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The general zeroth-order Randić index of maximal outerplanar graphs and trees with *k* maximum degree vertices

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ABSTRACT: For a graph, the general zeroth-order Randić index R^0_α is defined as the sum of the αth power of the vertex degrees ($\alpha \neq 0$, $\alpha \neq 1$). Let $\mathscr{H}_n$ be the class of all maximal outerplanar graphs on n vertices, and $\mathscr{T}_{n,k}$ be the class of trees with n vertices of which k vertices have the maximum degree. We first present a lower bound (respectively, upper bound) for the general zeroth-order Randić index of graphs in $\mathscr{H}_n$ (respectively, $\mathscr{T}_{n,k}$) when $\alpha \in (-\infty, 0) \cup (1, +\infty)$ (respectively, $\alpha \in (2, +\infty)$), and characterize the extremal graphs. Then we determine graphs of the class $\mathscr{T}_{n,k}$ with maximal and minimal general zeroth-order Randić index when $\alpha \in (-\infty, 0) \cup (1, +\infty)$, respectively.

KEYWORDS: graph invariant, extremal graphs

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INTRODUCTION

All graphs considered in this paper are finite and simple. For notation and terminology not defined here see Ref. 1. A graph invariant is a function on a graph that does not depend on the labelling of its vertices. It can be used to characterize some properties of the graph of a molecule. Up to now, hundreds of graph invariants based on vertex degrees of a graph have been considered in quantitative structure-activity relationship and quantitative structure-property relationship studies. Among the most important degree-based topological indices is the well-known *first Zagreb index*[2]:

$$M_1(G) = \sum_{u \in V} \big(d_G(u)\big)^2.$$

This graph invariant has been considered in connection with certain chemical applications[3,4]. A vast amount of research on the first Zagreb index has been done. For details of its mathematical theory see Refs. 5, 6. Recent contributions could be found in Refs. 7, 8. There are many other degree-based topological indices, such as the Zagreb index and Randić index[9–11].

The *zeroth-order Randić index* is[12]

$$R^0(G) = \sum_{u \in V} \big(d_G(u)\big)^{-1/2},$$

where the sum goes over all vertices of G. In analogy to the ordinary (first-order) Randić index, the *general zeroth-order Randić index* is[13]

$$R^0_\alpha(G) = \sum_{u \in V} \big(d_G(u)\big)^{\alpha},$$

where $\alpha \neq 0$, 1 is a pertinently chosen real number. It should be noted that the same quantity is sometimes referred to as 'general first Zagreb index'. Generally speaking, there are three groups of closely related problems which have attracted the attention of researchers for a long time.

Problem 1 *How does $R^0_\alpha(G)$ depend on the structure of graph G?*

Problem 2 *Given a set of molecular graph $\mathscr{G}_n$, find the upper and lower bounds for $R^0_\alpha(G)$ in $\mathscr{G}_n$ and characterize the graphs in which the maximal and minimal values are attained, respectively.*

Problem 3 *Compare the values of general zeroth-order Randić index and other topological indices of graphs.*

On concerning these problems, it is not surprising that in the chemical literature there are numerous studies of properties of the general zeroth-order Randić index of molecular graphs. Li and Zhao[14] determined the trees with the first three minimum and maximum zeroth-order general Randić index. An (n,m)-graph is a simple connected graph that has n vertices, m edges, and maximum degree at most 4. In Ref. 15 the authors investigated the general zeroth-order Randić index for molecular (n,m)-graphs. Zhang and Zhang[16] determined the unicyclic graphs with the first three minimum and maximum general zeroth-order Randić index. Zhang et al[17] determined the bicyclic graphs with the first three minimum and maximum general zeroth-order Randić index. Hu et al[18] investigated the general zeroth-order Randić index for general simple connected (n,m)-graphs and characterized the simple connected (n,m)-graphs with extremal (maximum and minimum) general zeroth-order Randić index. Li and Shi[19] did some further work on this topic following Ref. 18. Cheng et al[20] determined the minimum and maximum general zeroth-order Randić index values of bipartite graphs with a given number of vertices and edges for $\alpha = 2$. Su et al[21] presented several sufficient conditions for graphs to be maximally edge-connected in terms of the general zeroth-order Randić index, and generalized the results given in Ref. 22. We encourage the interested reader to consult Refs. 23–25. and therein for more information and details on the general zeroth-order Randić index.

