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THE ZEROTH-ORDER GENERAL RANDIĆ INDEX OF GRAPHS WITH A GIVEN CLIQUE NUMBER

Jianwei Du*, Yanling Shao, and Xiaoling Sun†

Abstract. The zeroth-order general Randić index ${}^0R_\alpha(G)$ of the graph G is defined as $\sum_{u\in V(G)} d(u)^\alpha$, where $d(u)$ is the degree of vertex u and α is an arbitrary real number. In this paper, the maximum value of zeroth-order general Randić index on the graphs of order n with a given clique number is presented for any $\alpha \neq 0, 1$ and $\alpha \notin (2, 2n-1]$, where $n = |V(G)|$. The minimum value of zeroth-order general Randić index on the graphs with a given clique number is also obtained for any $\alpha \neq 0, 1$. Furthermore, the corresponding extremal graphs are characterized.

1. Introduction

In this paper, we are concerned with undirected simple connected graphs only. Let $G = (V(G), E(G))$ denote a graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $u \in V(G)$ is denoted by $d_G(u)$ ($d(u)$ for short). Denote by $G-uv$ the graph that obtained from G by deleting the edge $uv \in E(G)$. Similarly, $G+uv$ is the graph that obtained from G by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$. A tree is a connected graph with n vertices and $n-1$ edges. The chromatic

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∗ Corresponding author.

number of a graph is the minimum number of colors such that the graph can be colored with these colors in such a way that no two adjacent vertices have the same color. We use $\chi(G)$ to denote the chromatic number of a graph G. A clique of a graph G is a subset S of V such that any two vertices in $G[S]$ (the subgraph of G induced by S) are adjacent. The number of vertices in a largest clique of G is called the clique number of G, and it is denoted by $\omega(G)$. As usual, we use P_n, S_n and K_n to denote the path, the star and the complete graph of order n, respectively.

The numerical quantities of a graph which are invariant under graph isomorphism are called topological indices [27]. The Randić (or connectivity) index of G, which is one of most popular topological indices, is defined as [23]

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

Randić himself [23] demonstrated that this index is well correlated with a variety of physico-chemical properties of various classes of organic compounds. Eventually, two books [12,13] are devoted for this structure-descriptor.

In [3], Bollobás and Erdős generalized $R(G)$ by replacing the exponent $-1/2$ with an arbitrary real number α, which is called the general Randić index and is denoted by R_α, i.e.,

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

The zeroth-order Randić index, conceived by Kier and Hall [14], is

$$^0R(G) = \sum_{u \in V(G)} d(u)^{-\frac{1}{2}}.$$

Li and Zheng [20] defined the zeroth-order general Randić index of a graph G as

$$^0R_\alpha(G) = \sum_{u \in V(G)} d(u)^{\alpha}.$$

for any real number α.

The zeroth-order general Randić index $^0R_2(G)$ is the well-known first Zagreb index $M_1(G) = \sum_{u \in V(G)} d(u)^2$ which is first introduced in [8], where Gutman and Trinajstić examined the dependence of total π-electron energy on molecular structure.

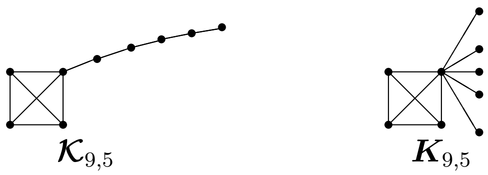

Fig. 1. The graphs $\boldsymbol{\mathcal{K}}_{9,5}$ and $\boldsymbol{K}_{9,5}$

Let $\boldsymbol{\mathcal{K}}_{n,n-k}$ and $\boldsymbol{K}_{n,n-k}$ be the graph obtained by identifying one vertex of K_k with a pendent vertex of path P_{n-k+1} and the graph obtained by identifying one vertex of K_k with the central vertex of star S_{n-k+1}, respectively. For example, $\boldsymbol{\mathcal{K}}_{9,5}$ and $\boldsymbol{K}_{9,5}$ are shown as Fig. 1. A complete k-partite graph whose partition sets differ in size by at most 1 is called Turán graph, which is denoted by $\boldsymbol{T}_n(k)$. Let us denote by $\boldsymbol{\chi}_{n,k}$ the set of the n-vertex graphs with chromatic number k, and $\boldsymbol{\mathcal{W}}_{n,k}$ the set of the n-vertex graphs with clique number k, respectively. We can see [4] for other notations.

In recent years, the zeroth-order general Randić index has been studied extensively. Pavlović [22] determined the (n,m)-graph with the maximum zeroth-order Randić index. Li and Zhao [19] presented trees with the first three minimum and maximum zeroth-order general Randić index, they also presented chemical trees with the minimum, second-minimum and maximum, second-maximum zeroth-order general Randić index. Zhang et al. [30] characterized the unicyclic graphs with the first three minimum and maximum zeroth-order general Randić index. Zhang, Wang and Cheng [31] determined bicyclic graphs with the first three minimum and maximum zeroth-order general Randić index. Hu, Li, Shi and Xu [9] obtained some bounds on connected (n,m)-graphs with the minimum and maximum zeroth-order general Randić index. Hu, Li, Shi, Xu and Gutman [10] determined the (n,m)-chemical graphs with the minimum and maximum zeroth-order general Randić index. For more results see [1,2,5,6,11,15−18,21,24−26,28].

