and G_{12} we have

(i) $R_\alpha^0(G_{12}) < R_\alpha^0(G_{11})$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G_{12}) > R_\alpha^0(G_{11})$ for $0 < \alpha < 1$.

The proof of Lemma 2.6 is completed.

Similarly, the unicycle graph in $\mathcal{G}_3$ with the second largest (smallest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ is G_3 and G_7. The unicycle graph in $\mathcal{G}_3$ with the third largest (smallest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ is one of G_4, G_5 and G_6. Comparing the zeroth-order general Randić indices of G_4, G_5 and G_6, we have

Lemma 2.7. (i) *The unicycle graph in* $\mathcal{G}_3$ *with the second largest* (*smallest*) *zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$ $(0 < \alpha < 1)$ *is* G_3 *or* G_7;

(ii) *The unicycle graph in* $\mathcal{G}_3$ *with the third largest* (*smallest*) *zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$ $(0 < \alpha < 1)$ *is* G_5.

Comparing the zeroth-order general Randić indices of G_3, G_7, G_1, G_{10} and G_{11}, we have

Theorem 2.8. *Among all unicycle graphs of order n*,

(i) *The unicycle graph with the second largest* (*smallest*) *zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$ $(0 < \alpha < 1)$ *is* G_{10};

(ii) *The unicycle graph with the third largest* (*smallest*) *zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$ $(0 < \alpha < 1)$ *is* G_3 *or* G_7.