An *outerplanar graph* is a planar graph that has a planar drawing with all vertices on the same face. From the definition, we know that a graph is outerplanar if it has an embedding in the plane such that all vertices lie on the outer face boundary. An edge of an outerplanar graph is said to be a *chord*, if it joins two vertices of the outer face boundary but is not itself an edge of the outer face boundary. A *maximal outerplanar graph* is an outerplanar graph such that all its faces except the outer face are composed of three edges. It can be easily verified that any maximal outerplanar graph possess the following properties[26].

Proposition 1 *Let G be a maximal outerplanar graph with $n \geqslant 4$ vertices. If v is a vertex of degree 2 whose neighbours are u and w, then u and w are adjacent in G.*

Proposition 2 *Let G be a maximal outerplanar graph with $n \geqslant 4$ vertices. If v is a vertex of degree 2 whose neighbours are u and w, then $|N(u) \cap N(w)| = 2$.*

For $n \geqslant 3$, we use $\mathscr{H}_n$ to denote the set of all the maximal outerplanar graphs with n vertices:

$$\mathscr{H}_n = \{G \mid G \text{ is a maximal outerplanar graph and } |V(G)| = n\}.$$

The maximal outerplanar graphs represent a series of an important class of molecules (see, e.g., Refs. 27, 28). In Ref. 26, the authors investigated sharp lower and upper bounds for Zagreb indices among all maximal outerplanar graphs, and the corresponding extremal graphs were also completely characterized.

Every tree consists of at least two pendent vertices and some maximum degree vertices. Hence it is interesting to consider the trees with a fixed number of maximum degree vertices. Let $\mathscr{T}_{n,k}$ be the class of trees with n vertices that have exactly k ($k \leqslant n-2$) vertices having the maximum degree:

$$\mathscr{T}_{n,k} = \{T \mid T \text{ is a tree with } n \text{ vertices and has exactly } k \text{ maximum degree vertices}\}.$$

More recently, Lin[11] determined the trees that maximize the Wiener index (which is defined as the sum of distances over all unordered vertex pairs in a graph) in the class of $\mathscr{T}_{n,k}$. Borovicanin et al[29] discussed the maximum and minimum Zagreb indices of trees with a given number of vertices of maximum degree, and the extremal graphs were also characterized.

To our best knowledge, the general zeroth-order Randić index of graphs in $\mathscr{H}_n$ and $\mathscr{T}_{n,k}$ have not been considered in the chemical literature so far. Inspired by the ideas of Refs. 26, 29, here we consider the problem of maximizing and minimizing the general zeroth-order Randić index among maximal outerplanar graphs. In addition, we investigate the maximum and minimum general zeroth-order Randić index of trees with a given number of vertices of maximum degree. The corresponding extremal graphs are also characterized.

THE GENERAL ZEROTH-ORDER RANDIĆ INDEX IN $\mathscr{H}_n$

In this section, we shall determine the trees with maximal and minimal general zeroth-order Randić index in the class $\mathscr{H}_n$. Let S be a subset of $V(G)$. Let $G[S]$ denote the subgraph of G induced by S. The distance between a vertex u and S is defined

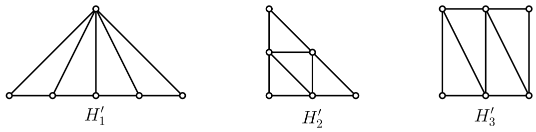

Fig. 1 Graphs $H_1' = K_1 \vee P_5$, H_2', and $H_3' = P_6^2$.

as $\min_{v\in S} d_G(u,v)$ and is denoted by $d_G(u,S)$. The neighbourhood of a vertex u of G is the set $\{x \in V(G) \mid d_G(x,u) = 1\}$ and is denoted by $N_G(u)$.

For a given graph G, we will use $G-x$ to denote the graph that arises from G by deleting the vertex x of G. The join of two graphs G and H, denoted by $G \vee H$, is obtained by adding an edge from each vertex in G to each vertex in H. For example the graph $H_1' = K_1 \vee P_5$ is the join of K_1 and P_5 in Fig. 1.

