On the zeroth-order general Randić index of cacti

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Abstract

The zeroth-order general Randić index of a graph G is defined as ${}^0R_\alpha = \sum_{v \in V(G)} d(v)^\alpha$, where $d(v)$ is the degree of the vertex v in G and α is an arbitrary real number. In the paper, we give sharp lower and upper bounds on the zeroth-order general Randić index of cacti.

Keywords: zeroth-order general Randić index, cacti, cycle

1. Introduction

Let $G = (V, E)$ be a graph. The Randić (or connectivity) index of G was introduced by Randić in 1975 and is defined as [21]

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

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where $d(u)$ and $d(v)$ are the degrees of u and v. This index had been showed closely correlated with many chemical properties [11] and found to parallel the boiling point, Kovats constants, and a calculated surface. So it has become one of the most popular molecular descriptors, the interesting reader is referred to [1]-[8], [16]-[19] and [22]. The zeroth-order Randić index of G, conceived by Kier and Hall [12], is $R^0(G) = \sum_{v \in V(G)} d(v)^{-\frac{1}{2}}$ and Pavlović determined the graphs with maximum value of $R^0(G)$ [20]. Li et al. [13] investigated the same problem for the topological index $M_1(G)$, also known as Zagreb indices, that is defined as $M_1(G) = \sum_{v \in V(G)} d(v)^2$. In 2005, Li and Zheng [15] defined the zeroth-order general Randić index of a graph G as ${}^0R_\alpha(G) = \sum_{v \in V(G)} d(v)^\alpha$, 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. We call G a *cacti* if all of blocks of G are either edges or cycles. Denote $G(n, r)$ the set of cacti of order n and with r cycles. Obviously, $G(n, 0)$ are trees and $G(n, 1)$ are unicyclic graphs. The degree and the neighborhood of a vertex $u \in V$ will be denoted by $d(u)$ and $N(u)$, respectively. Let $P = v_1 v_2 \cdots v_k$ be a path. We call P an *internal path*, if $d(v_1)$, $d(v_k) \geq 3$ and $d(v_2) = \cdots = d(v_{k-1}) = 2$ (if $k \geq 3$). 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. In [18], Lu et al. gave sharp lower bound on the Randić index of cacti. [17], Liu et al presented a unified approach to the cacti for some indices. In this paper, we will give sharp lower and upper bounds on the zeroth-order general Randić index of cacti.

Let $G \in G(n,r)$. Then $|E(G)| = m = n + r - 1$. If $\alpha = 0$, then ${}^0R_0(G) = \sum_{v \in V(G)} d(v)^0 = n$. If $\alpha = 1$, then ${}^0R_1(G) = \sum_{v \in V(G)} d(v) = 2m = 2(n + r - 1)$. Thus we always assume that $\alpha \neq 0, 1$ in the following sections.

2. Some Lemmas

Let $G \in G(n,r)$. Firstly, we will give some lemmas which will be used in Section 3.

Lemma 2.1. *Let $G \in G(n,r)$ and C_i a cycle of G. If ${}^0R_\alpha(G)$ is as small as possible for $0 < \alpha < 1$ or ${}^0R_\alpha(G)$ is as large as possible for $\alpha > 1$ or $\alpha < 0$, then $|A_{C_i}| = 1$, where $A_{C_i} = \{v : v \in V(C_i),\ d(v) \geq 3\}$.*

Proof. Suppose $|A_{C_i}| \geq 2$. Then there exist u, $v \in A_{C_i}$. Assume, without loss of generality, that $d(v) \geq d(u) \geq 3$. Set $N(u) \setminus V(C_i) = \{u_1, \cdots, u_k\}$, then $k \geq 1$. Since u, $v \in V(C_i)$ and $G \in G(n,r)$, $N(v) \cap \{u_1, \cdots, u_k\} = \emptyset$. Denote

$$G' = G - uu_1 - \cdots - uu_k + vu_1 + \cdots + vu_k.$$

Then $G' \in G(n,r)$ and

$$\begin{aligned} {}^0R_\alpha(G') - {}^0R_\alpha(G) &= [(d(u) - k)^\alpha + (d(v) + k)^\alpha] - [d(u)^\alpha + d(v)^\alpha] \\ &= [(d(v) + k)^\alpha - d(v)^\alpha] - [d(u)^\alpha - (d(u) - k)^\alpha] \\ &= \alpha k(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $d(v) < \xi < d(v) + k$ and $d(u) - k < \eta < d(u)$. Since $d(u) \leq d(v)$, we have $d(u) - k < \eta < d(u) \leq d(v) < \xi < d(v) + k$. Thus we have ${}^0R_\alpha(G') <{}^0R_\alpha(G)$ for $0 < \alpha < 1$, and ${}^0R_\alpha(G') >{}^0R_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$, a contradiction. ∎