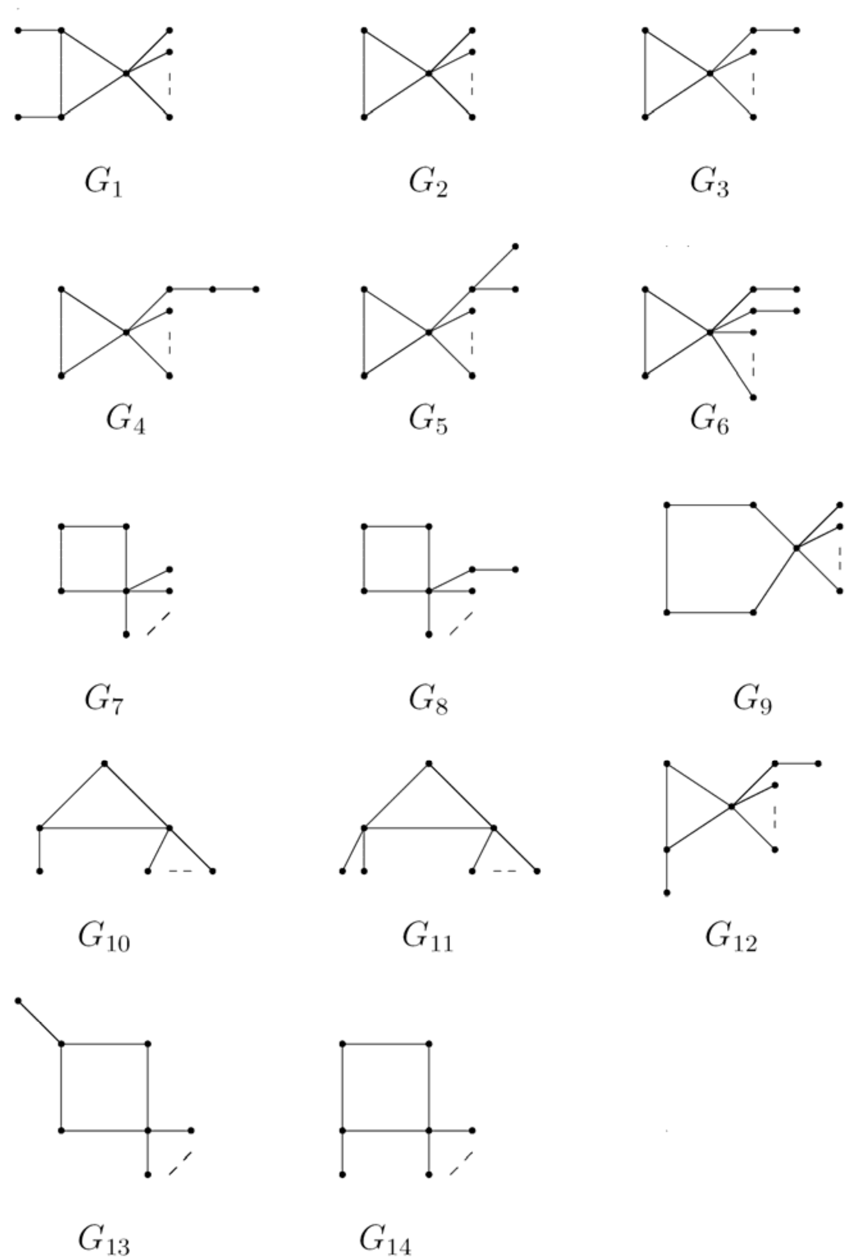

Figure 4.

3. The Unicycle Graphs with the First Three Smallest (Largest) Values of Zeroth-Order Randić Index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$

For convenience, we introduce some new transfer operations.

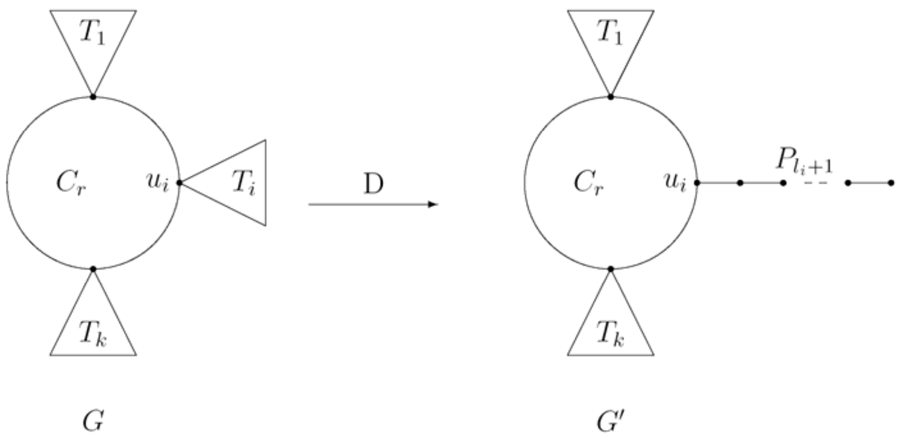

Figure 5. Transfer operation D.

Transfer operation *D*. Let $G = C_r^{u_1, u_2, \cdots, u_k}(T_1, \cdots, T_i, \cdots, T_k)$, $k \geq 1$. If T_i is not a path, or T_i is a path and u_i is not the end-vertex of the path, then G can be changed into $G' = C_r^{u_1, \cdots, u_i, \cdots, u_k}(T_1, \cdots, P_{l_i+1}, \cdots, T_k)$ after the transfer operation D, where $l_i + 1 = n(T_i)$ and u_i is the end-vertex of P_{l_i+1}, as shown in Figure 5.

Lemma 3.1. *For the two graphs G and G' above, we have*

(i) $R_\alpha^0(G') < R_\alpha^0(G)$ *for* $\alpha > 1$ *or* $\alpha < 0$;

(ii) $R_\alpha^0(G') > R_\alpha^0(G)$ *for* $0 < \alpha < 1$.

Proof. By the definition of $R_\alpha^0(G)$, we have

$$\begin{aligned}\Delta &= R_\alpha^0(G) - R_\alpha^0(G') \\ &= R_\alpha^0(T_i) - R_\alpha^0(P_{l_i+1}) + [(p+2)^\alpha - 3^\alpha] - [p^\alpha - 1^\alpha]\end{aligned}$$

$$= R_\alpha^0(T_i) - R_\alpha^0(P_{l_i+1}) + [(p+2)^\alpha - p^\alpha] - [3^\alpha - 1^\alpha]$$

$$= R_\alpha^0(T_i) - R_\alpha^0(P_{l_i+1}) + 2\alpha(\xi^{\alpha-1} - \eta^{\alpha-1}),$$

where $\xi \in (p,\ p+2),\ \eta \in (1,\ 3)$ (or $\xi \in (3,\ p+2),\ \eta \in (1,\ p)$).