In this paper, we present the maximum value of zeroth-order general Randić index on $\boldsymbol{\mathcal{W}}_{n,k}$ for any $\alpha \neq 0,1$ and $\alpha \notin (2, 2n-1]$. We also obtain the minimum value of zeroth-order general Randić index on $\boldsymbol{\mathcal{W}}_{n,k}$ for any $\alpha \neq 0,1$. Furthermore, the corresponding extremal graphs are characterized.

2. Preliminaries

Note that ${}^0R_0(G) = |V(G)| = n$ and ${}^0R_1(G) = 2|E(G)|$. Therefore, in the following we always assume that $\alpha \neq 0, 1$.

By the definition of zeroth-order general Randić index, these two lemmas are obvious and can be found in [28].

LEMMA 2.1. ([28]) *Let $G = (V, E)$ be a simple connected graph. If $e = uv \notin E(G)$, $u, v \in V(G)$, then*
(i) ${}^0R_\alpha(G) < {}^0R_\alpha(G + e)$ *for* $\alpha > 0$*;*
(ii) ${}^0R_\alpha(G) > {}^0R_\alpha(G + e)$ *for* $\alpha < 0$.

LEMMA 2.2. ([28]) *Let $G = (V, E)$ be a simple connected graph. If $e \in E(G)$, then*
(i) ${}^0R_\alpha(G) > {}^0R_\alpha(G - e)$ *for* $\alpha > 0$*;*
(ii) ${}^0R_\alpha(G) < {}^0R_\alpha(G - e)$ *for* $\alpha < 0$.

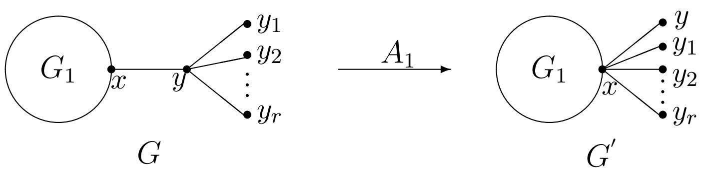

Fig. 2. Transformation A_1.

Transformation A_1: Let G be a graph as shown in Fig. 2, where $xy \in E(G)$, $d_G(x) \geq 2$, $N_G(y)/\{x\} = \{y_1, y_2, \cdots, y_r\}$ ($y_1, y_2, \cdots, y_r$ are pendant vertices). Set $G' = G - \{yy_1, yy_2, \cdots, yy_r\} + \{xy_1, xy_2, \cdots, xy_r\}$, as shown in Fig. 2.

LEMMA 2.3. ([5]) *Let G and G' be graphs in Fig. 2. Then*
(i) ${}^0R_\alpha(G') > {}^0R_\alpha(G)$ *for* $\alpha > 1$ *or* $\alpha < 0$*;*
(ii) ${}^0R_\alpha(G') < {}^0R_\alpha(G)$ *for* $0 < \alpha < 1$.

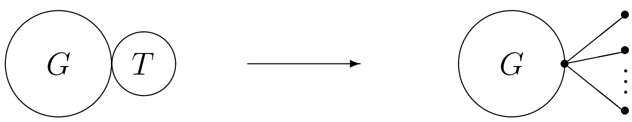

Fig. 3. The graphs in Remark 2.4.

Remark 2.4. By repeating Transformation A_1, any tree T attached to a graph G can be changed into a star as showed in Fig. 3. Furthermore, the zeroth-order general Randić indices increase for $\alpha > 1$ or $\alpha < 0$, and the zeroth-order general Randić indices decrease for $0 < \alpha < 1$.

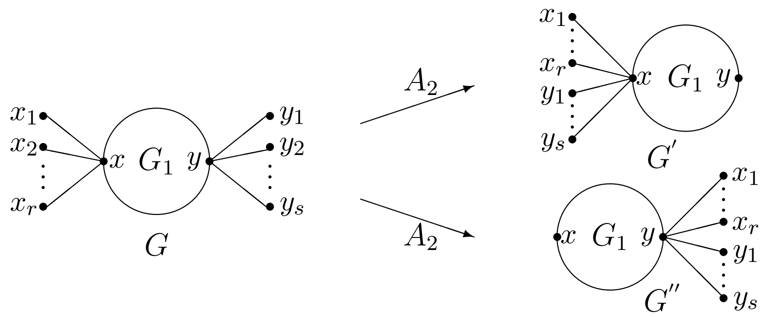

Fig. 4. Transformation A_2.

Transformation A_2: Let G be a graph as shown in Fig. 4, and $x, y \in V(G)$, where $x_1, x_2, \cdots, x_r$ are pendant vertices adjacent to x, and $y_1, y_2, \cdots, y_s$ are pendant vertices adjacent to y. Set $G' = G - \{yy_1, yy_2, \cdots, yy_s\} + \{xy_1, xy_2, \cdots, xy_s\}$, $G'' = G - \{xx_1, xx_2, \cdots, xx_r\} + \{yx_1, yx_2, \cdots, yx_r\}$, as shown in Fig. 4.