We use $\mathscr{G}_n^+$ to denote the class of n-vertex maximal outerplanar graphs each of which, say G, satisfies the following properties: (i) there exists a vertex v in G of degree 2 whose neighbours are u and w; (ii) for any vertex x in $V(G)-\{u,w\}$, at least one of $xu \in E(G)$ and $xw \in E(G)$ holds. It is easy to see that $K_1 \vee P_{n-1} \in \mathscr{G}_n^+$.

For any integer k, we use G^k to denote the *k-power graph* of G which is obtained from G by adding new edges joining all pairs of vertices a distance k apart. In particular, G^1 is the graph G itself. For example, H_3' in Fig. 1 is an illustration of P_6^2.

Lemma 1 (Ref. 26) *Let G be a maximal outerplanar graph on $n \geqslant 5$ vertices. If v is a vertex of degree 2 whose neighbours are u and w, then $7 \leqslant d(u)+d(w) \leqslant n+2$. The left equality holds if and only if $G[N(u)\cup N(w)] \cong P_5^2$, and the right equality holds if and only if $G \in \mathscr{G}_n^+$.*

The following lemma is easily checked.

Lemma 2 *For $n \geqslant 4$, we have*

$$R_\alpha^0(K_1 \vee P_{n-1}) = (n-1)^\alpha + 3^\alpha(n-3) + 2^{\alpha+1},$$
$$R_\alpha^0(P_n^2) = 4^\alpha(n-4) + 2\cdot 3^\alpha + 2^{\alpha+1}.$$

Theorem 1 *Let G be a maximal outerplanar graph on $n \geqslant 4$ vertices. Then for any $\alpha > 1$ or $\alpha < 0$, we have*

$$R_\alpha^0(G) \geqslant 4^\alpha(n-4) + 2\cdot 3^\alpha + 2^{\alpha+1}$$

with the equality if and only if $G \cong P_n^2$.

Proof: Note that for $n = 4$, $\mathscr{H}_n$ contains exactly one graph P_n^2. The result is clearly true. In the following we proceed by induction on $n \geqslant 5$. Without loss of generality, we assume that the result holds for all maximal outerplanar graphs of order less than n. Let G be a maximal outerplanar graph on n vertices. If $G \cong P_n^2$, then by Lemma 2, we are done. It suffices to prove that $R_\alpha^0(G) > 4^\alpha(n-4) + 2\cdot 3^\alpha + 2^{\alpha+1}$ if $G \ncong P_n^2$.

Since G is a maximal outerplanar graph, there must exist vertices of degree two. We can choose a vertex v of degree 2 whose neighbours are u, w such that $d(u)+d(w)$ is as small as possible. Let $G' = G-v$. Then G' is a maximal outerplanar graph of order $n-1$. It is also clear that $d_{G'}(u) = d_G(u)-1$, $d_{G'}(w) = d_G(w)-1$, and $d_{G'}(z) = d_G(z)$ for all vertices z in $V_G\setminus\{v,u,w\}$.

Note that $G \ncong P_n^2$ and we have $G' \ncong P_{n-1}^2$ by the choice of v. By inductive hypothesis we have

$$R_\alpha^0(G') > R_\alpha^0(P_{n-1}^2).$$

It follows from Lemma 1 that $d_G(u)+d_G(w) \geqslant 7$ and the equality holds if and only if $G[N(u)\cup N(w)] \cong P_5^2$. Combining Proposition 1 and Proposition 2, we conclude that $d_G(u) \geqslant 3$, $d_G(w) \geqslant 3$. Without loss of generality, we assume that $d_G(u) \geqslant 3$ and $d_G(w) \geqslant 4$. Hence

$$\big(d_G(u)\big)^\alpha - \big(d_G(u)-1\big)^\alpha \geqslant 3^\alpha - 2^\alpha,$$
$$\big(d_G(w)\big)^\alpha - \big(d_G(w)-1\big)^\alpha \geqslant 4^\alpha - 3^\alpha.$$