Let $\Delta_1 = f(T_i) - f(P_{l_i+1}),\ \Delta_2 = \alpha(\xi^{\alpha-1} - \eta^{\alpha-1})$.

If $\alpha > 1$ or $\alpha < 0$, then $\Delta_2 \geq 0$; and $\Delta_1 \geq 0$ from [9]. And at least one of the equalities strictly holds. So, $\Delta > 0$.

If $0 < \alpha < 1$, then $\Delta_2 < 0$; and $\Delta_1 < 0$ from [9]. And at least one of the inequalities strictly holds. So, $\Delta < 0$.

The proof of Lemma 3.1 is completed.

Remark. Repeating the operations D, any unicycle graph

$G = C_r^{u_1, u_2, \cdots, u_k}(T_1, T_2, \cdots, T_k)$ can be changed into

$C_r^{u_1, u_2, \cdots, u_k}(P_{l_1+1}, P_{l_2+1}, \cdots, P_{l_k+1})$.

For any unicycle graph $G = C_r^{u_1, u_2, \cdots, u_k}(T_1, T_2, \cdots, T_k)$, we can see from Lemma 3.1 that

(i) $R_\alpha^0(G) \geq R_\alpha^0(C_r^{u_1, u_2, \cdots, u_k}(P_{l_1+1}, P_{l_2+1}, \cdots, P_{l_k+1}))$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G) \leq R_\alpha^0(C_r^{u_1, u_2, \cdots, u_k}(P_{l_1+1}, P_{l_2+1}, \cdots, P_{l_k+1}))$ for $0 < \alpha < 1$.

And the equality holds if and only if

$$G = C_r^{u_1, u_2, \cdots, u_k}(P_{l_1+1}, P_{l_2+1}, \cdots, P_{l_k+1}).$$

Transfer operation *F*. Let $G = C_r^{u_1, u_2, \cdots, u_k}(P_{l_1+1}, P_{l_2+1}, \cdots, P_{l_k+1})$. If $k > 1$, then G can be changed into

$$G' = C_r^{u_1, \cdots, u_{k-1}}(P_{l_1+1}, P_{l_2+1}, \cdots, P_{l_{k-1}+l_k+1}).$$

Lemma 3.2. *For the two graphs G and G' above, we have*

(i) $R_\alpha^0(G') < R_\alpha^0(G)$ *for* $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G') > R_\alpha^0(G)$ *for* $0 < \alpha < 1$.

Proof. By the definition of $R_\alpha^0(G)$, we have

$$\begin{aligned}\Delta &= R_\alpha^0(G') - R_\alpha^0(G)\\ &= [2^\alpha + 2^\alpha] - [3^\alpha + 1^\alpha]\\ &= [2^\alpha - 1^\alpha] - [3^\alpha - 2^\alpha]\\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}),\end{aligned}$$

where $\xi \in (1, 2)$, $\eta \in (2, 3)$. And $\xi < \eta$, $\Delta < 0$ for $\alpha > 1$ or $\alpha < 0$, $\Delta > 0$ for $0 < \alpha < 1$. The proof of Lemma 3.2 is completed.

Remark. Repeating the operation F, any unicycle graph $G = C_r^{u_1, u_2, \cdots, u_k}(P_{l_1+1}, P_{l_2+1}, \cdots, P_{l_k+1})$ can be changed into $C_r^{u_1}(P_{n-r+1})$, as shown in Figure 6.

Therefore, any unicycle graph $G = C_r^{u_1, u_2, \cdots, u_k}(T_1, T_2, \cdots, T_k)$ can be changed into $C_r^{u_1}(P_{n-r+1})$ after the operations D and F.