Lemma 2.5. *Let G, G' and G'' be graphs in Fig. 4. Then*

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

(ii) either ${}^0R_\alpha(G') < {}^0R_\alpha(G)$ or ${}^0R_\alpha(G'') < {}^0R_\alpha(G)$ for $0 < \alpha < 1$.

Proof. By the definition of zeroth-order general Randić index and the Lagrange mean value theorem, we have

$$\begin{aligned}{}^0R_\alpha(G') - {}^0R_\alpha(G) &= (d_G(x)+s)^\alpha + (d_G(y)-s)^\alpha - (d_G(x)^\alpha + d_G(y)^\alpha)\\ &= (d_G(x)+s)^\alpha - d_G(x)^\alpha - [d_G(y)^\alpha - (d_G(y)-s)^\alpha]\\ &= s\alpha(\xi_1^{\alpha-1} - \eta_1^{\alpha-1}),\end{aligned}$$

where $d_G(x) < \xi_1 < d_G(x)+s$, $d_G(y)-s < \eta_1 < d_G(y)$.

$$\begin{aligned}{}^0R_\alpha(G'') - {}^0R_\alpha(G) &= (d_G(x)-r)^\alpha + (d_G(y)+r)^\alpha - (d_G(x)^\alpha + d_G(y)^\alpha)\\ &= (d_G(y)+r)^\alpha - d_G(y)^\alpha - [d_G(x)^\alpha - (d_G(x)-r)^\alpha]\\ &= r\alpha(\eta_2^{\alpha-1} - \xi_2^{\alpha-1}),\end{aligned}$$

where $d_G(x)-r < \xi_2 < d_G(x)$, $d_G(y) < \eta_2 < d_G(y)+r$.

If $d_G(y) \leq d_G(x)$, then ${}^0R_\alpha(G^{'}) - {}^0R_\alpha(G) > 0$, i.e., ${}^0R_\alpha(G^{'}) > {}^0R_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$; otherwise, ${}^0R_\alpha(G^{''}) > {}^0R_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$.

If $d_G(y) \leq d_G(x)$, then ${}^0R_\alpha(G^{'}) < {}^0R_\alpha(G)$ for $0 < \alpha < 1$; otherwise, ${}^0R_\alpha(G^{''}) < {}^0R_\alpha(G)$ for $0 < \alpha < 1$. □

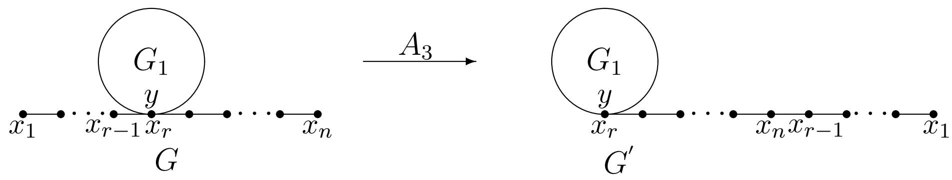

Fig. 5. Transformation A_3.

Transformation A_3: Let G be a graph as shown in Fig. 5, where $G_1 \ncong K_1$ and $y \in V(G_1)$. That is, we use G to denote the graph obtained from identifying y with the vertex x_r of a path $x_1x_2 \cdots x_{r-1}x_r \cdots x_n$, $1 < r < n$. Set $G^{'} = G - x_{r-1}x_r + x_nx_{r-1}$, as shown in Fig. 5.

Lemma 2.6. *Let G and $G^{'}$ be graphs in Fig. 5. Then*
(i) ${}^0R_\alpha(G^{'}) < {}^0R_\alpha(G)$ *for* $\alpha > 1$ *or* $\alpha < 0$;
(ii) ${}^0R_\alpha(G^{'}) > {}^0R_\alpha(G)$ *for* $0 < \alpha < 1$.

Proof. We notice that

$$\begin{aligned} {}^0R_\alpha(G^{'}) - {}^0R_\alpha(G) &= (d_{G_1}(y) + 1)^\alpha + 2^\alpha - (d_{G_1}(y) + 2)^\alpha - 1 \\ &= 2^\alpha - 1 - [(d_{G_1}(y) + 2)^\alpha - (d_{G_1}(y) + 1)^\alpha] \\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $1 < \xi < 2$, $d_{G_1}(y)+1 < \eta < d_{G_1}(y)+2$. This finishes the proof. □

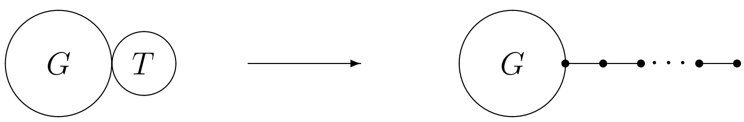

Fig. 6. The graphs in Remark 2.7.