Hence we have

$$\begin{aligned} R_\alpha^0(G) &= R_\alpha^0(G') + \big(d_G(v)\big)^\alpha + \Big(\big(d_G(u)\big)^\alpha \\ &\quad - \big(d_{G'}(u)\big)^\alpha\Big) + \Big(\big(d_G(w)\big)^\alpha - \big(d_{G'}(w)\big)^\alpha\Big) \\ &= R_\alpha^0(G') + \Big(\big(d_G(u)\big)^\alpha - \big(d_G(u)-1\big)^\alpha\Big) \\ &\quad + 2^\alpha + \Big(\big(d_G(w)\big)^\alpha - \big(d_G(w)-1\big)^\alpha\Big) \\ &\geqslant R_\alpha^0(P_{n-1}^2) + 2^\alpha + \big(3^\alpha - 2^\alpha\big) + \big(4^\alpha - 3^\alpha\big) \\ &= 4^\alpha(n-5) + 2\cdot 3^\alpha + 2^{\alpha+1} + 4^\alpha \\ &= 4^\alpha(n-4) + 2\cdot 3^\alpha + 2^{\alpha+1} \\ &= R_\alpha^0(P_n^2). \end{aligned}$$

□

If $\alpha = 2$ in Theorem 1, we immediately obtain the following result.

Corollary 1 (Ref. 26) *Let G be a maximal outerplanar graph on $n \geqslant 4$ vertices. Then $M_1(G) \geqslant 16n-38$, with the equality if and only if $G \cong P_n^2$.*

Finally, we will give a complete characterization of maximal outerplanar graphs with maximal general zeroth-order Randić index.

Theorem 2 *Let G be a maximal outerplanar graph on $n \geqslant 4$ vertices. Then for $\alpha > 2$, we have*

$$R^0_\alpha(G) \leqslant (n-1)^\alpha + (n-3)3^\alpha + 2^{\alpha+1}$$

with equality if and only if $G \cong K_1 \vee P_{n-1}$.

Proof: Note that for $n = 4$, $\mathscr{H}_n$ contains exactly one graph P^2_n. The result is clearly true. Now we consider the case of $n \geqslant 5$. Assume that the result holds for all maximal outerplanar graphs of order less than n. Let G be a maximal outerplanar graph on n vertices, and v be a vertex of degree 2 in G whose neighbours are u, w.

Let $G' = G - v$, which is also a maximal outerplanar graph of order $n-1$. By inductive hypothesis, $R^0_\alpha(G') \leqslant R^0_\alpha(K_1 \vee P_{n-2}) = (n-2)^\alpha + (n-4)\cdot 3^\alpha + 2^{\alpha+1}$, and the equality holds if and only if $G' \cong K_1 \vee P_{n-2}$. Note that $G' = G - v$. We have $d_{G'}(u) = d_G(u) - 1$, $d_{G'}(w) = d_G(w) - 1$, and for all vertices z in $V_G \backslash \{v, u, w\}$, $d_{G'}(z) = d_G(z)$. It follows from Lemma 1 that $7 \leqslant d_G(u) + d_G(w) \leqslant n+2$ and so

$$5 \leqslant (d_G(u)-1) + (d_G(w)-1) \leqslant n+2-2.$$

By Proposition 1 and 2, we immediately obtain

$$(d_G(u)-1) \geqslant 2\ ,\ \ (d_G(u)-1) \geqslant 2.$$

Let $f(x)$ be a function defined above. For any positive integers x_1, x_2, x_3, x_4 with $x_1 < x_3 < x_4 < x_2$, we have $f(x_1) + f(x_2) \geqslant f(x_3) + f(x_4)$. From this and the inductive hypothesis we obtain

$$\begin{aligned}
R^0_\alpha(G) &= R^0_\alpha(G') + \big(d_G(v)\big)^\alpha + \big(d_G(u)\big)^\alpha \\
&\quad - \big(d_{G'}(u)\big)^\alpha + \big(d_G(w)\big)^\alpha - \big(d_{G'}(w)\big)^\alpha \\
&= R^0_\alpha(G') + 2^\alpha + \big(d_{G'}(u)+1\big)^\alpha \\
&\quad - \big(d_{G'}(u)\big)^\alpha + \big(d_{G'}(w)+1\big)^\alpha - \big(d_{G'}(w)\big)^\alpha \\
&\leqslant \big((n-2)^\alpha + (n-4)3^\alpha + 2^{\alpha+1}\big) \\
&\quad + 2^\alpha + 3^\alpha - 2^\alpha + (n-1)^\alpha - (n-2)^\alpha \\
&= (n-1)^\alpha + (n-3)3^\alpha + 2^{\alpha+1}.
\end{aligned}$$