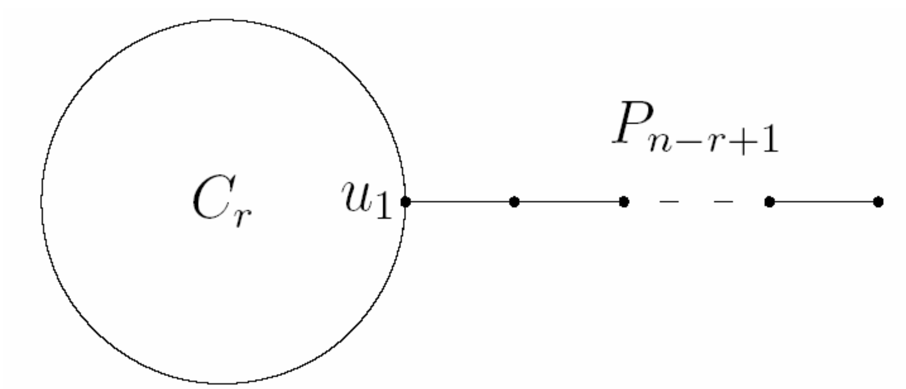

Figure 6. $C_r^{u_1}(P_{n-r+1})$.

Lemma 3.3. *If* $3 \leq r < n$, *then*

(i) $R_\alpha^0(C_r^{u_1}(P_{n-r+1})) > R_\alpha^0(C_n)$ *for* $\alpha > 1$ *or* $\alpha < 0$;

(ii) $R_\alpha^0(C_r^{u_1}(P_{n-r+1})) < R_\alpha^0(C_n)$ *for* $0 < \alpha < 1$.

Proof. If $3 \leq r < n$, then the degree sequence of $C_r^{u_1}(P_{n-r+1})$ is $[1, 2, \cdots, 2 \cdots, 3]$. The degree sequence of C_n is $[2, 2, \cdots, 2 \cdots, 2]$. By the definition of $R_\alpha^0(G)$, we have

$$\begin{aligned} \Delta &= R_\alpha^0(C_r^{u_1}(P_{n-r+1})) - R_\alpha^0(C_n) \\ &= [1^\alpha + 3^\alpha] - [2^\alpha + 2^\alpha] \\ &= [3^\alpha - 2^\alpha] - [2^\alpha - 1^\alpha] \\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $\xi \in (2, 3)$, $\eta \in (1, 2)$. And $\Delta > 0$ for $\alpha > 1$ or $\alpha < 0$, $\Delta < 0$ for $0 < \alpha < 1$. The proof of Lemma 3.3 is completed.

From Lemmas 3.1 and 3.2, the following result is immediate.

Theorem 3.4. *Among all unicycle graphs*,

(i) C_n *is the unique unicycle graph with the smallest* (*largest*) *zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$ $(0 < \alpha < 1)$;

(ii) *the unicycle graphs with the second smallest* (*largest*) *zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$ $(0 < \alpha < 1)$ *are* $C_r^{u_1}(P_{n-r+1})$, $3 \leq r \leq n-1$, *their degree sequences are* $[1, 2, \cdots, 2 \cdots, 3]$.

In the following, we consider the unicycle graph with third smallest (largest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$.

Let

$$\mathcal{F}_1 = \{C_r^{u_1, u_2}(P_{l_1+1}, P_{l_2+1}) | l_1, l_2 \geq 1, l_1 + l_2 = n - r, r \geq 3\}$$

$$\mathcal{F}_2 = \{C_r^{u_1}(T_1) | 3 \leq r \leq n - 1\}.$$

For any unicycle $G = C_r^{u_1, u_2, \cdots, u_k}(T_1, \cdots, T_i, \cdots, T_k)$, if $k \geq 3$, then by the operations D and F, there is $G' \in \mathcal{F}_1$ such that

(i) $R_\alpha^0(G) > R_\alpha^0(G')$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G) < R_\alpha^0(G')$ for $0 < \alpha < 1$.

Similarly, for any unicycle graph $G \in \mathcal{F}_1$, there is $G' \in \mathcal{F}_2$ such that

(i) $R_\alpha^0(G) > R_\alpha^0(G')$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G) < R_\alpha^0(G')$ for $0 < \alpha < 1$.

Therefore, the smallest value of zeroth-order general Randić indices of the unicycle graphs in $\mathcal{F}_1$ is not less than the third smallest value of zeroth-order general Randić indices of all unicycle graphs for $\alpha > 1$ or $\alpha < 0$; and the largest value of zeroth-order general Randić indices of the unicycle graphs in $\mathcal{F}_1$ is not more than the third largest value of zeroth-order general Randić indices of all unicycle graphs for $0 < \alpha < 1$.