Remark 2.7. By repeating Transformation A_3, any tree T attached to a graph G can be changed into a path as shown in Fig. 6. Furthermore, the zeroth-order general Randić indices decrease for $\alpha > 1$ or $\alpha < 0$, and the zeroth-order general Randić indices increase for $0 < \alpha < 1$.

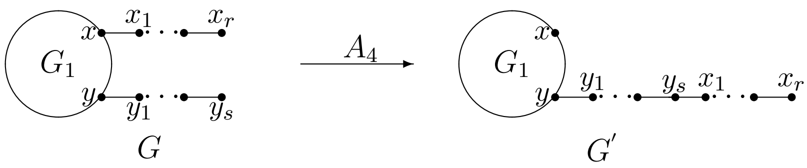

Fig. 7. Transformation A_4.

Transformation A_4: Let G be a graph as shown in Fig. 7, where $x, y \in V(G_1)$. That is, we use G to denote the graph obtained from identifying x with the vertex x_0 of a path $x_0x_1 \cdots x_r$ and identifying y with the vertex y_0 of a path $y_0y_1 \cdots y_s$, where $r, s \geq 1$. Set $G' = G - xx_1 + y_sx_1$, as shown in Fig. 7.

LEMMA 2.8. *Let G and G' be graphs in Fig. 7. Then*
(i) ${}^0R_\alpha(G') < {}^0R_\alpha(G)$ *for* $\alpha > 1$ *or* $\alpha < 0$*;*
(ii) ${}^0R_\alpha(G') > {}^0R_\alpha(G)$ *for* $0 < \alpha < 1$.

Proof. The proof is similar to Lemma 2.6, omitted. □

LEMMA 2.9. *Let*

$$f(x) = x(n-x)^\alpha,$$

where $1 \leq x \leq n-1$, $n \geq 3$. *Then* $f''(x) < 0$ *for* $0 < \alpha < 1$, *and* $f''(x) > 0$ *for* $\alpha < 0$ *or* $\alpha > 2n-1$.

Proof. Note that

$$f'(x) = (n-x)^{\alpha-1}(n - \alpha x - x),$$
$$f''(x) = -\alpha(n-x)^{\alpha-2}[2n - (\alpha+1)x].$$

This completes the proof. □

LEMMA 2.10. *Let n_i, n_j, t be positive integers and α be a real number, where $n_j - n_i \geq 2$ and $1 < \alpha \leq 2$. Then*

$$n_j(n_i+t)^{\alpha-1} - n_i(n_j+t)^{\alpha-1} > 0.$$

Proof. Let $g(x) = (\alpha-1)\ln(x+t) - \ln x$, where $x \geq 1$. Then

$$g'(x) = \frac{(\alpha-2)x - t}{x(x+t)} < 0.$$

So $g(n_i) > g(n_j)$. Thus we have

$$\begin{aligned}&(\alpha-1)\ln(n_i+t)-\ln n_i > (\alpha-1)\ln(n_j+t)-\ln n_j\\ \Longrightarrow\,&\ln n_j+(\alpha-1)\ln(n_i+t) > \ln n_i+(\alpha-1)\ln(n_j+t)\\ \Longrightarrow\,&\ln[n_j(n_i+t)^{\alpha-1}] > \ln[n_i(n_j+t)^{\alpha-1}]\\ \Longrightarrow\,&n_j(n_i+t)^{\alpha-1} > n_i(n_j+t)^{\alpha-1}.\end{aligned}$$

This completes the proof. □

3. Main result

Let $G \in \boldsymbol{\mathcal{W}}_{n,k}$. If $k = 1$, $G \cong K_1$. If $k = n$, $G \cong K_n$. So, next, we always assume that $1 < k < n$.

THEOREM 3.1. *Let* $H_1 \in \boldsymbol{\mathcal{W}}_{n,k}$. *Then* ${}^0R_\alpha(H_1) \geq (k-1)^{\alpha+1} + k^\alpha + 2^\alpha(n-k-1) + 1$ *for* $\alpha > 1$, *with the equality holding if and only if* $H_1 \cong \boldsymbol{\mathcal{K}}_{n,n-k}$.

Proof. Choose a graph $H_1 \in \boldsymbol{\mathcal{W}}_{n,k}$ such that H_1has the minimum zeroth-order general Randić index. By the definition of the set $\boldsymbol{\mathcal{W}}_{n,k}$, H_1 contains a clique K_k as a subgraph. From Lemma 2.2, H_1 must be the graph that results from K_k by attaching some trees rooted at some vertices of K_k. By Remark 2.7, we conclude that, in H_1, all the trees attached at some vertices of K_k must be paths. Now we claim that $H_1 \cong \boldsymbol{\mathcal{K}}_{n,n-k}$. Otherwise, suppose that there are two paths P_1 and P_2 attached at two vertices v_1 and v_2 of K_k, respectively. From Lemma 2.8, H_1 can be changed to H_1' by transformation A_4 with a smaller zeroth-order general Randić index, which contradicts the choice of H_1. Therefore $H_1 \cong \boldsymbol{\mathcal{K}}_{n,n-k}$.