The equality holds if and only if $G' \cong K_1 \vee P_{n-2}$ and $G \in \mathscr{G}^+_n$, which is equivalent to $G \cong K_1 \vee P_{n-1}$. □

The following is an immediate consequence of Theorem 2, which was also proved by Hou et al in Ref. 26.

Corollary 2 *Let G be a maximal outerplanar graph on $n \geqslant 4$ vertices. Then (i) if $n = 6$, $M_1(G) \leqslant 60$, with equality if and only if $G \cong K_1 \vee P_5$ or H'_2 which is depicted in Fig. 1; (ii) if $n \neq 6$, then $M_1(G) \leqslant n^2 + 7n - 18$, with equality if and only if $G \cong K_1 \vee P_{n-1}$.*

THE GENERAL ZEROTH-ORDER RANDIĆ INDEX IN $\mathscr{T}_{n,k}$

In this section, we shall determine the trees with maximal and minimal general zeroth-order Randić index in the class $\mathscr{T}_{n,k}$.

Lemma 3 (Ref. 29) *If $T \in \mathscr{T}_{n,k}$ is a tree with the maximum vertex degree Δ, then $\Delta \leqslant \lfloor((n-2)/k)\rfloor + 1$.*

Let $\pi = (d_1, d_2, \dots, d_n)$ be a sequence of positive integers, which is called a *degree sequence* of G if $d_i = d_G(v)$ holds for $i = 1, 2, \dots, n$ and $v \in V(G)$. For convenience, in the following we always assume that $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$.

Lemma 4 (Ref. 30) *A non-decreasing sequence $\pi = (d_1, d_2, \dots, d_n)$ of non-negative integers, whose sum is even is graphic if and only if*

$$\sum_{l=1}^{k} d_l \leqslant k(k-1) + \sum_{l=k+1}^{n} \min\{d_l, k\}$$

for every k, $1 \leqslant k \leqslant n$.

Lemma 5 *Let $T_{\max}$ be the tree with maximum general zeroth-order Randić index for $\alpha > 1$ or $\alpha < 0$ in $\mathscr{T}_{n,k}$. Then its maximum vertex degree is equal to $\lfloor((n-2)/k)\rfloor + 1$.*

Proof: Let $\{v_1, v_2, \dots, v_n\}$ be the vertex set of the tree $T_{\max}$ with the degree sequence $\pi = (d_1, d_2, \dots, d_n)$, and Δ be the maximum vertex degree in the tree $T_{\max}$. From Lemma 3, it follows that $\Delta \leqslant \lfloor((n-2)/k)\rfloor + 1$.

To show the result, it suffices to prove that $\Delta < \lfloor((n-2)/k)\rfloor + 1$ cannot occur. In the following we use induction, and so

$$\begin{aligned}
\Delta = d_1 = d_2 = \cdots = d_k &= \left\lfloor \frac{n-2}{k} \right\rfloor + 1 - t \\
&= \frac{n-2}{k} - a + 1 - t,
\end{aligned}$$

where $0 \leqslant a < 1$ and $t \geqslant 1$. Denote the number of vertices of degree i in $T_{\max}$ by n_i. Then $\sum_{i=1}^{\Delta} n_i = n$ and $\sum_{i=1}^{\Delta} i n_i = 2(n-1)$. Hence

$$\sum_{i=2}^{\Delta} (i-1) n_i = n-2.$$

Hence

$$\sum_{i=2}^{\Delta-1}(i-1)n_i = n-2-k(\Delta-1) = n-2-k\left(\left\lfloor\frac{n-2}{k}\right\rfloor - t\right) = n-2-k\left(\frac{n-2}{k}-a-t\right) = k(a+t)\geqslant k.$$