Lemma 2.2. *Let $G \in G(n,r)$ and uv be an edge which is not in any cycle of G. If ${}^0R_\alpha(G)$ is as small as possible for $0 < \alpha < 1$ or ${}^0R_\alpha(G)$ is as large as possible for $\alpha > 1$ or $\alpha < 0$, then $d(u) = 1$ or $d(v) = 1$.*

Proof. Suppose there exists an edge uv which is not in any cycle of G and $d(v) \geq d(u) \geq 2$. Set $N(u) \setminus \{v\} = \{u_1, \cdots, u_k\}$, then $k \geq 1$. Since uv does not contain in any cycle of G and $G \in G(n,r)$, $N(v) \cap \{u_1, \cdots, u_k\} = \emptyset$. Denote

$$G' = G - uu_1 - \cdots - uu_k + vu_1 + \cdots + vu_k.$$

Then $G' \in G(n,r)$ and by the same argument as that of Lemma 2.1, we have ${}^0R_\alpha(G') < {}^0R_\alpha(G)$ for $0 < \alpha < 1$ and ${}^0R_\alpha(G') >{}^0R_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$, a contradiction. ∎

Let $G \in G(n,r)$ and $C_1, C_2, \cdots, C_r$ the cycles of G. Denote $V(C) = \cup_{i=1}^{r} V(C_i)$.

Lemma 2.3. *Let $G \in G(n,r)$ with $r \geq 1$. If ${}^0R_\alpha(G)$ is as large as possible for $0 < \alpha < 1$ or ${}^0R_\alpha(G)$ is as small as possible for $\alpha > 1$ or $\alpha < 0$, then $d(u) \geq 2$ for any $u \in V(G)$.*

Proof. Suppose there exists $u \in V(G)$ such that $d(u) = 1$. Since $G \in G(n,r)$ and $r \geq 1$, there exists a cycle C_i and a vertex $v \in V(C_i)$ such that there is a path P connected u and v in G and $V(P) \cap V(C) = \{v\}$. Obviously, $d(v) \geq 3$. Let $w \in V(C_i)$ with

$wv \in E(G)$. Denote $G' = G - vw + wu$. Then $G' \in G(n,r)$ and

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

where $1 < \xi < 2$ and $d(v) - 1 < \eta < d(v)$. Since $d(v) \geq 3$, we have $1 < \xi < 2 \leq d(v) - 1 < \eta < d(v)$. Thus we have ${}^0R_\alpha(G') > {}^0R_\alpha(G)$ for $0 < \alpha < 1$ and ${}^0R_\alpha(G') < {}^0R_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$, a contradiction. ∎

Lemma 2.4. *Let $G \in G(n,r)$ with $r \geq 1$. If ${}^0R_\alpha(G)$ is as large as possible for $0 < \alpha < 1$ or ${}^0R_\alpha(G)$ is as small as possible for $\alpha > 1$ or $\alpha < 0$, then $d(u) \leq 4$ for any $u \in V(C)$.*

Proof. Suppose there exists a cycle C_i and $u \in V(C_i)$ such that $d(u) \geq 5$. Assume $N(u) \setminus V(C_i) = \{v_1, v_2, \cdots, v_k\}$. Then $k \geq 3$. Let H_i be the components contained v_i in $G - u$, $1 \leq i \leq k$. We will complete the proof by considering the following two cases.

Case 1. There exists i, say $i = 1$, such that $H_1 \neq H_j$ for any $2 \leq j \leq k$.

By $G \in G(n,r)$ and Lemma 2.3, there exists $v \in V(H_2)$ such that $d(v) = 2$. Denote $G' = G - uv_1 + vv_1$. Then $G' \in G(n,r)$ and

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

where $2 < \xi < 3$ and $d(u) - 1 < \eta < d(u)$. Since $d(u) \geq 5$, we have $2 < \xi < 3 < d(u) - 1 < \eta < d(u)$. Thus we have ${}^0R_\alpha(G') > {}^0R_\alpha(G)$

for $0 < \alpha < 1$ and ${}^0R_\alpha(G') <{}^0R_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$, a contradiction.

Case 2. For any i $(1 \leq i \leq k)$, there exists j such that $H_i = H_j$, where $1 \leq j \leq k$ and $i \neq j$.

In the case, we have $d(u) \geq 6$. Assume, without loss of generality, that $H_1 = H_2$. Then v_1, v_2 contain in a common cycle and $H_3 \neq H_1$ by the definition of cacti. By Lemma 2.3, there exists $v \in V(H_3)$ such that $d(v) = 2$. Denote $G' = G - uv_1 - uv_2 + vv_1 + vv_2$. Then $G' \in G(n,r)$ and

$$\begin{aligned} {}^0R_\alpha(G') -{}^0 R_\alpha(G) &= [(d(u)-2)^\alpha + 4^\alpha] - [d(u)^\alpha + 2^\alpha] \\ &= (4^\alpha - 2^\alpha) - [d(u)^\alpha - (d(u)-2)^\alpha] \\ &= 2\alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $2 < \xi < 4$ and $d(u) - 2 < \eta < d(u)$. Since $d(u) \geq 6$, we have $2 < \xi < 4 \leq d(u) - 1 < \eta < d(u)$. Thus when $0 < \alpha < 1$, we have ${}^0R_\alpha(G') >{}^0R_\alpha(G)$ and when $\alpha > 1$ or $\alpha < 0$, we have ${}^0R_\alpha(G') <{}^0R_\alpha(G)$, a contradiction. ∎