By the definition of zeroth-order general Randić index, we have

$${}^0R_\alpha(\boldsymbol{\mathcal{K}}_{n,n-k}) = (k-1)^{\alpha+1} + k^\alpha + 2^\alpha(n-k-1) + 1.$$

The proof is completed. □

THEOREM 3.2. *Let* $H_2 \in \boldsymbol{\mathcal{W}}_{n,k}$. *Then*

(*i*) ${}^0R_\alpha(H_2) \geq (k-1)^{\alpha+1} + (n-1)^\alpha + n - k$ *for* $0 < \alpha < 1$, *with the equality holding if and only if* $H_2 \cong \boldsymbol{K}_{n,n-k}$;

(*ii*) ${}^0R_\alpha(H_2) \leq (k-1)^{\alpha+1} + (n-1)^\alpha + n - k$ *for* $\alpha < 0$, *with the equality holding if and only if* $H_2 \cong \boldsymbol{K}_{n,n-k}$.

Proof. We discuss in two cases.

Case 1. $0 < \alpha < 1$.

Choose a graph $H_2 \in \boldsymbol{\mathcal{W}}_{n,k}$ such that H_2 has the minimum zeroth-order general Randić index. Similarly as the proof of Theorem 3.1, by Remark 2.4, all the trees in H_2 attached at some vertices of K_k must be stars; furthermore, if $H_2 \ncong \boldsymbol{K}_{n,n-k}$, from Lemma 2.5, H_2 can be changed to H_2' or H_2'' by transformation A_2 with a smaller zeroth-order general Randić index which is a contradiction to the choice of H_2. Therefore $H_2 \cong \boldsymbol{K}_{n,n-k}$.

Case 2. $\alpha < 0$.

Choose a graph $H_2 \in \boldsymbol{\mathcal{W}}_{n,k}$ such that H_2 has the largest zeroth-order general Randić index. The rest of the proof is analogous to that of Case 1, omitted.

From the definition of zeroth-order general Randić index, we have

$$^0R_\alpha(\boldsymbol{K}_{n,n-k}) = (k-1)^{\alpha+1} + (n-1)^\alpha + n - k.$$

The proof is completed. □

Let $K_{n_1,n_2,\cdots,n_k}$ denote the n-vertex complete k-partite graph whose partition sets size are $n_1, n_2, \cdots, n_k$, respectively. Then $n_1 + n_2 + \cdots + n_k = n$.

LEMMA 3.3. *Let $G \in \boldsymbol{\chi}_{n,k}$ be a graph with maximum zeroth-order general Randić index for $\alpha > 0$, and with minimum zeroth-order general Randić index for $\alpha < 0$. Then $G \cong K_{n_1,n_2,\cdots,n_k}$.*

Proof. By the definition of the set $\boldsymbol{\chi}_{n,k}$ and Lemma 2.1, the lemma holds obviously. □

In order to get our other results, we first consider the zeroth-order general Randić indices of graphs $G \in \boldsymbol{\chi}_{n,k}$. Let $n = kp + q$, where $0 \le q < k$, i.e., $p = \lfloor \frac{n}{k} \rfloor$.

THEOREM 3.4. *Let $G \in \boldsymbol{\chi}_{n,k}$. Then*

(i) $^0R_\alpha(G) \le {^0R_\alpha}(\boldsymbol{T}_n(k)) = (k-q)(n-\lfloor \frac{n}{k} \rfloor)^\alpha + q(\lfloor \frac{n}{k} \rfloor + 1)(n - \lfloor \frac{n}{k} \rfloor - 1)^\alpha$ *for $0 < \alpha < 1$ or $1 < \alpha \le 2$, with the equality holding if and only if $G \cong \boldsymbol{T}_n(k)$;*

(ii) $^0R_\alpha(G) \ge {^0R_\alpha}(\boldsymbol{T}_n(k)) = (k-q)(n-\lfloor \frac{n}{k} \rfloor)^\alpha + q(\lfloor \frac{n}{k} \rfloor + 1)(n - \lfloor \frac{n}{k} \rfloor - 1)^\alpha$ *for $\alpha < 0$, with the equality holding if and only if $G \cong \boldsymbol{T}_n(k)$.*

Proof. In view of the definition of chromatic number, any graph $G \in \boldsymbol{\chi}_{n,k}$ has k color classes each of which is an independent set. Let the size of the k classes be $n_1, n_2, \cdots, n_k$, respectively. By Lemma 3.3, the graph $G \in \boldsymbol{\chi}_{n,k}$ which reaches the maximum zeroth-order general Randić indices for $0 < \alpha < 1$ or $1 < \alpha \leq 2$, and reaches the minimum zeroth-order general Randić indices for $\alpha < 0$ will be a complete k-partite graph $K_{n_1,n_2,\cdots,n_k}$. Choose the graph $G \in \boldsymbol{\chi}_{n,k}$ such that G has the maximum zeroth-order general Randić indices for $0 < \alpha < 1$ or $1 < \alpha \leq 2$, and has the minimum zeroth-order general Randić indices for $\alpha < 0$, respectively.