For any integer $k<i\leqslant n$, let $v_i \in V(T_{\max})$ be a vertex with degree $d_i \in [2,\Delta-1]$. Define the following sequence

$$\pi_1 = (\underline{d_1^1}, d_2^1, \dots, d_{i-1}^1, \underline{d_i^1}, d_{i+1}^1, \dots, d_{j-1}^1, d_j^1, d_{j+1}^1, \dots, d_n^1) = (\underline{d_1+1}, d_2, \dots, d_{i-1}, \underline{d_i-1}, d_{i+1}, \dots, d_{j-1}, d_j, d_{j+1}, \dots, d_n).$$

It follows from Lemma 4 that π_1 is a degree sequence of some graph, say G'. Comparing the structure of G' and $T_{\max}$, one can find that G' is exactly a tree, say T_1. By simple calculation,

$$R_\alpha^0(T_1)-R_\alpha^0(T_{\max}) = (d_1+1)^\alpha - d_1^\alpha + (d_i-1)^\alpha - d_i^\alpha = (d_1+1)^\alpha - d_1^\alpha - (d_i^\alpha - (d_i-1)^\alpha) > 0.$$

It follows from this fact that the transformation $T_1 \to T_{\max}$ increases the value of the general zeroth-order Randić index, but $T_1 \notin \mathscr{T}_{n,k}$.

Note that $\sum_{i=2}^{\Delta-1}(i-1)n_i$ is at least k. We can repeat the above transformation k times on every vertex of degree Δ in the tree $T_{\max}$. Each step produces a tree T_l, $l=1,2,\dots,k$, with the degree sequence

$$\pi_l = (\underline{d_1^l}, d_2^l, \dots, d_{i-1}^l, \underline{d_i^l}, d_{i+1}^l, \dots, d_{j-1}^l, d_j^l, d_{j+1}^l, \dots, d_n^l) = (\underline{\Delta+1}, d_2^{l-1}, \dots, d_{i-1}^{l-1}, \underline{d_i^{l-1}-1}, d_{i+1}^{l-1}, \dots, d_{j-1}^{l-1}, d_j^{l-1}, d_{j+1}^{l-1}, \dots, d_n^{l-1})$$

where $j \in \{1,2,\dots,n\}$ and $j \neq i,l$, and d_i^{l-1} is the degree of an arbitrary vertex v_i in the resulting tree T_{l-1} for $k<i\leqslant n$.

By using a similar approach, we obtain

$$R_\alpha^0(T_k) > R_\alpha^0(T_{k-1}) > \cdots > R_\alpha^0(T_1) > R_\alpha^0(T_{\max})$$

and easily see that $T_k \in \mathscr{T}_{n,k}$ is a tree with maximal vertex degree $\Delta+1$, which contradicts the initial hypothesis. This proves that $\Delta = \lfloor((n-2)/k)\rfloor + 1$. □

Theorem 3 *Let $T\in\mathscr{T}_{n,k}$, $1\leqslant k\leqslant \frac{1}{2}n-1$. Then for $\alpha>1$ or $\alpha<0$, we have*

$$R_\alpha^0(T) \leqslant k\Delta^\alpha + p(\Delta-1)^\alpha + \mu^\alpha + n-k-p-1$$

with equality if and only if T has the degree sequence

$$(\underbrace{\Delta,\dots,\Delta}_{k}, \underbrace{\Delta-1,\dots,\Delta-1}_{p}, \mu, \underbrace{1,\dots,1}_{n-k-p-1})$$

for $\Delta = \lfloor((n-2)/k)\rfloor+1$, $p=\lfloor((n-2-k(\Delta-1))/(\Delta-2))\rfloor$ and $\mu = n-1-k(\Delta-1)-p(\Delta-2)$.

Proof: Let $\pi=(d_1,d_2,\dots,d_n)$ be the degree sequence of a tree $T_{\max}$ with maximal general zeroth-order Randić index in the class $\mathscr{T}_{n,k}$. Then, by Lemma 5, we have that $d_1=d_2=\cdots=d_k=\Delta=\lfloor((n-2)/k)\rfloor+1$.