In order to find the unicycle graph with the third smallest (largest) zeroth-order general Randić index for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$, we only need to find

(i) the unicycle graph with the smallest (largest) zeroth-order general Randić index in $\mathcal{F}_1$ for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$; and

(ii) the unicycle graphs with the second smallest (largest) zeroth-order general Randić index in $\mathcal{F}_2$ for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$ and, then compare them in turn.

Note that the degree sequences of graphs in $\mathcal{F}_1$ are $[1, 1, 2, \cdots, 2, 3, 3]$, and their zeroth-order general Randić indices are the same value:

$$R_\alpha^0(G) = 2 + 2^\alpha(n-4) + 2 \cdot 3^\alpha.$$

So, we only need to find the unicycle graphs with the second smallest (largest) zeroth-order general Randić index in $\mathcal{F}_2$ for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$.

Let $D(G) = [d_1, d_2, \cdots, d_n]$ be the degree sequence of unicycle graph G with order n, where $d_i \geq d_j + 2$. G' is obtained by replacing (d_i, d_j) with $(d_i - 1, d_j + 1)$ in $D(G)$, i.e.,

$$D(G') = [d_1, \cdots, d_{i-1}, d_i - 1, d_{i+1}, \cdots, d_{j-1}, d_j + 1, d_{j+1}, \cdots, d_n].$$

Lemma 3.4 ([9]). *For the two graphs G and G' above, we have*

(i) $R_\alpha^0(G) > R_\alpha^0(G')$ *for* $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G) < R_\alpha^0(G')$ *for* $0 < \alpha < 1$.

Lemma 3.5. *The graphs in $\mathcal{F}_2$ with the degree sequence $D(G) =$ $[1, 1, 2, \cdots, 2, 3, 3]$ are the unicycle graphs with the second smallest (largest) zeroth-order general Randić index in $\mathcal{F}_2$ for* $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$.

Proof. Let $G = C_r^{u_1}(T_1)$ be the unicycle graph in $\mathcal{F}_2$ with the second smallest (largest) for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$. Since $r \leq n - 1$, G must have at least one vertex with degree more than 2.

If $\mathcal{F}_0$ is the unicycle graph with the smallest (largest) zeroth-order general Randić index in $\mathcal{F}_2$ for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$, then, by Theorem 3.1, the degree sequence of $\mathcal{F}_0$ is $[1, 2, \cdots, 2, 3]$.

Therefore, G must have at least two vertices with degree more than 2.

If the degree sequence of G is not $[1, 1, 2, \cdots, 2, 3, 3]$, then, by Lemma 3.4, there is an unicycle graph $G' \in \mathcal{F}_2$ such that $D(G') = [1, 1, 2, \cdots, 2, 3, 3]$, and

(i) $R_\alpha^0(G) > R_\alpha^0(G') > R_\alpha^0(\mathcal{F}_0)$ for $\alpha > 1$ or $\alpha < 0$;

(ii) $R_\alpha^0(G) < R_\alpha^0(G') < R_\alpha^0(\mathcal{F}_0)$ for $0 < \alpha < 1$.

This contradicts that G is the unicycle graph in $\mathcal{F}_2$ with the second smallest (largest) for $\alpha > 1$ or $\alpha < 0$ $(0 < \alpha < 1)$. So, the degree sequence of G is $D(G) = [1, 1, 2, \cdots, 2, 3, 3]$.

Since the degree sequence of the graph in $\mathcal{F}_1$ is $[1, 1, 2, \cdots, 2, 3, 3]$, combining Lemma 3.5 and the above, we have

Theorem 3.2. *Among all the unicycle graphs of order n, the unicycle graphs with the third smallest* (*largest*) *zeroth-order general Randić index for* $\alpha > 1$ *or* $\alpha < 0$ $(0 < \alpha < 1)$ *are the graphs whose degree sequences are* $[1, 1, 2, \cdots, 2, 3, 3]$.

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