Now we claim that $G \in \boldsymbol{T}_n(k)$. Otherwise, there exist two classes of size n_i and n_j, respectively, satisfy $n_j - n_i \geq 2$, that is, $n_j - 1 \geq n_i + 1$, without loss of generality, we assume that $1 \leq i < j \leq k$. We will find a contradiction.

Case 1. $0 < \alpha < 1$ or $1 < \alpha \leq 2$.

Subcase 1.1. $1 < \alpha \leq 2$.

Note that

$$\begin{aligned}
&{}^0R_\alpha(K_{n_1,\cdots,n_i+1,\cdots,n_j-1,\cdots,n_k}) - {}^0R_\alpha(K_{n_1,\cdots,n_i,\cdots,n_j,\cdots,n_k}) \\
=&(n_i+1)(n-n_i-1)^\alpha + (n_j-1)(n-n_j+1)^\alpha - n_i(n-n_i)^\alpha - n_j(n-n_j)^\alpha \\
=&n_j[(n-n_j+1)^\alpha - (n-n_j)^\alpha] - n_i[(n-n_i)^\alpha - (n-n_i-1)^\alpha] \\
&+ (n-n_i-1)^\alpha - (n-n_j+1)^\alpha \\
=&\alpha(n_j\xi_1^{\alpha-1} - n_i\eta_1^{\alpha-1}) + (n-n_i-1)^\alpha - (n-n_j+1)^\alpha,
\end{aligned}$$

where $n - n_j < \xi_1 < n - n_j + 1$, $n - n_i - 1 < \eta_1 < n - n_i$. Since $(n - n_i - 1) \geq (n - n_j + 1)$, we have

$$\begin{aligned}
&{}^0R_\alpha(K_{n_1,\cdots,n_i+1,\cdots,n_j-1,\cdots,n_k}) - {}^0R_\alpha(K_{n_1,\cdots,n_i,\cdots,n_j,\cdots,n_k}) \\
\geq&\alpha(n_j\xi_1^{\alpha-1} - n_i\eta_1^{\alpha-1}) \\
>&\alpha[n_j(n-n_j)^{\alpha-1} - n_i(n-n_i)^{\alpha-1}].
\end{aligned}$$

If $k = 2$, then $n_i + n_j = n_1 + n_2 = n$, and we have ${}^0R_\alpha(K_{n_1+1,n_2-1}) - {}^0R_\alpha(K_{n_1,n_2}) > \alpha[n_2(n-n_2)^{\alpha-1} - n_1(n-n_1)^{\alpha-1}] = \alpha(n_1n_2)^{\alpha-1}(n_2^{2-\alpha} - n_1^{2-\alpha}) \geq 0$, which contradicts the choice of G.

If $k \geq 3$, let $n_i + n_j + t = n$, where $t = \sum_{r=1, r\neq i,j}^{k} n_r \geq k - 2 \geq 1$, by Lemma 2.10, we have

$$\begin{aligned}
&{}^0R_\alpha(K_{n_1,\cdots,n_i+1,\cdots,n_j-1,\cdots,n_k}) - {}^0R_\alpha(K_{n_1,\cdots,n_i,\cdots,n_j,\cdots,n_k}) \\
>&\alpha[n_j(n_i+t)^{\alpha-1} - n_i(n_j+t)^{\alpha-1}] > 0,
\end{aligned}$$

which contradicts the choice of G, again.

Subcase 1.2. $0 < \alpha < 1$.

Note that

$$\begin{aligned}&{}^0R_\alpha(K_{n_1,\cdots,n_i+1,\cdots,n_j-1,\cdots,n_k}) - {}^0R_\alpha(K_{n_1,\cdots,n_i,\cdots,n_j,\cdots,n_k})\\ =&(n_i+1)(n-n_i-1)^\alpha+(n_j-1)(n-n_j+1)^\alpha - n_i(n-n_i)^\alpha - n_j(n-n_j)^\alpha\\ =&f(n_i+1) - f(n_i) - [f(n_j) - f(n_j-1)]\\ =&f'(\xi_2) - f'(\eta_2),\end{aligned}$$

where $n_i < \xi_2 < n_i+1$, $n_j-1 < \eta_2 < n_j$. By Lemma 2.9, we have $f'(\xi_2)-f'(\eta_2) > 0$, i.e., ${}^0R_\alpha(K_{n_1,\cdots,n_i+1,\cdots,n_j-1,\cdots,n_k}) > {}^0R_\alpha(K_{n_1,\cdots,n_i,\cdots,n_j,\cdots,n_k})$, which is a contradiction to the choice of G.

Case 2. $\alpha < 0$.

Note that

$$\begin{aligned}&{}^0R_\alpha(K_{n_1,\cdots,n_i+1,\cdots,n_j-1,\cdots,n_k}) - {}^0R_\alpha(K_{n_1,\cdots,n_i,\cdots,n_j,\cdots,n_k})\\ =&f(n_i+1) - f(n_i) - [f(n_j) - f(n_j-1)]\\ =&f'(\xi_3) - f'(\eta_3),\end{aligned}$$

where $n_i < \xi_3 < n_i+1$, $n_j-1 < \eta_3 < n_j$. By Lemma 2.9, we have $f'(\xi_3)-f'(\eta_3) < 0$, i.e., ${}^0R_\alpha(K_{n_1,\cdots,n_i+1,\cdots,n_j-1,\cdots,n_k}) < {}^0R_\alpha(K_{n_1,\cdots,n_i,\cdots,n_j,\cdots,n_k})$, which is a contradiction to the choice of G.