The number of vertices of degree $\Delta-1$ is equal to

$$p = n_{\Delta-1} = \left\lfloor \frac{n-2-k(\Delta-1)}{\Delta-2}\right\rfloor. \qquad (1)$$

To show this, as is mentioned in Lemma 5

$$\sum_{i=2}^{\Delta-1}(i-1)n_i = n-2-k(\Delta-1) = n-2-k\left(\left\lfloor\frac{n-2}{k}\right\rfloor - t\right) = ka = r,$$

where $0\leqslant r<k$. Note that n_i is a positive integer for each $i=2,3,\dots,\Delta-1$, it follows that $p=n_{\Delta-1}\leqslant r/(\Delta-2)$ and consequently we obtain $p\leqslant\lfloor(r/(\Delta-2))\rfloor$. This completes the proof of (1).

In the following we will show that $p=\lfloor(r/(\Delta-2))\rfloor$. Without loss of generality, we assume that $p<\lfloor(r/(\Delta-2))\rfloor$, i.e., $p\leqslant\lfloor(r/(\Delta-2))\rfloor-1$. Then

$$\sum_{i=2}^{\Delta-2}(i-1)n_i = r-(\Delta-2)p \geqslant r-(\Delta-2)\left(\left\lfloor\frac{r}{\Delta-2}\right\rfloor - 1\right) \geqslant \Delta-2.$$

Furthermore, according to the analysis we have

$$\pi = (d_1,d_2,\dots,d_n) = (\underbrace{\Delta,\Delta,\dots,\Delta}_{k}, d_{k+1}, d_{k+2}, \dots, d_{k+j_1}, \cdots, d_{k+i_1}, \dots, d_{k+r}, 1,1,\dots,1)$$

and there exists two distinct numbers d_{k+j_1} and d_{k+i_1} for $1\leqslant j_1<i_1\leqslant r$ such that $d_{k+j_1}=j>d_{k+i_1}=i$ or there exists two numbers such that $d_{k+j_1} = d_{k+i_1} = i$ for $n_i \geqslant 2$.

Define a degree sequence of positive integers as follows

$$\begin{aligned}\pi' &= (d'_1, d'_2, \dots, d'_k, d'_{k+1}, \dots, d'_{k+j_1-1}, \underline{d'_{k+j_1}},\\ &\quad d'_{k+j_1+1}, \dots, d'_{k+i_1-1}, \underline{d'_{k+i_1}}, d'_{k+i_1+1}, \dots, d'_n)\\ &= (d_1, d_2, \dots, d_k, d_{k+1}, \dots, d_{k+j_1-1}, \underline{d_{k+j_1}+1},\\ &\quad \cdots, d_{k+i_1-1}, \underline{d_{k+i_1}-1}, d_{k+i_1+1}, \dots, d_n).\end{aligned}$$

Note that $\sum_{i=1}^{n} d'_i = 2n-2$. Hence π' must be the degree sequence of a tree T' with k maximum degree vertices. Equivalently, $T' \in \mathscr{T}_{n,k}$. On the other hand,

$$\begin{aligned}&R^0_\alpha(T') - R^0_\alpha(T_{\max})\\ &\quad = (j+1)^\alpha - j^\alpha + (i-1)^\alpha - i^\alpha\\ &\quad = (j+1)^\alpha - j^\alpha - (i^\alpha - (i-1)^\alpha) > 0,\end{aligned}$$

again a contradiction with the initial hypothesis. Hence

$$p = n_{\Delta-1} = \left\lfloor \frac{r}{\Delta-2} \right\rfloor = \left\lfloor \frac{n-2-k(\Delta-1)}{\Delta-2} \right\rfloor.$$

We now show that there exists one vertex with degree $\mu = n-1-k(\Delta-1)-p(\Delta-2)$. To show this it is easy to prove that it has to be $n_\mu = 1$, where $\mu = r-p(\Delta-2)+1$, i.e., $\mu = n-1-k(\Delta-1)-p(\Delta-2)$, otherwise, there would produce a tree T'' whose R^0_α-value is greater than that of $T_{\max}$. Hence it follows from this and (1) that the tree $T_{\max}$ with maximal general zeroth-order Randić index in the class $\mathscr{T}_{n,k}$ has the vertex degree sequence

$$\pi = (\underbrace{\Delta, \dots, \Delta}_{k}, \underbrace{\Delta-1, \dots, \Delta-1}_{p}, \mu, \underbrace{1, \dots, 1}_{n-k-p-1})$$

and consequently we obtain $R^0_\alpha(T_{\max}) = k\Delta^\alpha + p(\Delta-1)^\alpha + \mu^\alpha + n - k - p - 1$. □