Recall that $n = k\lfloor \frac{n}{k} \rfloor + q = (k-q)\lfloor \frac{n}{k} \rfloor + q(\lfloor \frac{n}{k} \rfloor + 1)$. By the definition of the zeroth-order general Randić index, we obtain the value of ${}^0R_\alpha(\boldsymbol{T}_n(k))$ immediately.

Conversely, it is easy to see that the equality holds in (i) or (ii) when $G \cong \boldsymbol{T}_n(k)$. The proof is completed. □

THEOREM 3.5. *Let $G \in \boldsymbol{\chi}_{n,k}$. Then ${}^0R_\alpha(G) \leq {}^0R_\alpha(K_{n+1-k,1,1,\cdots,1}) = (k-1)(n-1)^\alpha + (n-k+1)(k-1)^\alpha$ for $\alpha > 2n-1$, with the equality holding if and only if $G \cong K_{n+1-k,1,1,\cdots,1}$, where $K_{n+1-k,1,1,\cdots,1}$ is the complete k-partite graph with n vertices whose partition sets size are $n+1-k, 1, 1, \cdots, 1$, respectively.*

Proof. Similar to the proof of theorem 3.4, the graph $G \in \boldsymbol{\chi}_{n,k}$ which reaches the maximum zeroth-order general Randić indices for $\alpha > 2n-1$ will be a complete k-partite graph $K_{n_1,n_2,\cdots,n_k}$. Suppose that the graph $G \in \boldsymbol{\chi}_{n,k}$ has the maximum zeroth-order general Randić indices for $\alpha > 2n-1$.

Now we claim that $G \in K_{n+1-k,1,1,\cdots,1}$. Otherwise, there exist two classes of size n_i and n_j, respectively, satisfy $n_j \geq n_i \geq 2$, without loss of generality, we assume that $1 \leq i < j \leq k$.

Note that

$$\begin{aligned}&{}^0R_\alpha(K_{n_1,\cdots,n_i-1,\cdots,n_j+1,\cdots,n_k}) - {}^0R_\alpha(K_{n_1,\cdots,n_i,\cdots,n_j,\cdots,n_k})\\ =&f(n_j+1) - f(n_j) - [f(n_i) - f(n_i-1)]\\ =&f'(\xi) - f'(\eta),\end{aligned}$$

where $n_j < \xi < n_j+1$, $n_i - 1 < \eta < n_i$. By Lemma 2.9, we have $f'(\xi) - f'(\eta) > 0$, i.e., ${}^0R_\alpha(K_{n_1,\cdots,n_i-1,\cdots,n_j+1,\cdots,n_k}) > {}^0R_\alpha(K_{n_1,\cdots,n_i,\cdots,n_j,\cdots,n_k})$, which contradicts the choice of G.

From the definition of zeroth-order general Randić index, we have

$${}^0R_\alpha(K_{n+1-k,1,1,\cdots,1}) = (k-1)(n-1)^\alpha + (n-k+1)(k-1)^\alpha.$$

Conversely, it is easy to see that the equality holds when $G \cong K_{n+1-k,1,1,\cdots,1}$. This completes the proof. □

Lemma 3.6. ([7]) *Let $G = (V, E)$ be a graph with $\omega(G) \le k$. Then there is a k-partite graph $G' = (V, E')$ such that for every vertex $v \in V$, $d_G(v) \le d_{G'}(v)$.*

Theorem 3.7. *Let $G \in \boldsymbol{\mathcal{W}}_{n,k}$. Then*

(i) ${}^0R_\alpha(G) \le (k-q)(n-\lfloor\frac{n}{k}\rfloor)^\alpha + q(\lfloor\frac{n}{k}\rfloor+1)(n-\lfloor\frac{n}{k}\rfloor-1)^\alpha$ for $0<\alpha<1$ or $1<\alpha\le 2$, with the equality holding if and only if $G \cong \boldsymbol{T}_n(k)$;

(ii) ${}^0R_\alpha(G) \ge (k-q)(n-\lfloor\frac{n}{k}\rfloor)^\alpha + q(\lfloor\frac{n}{k}\rfloor+1)(n-\lfloor\frac{n}{k}\rfloor-1)^\alpha$ for $\alpha<0$, with the equality holding if and only if $G \cong \boldsymbol{T}_n(k)$.

(iii) ${}^0R_\alpha(G) \le (k-1)(n-1)^\alpha + (n-k+1)(k-1)^\alpha$ for $\alpha > 2n-1$, with the equality holding if and only if $G \cong K_{n+1-k,1,1,\cdots,1}$, where $K_{n+1-k,1,1,\cdots,1}$ is the complete k-partite graph of order n whose partition sets size are $n+1-k, 1, 1, \cdots, 1$, respectively.

Proof. If $k = n$, then $G \cong K_n$. Thus, we assume that $k < n$. Pick a graph $G \in \boldsymbol{\mathcal{W}}_{n,k}$ such that G has the maximum zeroth-order general Randić indices for $0<\alpha<1$, $1<\alpha\le 2$ or $\alpha > 2n-1$, and has the minimum zeroth-order general Randić indices for $\alpha<0$, respectively. Now we claim that $G \in \boldsymbol{\chi}_{n,k}$. To the contrary, since $\omega(G) = k$, by Lemma 3.6, we can get a k-partite graph G^* with $V(G^*) = V(G)$ such that for every vertex $v \in V(G) = V(G^*)$, $d_G(v) \le d_{G^*}(v)$. Obviously, $G^* \in \boldsymbol{\mathcal{W}}_{n,k}$. By the definition of zeroth-order general Randić index, we have ${}^0R_\alpha(G^*) \ge {}^0R_\alpha(G)$ for $0<\alpha<1$, $1<\alpha\le 2$ or $\alpha>2n-1$, and ${}^0R_\alpha(G^*) \le {}^0R_\alpha(G)$ for $\alpha<0$, respectively.

By Theorem 3.4 and 3.5, considering the uniqueness of the extremal graph in the set $\boldsymbol{\chi}_{n,k}$, the theorem holds immediately. □

If $\alpha = 2$, then ${}^0R_2(G)$ is the first Zagreb index $M_1(G)$ and by using $\alpha = 2$ in Theorem 3.5 and 3.6, we obtain the following corollary which is the result given in [29].

COROLLARY 3.8. ([29])*Let* $G \in \boldsymbol{\mathcal{W}}_{n,k}$*. Then*
(*i*) $M_1(G) \leq (k-q)(n - \lfloor \frac{n}{k} \rfloor)^2 + q\lceil \frac{n}{k} \rceil (n - \lceil \frac{n}{k} \rceil)^2$ *with the equality holding if and only if* $G \cong \boldsymbol{T}_n(k)$*;*
(*ii*) $M_1(G) \geq k^3 - 2k^2 - k + 4n - 4$ *with the equality holding if and only if* $G \cong \boldsymbol{\mathcal{K}}_{n,n-k}$*.*

REMARK 3.9. Another question is to consider the maximum zeroth-order general Randić index for $\alpha \in (2, 2n-1]$ on the graphs $G \in \boldsymbol{\mathcal{W}}_{n,k}$. By inspecting some special graphs $G \in \boldsymbol{\mathcal{W}}_{n,k}$, we found that for $\alpha \in (2, a)$, $\mathbf{T}_n(k)$ has maximum zeroth-order general Randić index, and for $\alpha \in (b, 2n-1]$, $K_{n+1-k,1,1,\cdots,1}$ has maximum zeroth-order general Randić index, where $a \leq b$. So further research is needed in future.

4. Conclusion

In this article, for $G \in \boldsymbol{\mathcal{W}}_{n,k}$, we got that $\boldsymbol{K}_{n,n-k}$ (resp. $\mathbf{T}_n(k)$) has the maximum (resp. minimum) ${}^0R_\alpha(G)$ for $\alpha < 0$, and $\mathbf{T}_n(k)$ (resp. $\boldsymbol{K}_{n,n-k}$) has the maximum (resp. minimum) ${}^0R_\alpha(G)$ for $0 < \alpha < 1$. Furthermore, for $G \in \boldsymbol{\mathcal{W}}_{n,k}$, we proved that $\boldsymbol{\mathcal{K}}_{n,n-k}$ has the minimum ${}^0R_\alpha(G)$ for $\alpha > 1$, and $\mathbf{T}_n(k)$ (resp. $K_{n+1-k,1,1,\cdots,1}$) has the maximum ${}^0R_\alpha(G)$ for $1 < \alpha \leq 2$ (resp. for $\alpha > 2n-1$).

The maximum ${}^0R_\alpha(G)$ for $\alpha \in (2, 2n-1]$ on the graphs $G \in \boldsymbol{\mathcal{W}}_{n,k}$ has not been obtained. By inspecting some special graphs $G \in \boldsymbol{\mathcal{W}}_{n,k}$, it seems that for $\alpha \in (2, a)$, $\mathbf{T}_n(k)$ has maximum ${}^0R_\alpha(G)$, and for $\alpha \in (b, 2n-1]$, $K_{n+1-k,1,1,\cdots,1}$ has maximum ${}^0R_\alpha(G)$, where $a \leq b$. So further study is needed in future.

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Jianwei Du
School of Science, North University of China
Taiyuan 030051, China
E-mail: jianweidu@nuc.edu.cn

Yanling Shao
School of Science, North University of China
Taiyuan 030051, China
E-mail: ylshao@nuc.edu.cn

Xiaoling Sun
School of Science, North University of China
Taiyuan 030051, China
E-mail: sunxiaoling@nuc.edu.cn