In the following, we will describe the tree with minimum general zeroth-order Randić index in $\mathscr{T}_{n,k}$, using a similar idea to that used in Ref. 31.

Lemma 6 *Let $T_{\min}$ be a tree with minimal general zeroth-order Randić index for $\alpha > 1$ or $\alpha < 0$ in the class $\mathscr{T}_{n,k}$, where $1 \leqslant k \leqslant \frac{1}{2}n - 1$. Then its maximum vertex degree Δ equals 3.*

Proof by contradiction: In what follows we assume that $\Delta \geqslant 4$. Let u be a vertex of maximum degree Δ in $T_{\min}$ and $P = v_0 v_1 \cdots v_{i-1} v_i v_{i+1} \cdots v_l$ be the longest path in $T_{\min}$ that contains $u = v_i$. In addition, let v_{i-1}, v_{i+1} and $u_1, u_2, \dots, u_{\Delta-2}$ be the vertices adjacent to u in $T_{\min}$, and z_1 a pendent vertex connected to u via u_1 (it is possible that $z_1 \equiv u_1$). Let T^1 be a tree obtained in the following way:

$$T^1 = T_{\min} - uu_2 + u_2 z_1.$$

By some computations, for $\alpha < 0$ or $\alpha > 1$, we have

$$\begin{aligned}&R^0_\alpha(T^1) - R^0_\alpha(T_{\min})\\ &\quad = (\Delta-1)^\alpha + 2^\alpha - \Delta^\alpha - 1\\ &\quad = 2^\alpha - 1 - (\Delta^\alpha - (\Delta-1)^\alpha)\\ &\quad < 0\end{aligned}$$

which shows that the transformation $T_{\min} \to T^1$ decreases the R^0_α-value, but $T^1 \notin \mathscr{T}_{n,k}$. The transformation described above repeated k times on every vertex u of degree Δ would produce a sequence of trees $T^1, T^2, \dots, T^k$, which satisfy

$$R^0_\alpha(T^k) < R^0_\alpha(T^{k-1}) < \cdots < R^0_\alpha(T^2) < R^0_\alpha(T^1).$$

It follows that T^k has exactly k maximum degree vertices with degree $\Delta - 1$. Consequently, we have $T^k \in \mathscr{T}_{n,k}$. Again a contradiction. □

Theorem 4 *Let $T \in \mathscr{T}_{n,k}$, where $1 \leqslant k \leqslant \frac{1}{2}n - 1$. Then for $\alpha > 1$ or $\alpha < 0$ we have*

$$R^0_\alpha(T) \geqslant 3^\alpha k + 2^\alpha(n-2k-2) + k + 2$$

with equality if and only if the tree T has the degree sequence

$$(\underbrace{3, 3, \dots, 3}_{k}, \underbrace{2, 2, \dots, 2}_{n-2k-2}, \underbrace{1, 1, \dots, 1}_{k+2}).$$

Proof: Let $T_{\min}$ be a tree with minimal general zeroth-order Randić index in the class $\mathscr{T}_{n,k}$. By Lemma 6, the vertex degree sequence of $T_{\min}$ is

$$\pi = (\underbrace{3, 3, \dots, 3}_{k}, \underbrace{2, 2, \dots, 2}_{n_2}, \underbrace{1, 1, \dots, 1}_{n_1}),$$

when $k \leqslant \frac{1}{2}n - 1$. It follows that $n_1 + 2n_2 + 3k = 2(n_1 + n_2 + k) - 2$, which implies that $n_1 = k + 2$ and $n_2 = n - 2k - 2$. Hence $R^0_\alpha(T_{\min}) = 3^\alpha k + 2^\alpha(n - 2k - 2) + k + 2$. □

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