Lemma 2.5. *Let $G \in G(n,r)$ with $r \geq 1$. If ${}^0R_\alpha(G)$ is as large as possible for $0 < \alpha < 1$ or ${}^0R_\alpha(G)$ is as small as possible for $\alpha > 1$ or $\alpha < 0$, then $d(u) \leq 3$ for any vertex $u \notin V(C)$.*

Proof. Suppose there exists a vertex $u \notin V(C)$ such that $d(u) \geq 4$. Assume $N(u) = \{v_1, v_2, \cdots, v_k\}$. Then $k \geq 4$. Let H_i be the components contained v_i in $G - u$, $1 \leq i \leq k$. Then $H_i \neq H_j$ for $i \neq j$. By $G \in G(n,r)$ and Lemma 2.3, there exists $v \in V(H_2)$ such that $d(v) = 2$. Denote $G' = G - uv_1 + vv_1$. Then $G' \in G(n,r)$ and

$${}^0R_\alpha(G') -{}^0 R_\alpha(G) = [(d(u)-1)^\alpha + 3^\alpha] - [d(u)^\alpha + 2^\alpha]$$

$$= (3^\alpha - 2^\alpha) - [d(u)^\alpha - (d(u)-1)^\alpha]$$

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

where $2 < \xi < 3$ and $d(u) - 1 < \eta < d(u)$. Since $d(u) \geq 4$, we have $2 < \xi < 3 \leq d(u) - 1 < \eta < d(u)$. Thus we have ${}^0R_\alpha(G') > {}^0R_\alpha(G)$ for $0 < \alpha < 1$ and ${}^0R_\alpha(G') < {}^0R_\alpha(G)$ for $\alpha > 1$ or $\alpha < 0$, a contradiction. ■

Denote $A_4 = \{v \in V(G) : d(v) = 4\}$. Then we have the following result.

Lemma 2.6. *Let $G \in G(n,r)$ $(r \geq 1)$ and $n = 2r + k$, where $k \geq 1$. If ${}^0R_\alpha(G)$ is as large as possible for $0 < \alpha < 1$ or ${}^0R_\alpha(G)$ is as small as possible for $\alpha > 1$ or $\alpha < 0$, then $|A_4| = r - k$ when $1 \leq k \leq r-1$ and $|A_4| = 0$ when $k \geq r$.*

Proof. If $r = 1$, then G is a cycle by Lemma 2.3 and the result holds immediately. So we can assume that $r \geq 2$. Denote $A_3(G) = \{u : d(u) = 3,\ u \notin V(C)\}$. Choose $G \in G(n,r)$ $(r \geq 2)$ and $n = 2r+k$ such that ${}^0R_\alpha(G)$ is as large as possible for $0 < \alpha < 1$ or ${}^0R_\alpha(G)$ is as small as possible for $\alpha > 1$ or $\alpha < 0$ and $|A_3(G)|$ is as small as possible. We first show that $|A_3(G)| = 0$.

Suppose there exists $u \in A_3(G)$. Let $N(u) = \{u_1, u_2, u_3\}$. Then there exists v with $d(v) = 2$ such that v and u_1 do not contain in the same component in $G - u$ by Lemma 2.3. Denote $G' = G - uu_1 + vu_1$. Then $G' \in G(n,r)$ and ${}^0R_\alpha(G') = {}^0R_\alpha(G)$, but $|A_3(G')| < |A_3(G)|$, a contradiction. Hence $|A_3(G)| = 0$.

Now we complete the proof.

If $k = 1$, then $|A_4| = r - 1$ by the definition of cacti. Suppose $2 \leq k \leq r-1$. Then $|A_4| \geq r - k$ by the definition of cacti. Assume

$|A_4| \geq r - k + 1 \geq 1$. Then there exists a cycle of length at least 4 or an internal path of length at least 2 by Lemmas 2.3, 2.4 and $|A_3(G)| = 0$. Choose $u \in A_4$ such that there is a cycle, say C_1, contained u and $(V(C_1)\backslash\{u\}) \cap A_4 = \emptyset$. By the definition of ${}^0R_\alpha(G)$, we can assume, without loss of generality, that length of C_1 at least 4. Let $C_1 = u_1(= u)u_2 \cdots u_s u_1$ $(s \geq 4)$. Denote $G' = G - u_1u_2 + u_su_2$. Then $G' \in G(n, r)$ and

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

where $2 < \xi < 3$ and $d(u) - 1 < \eta < d(u)$. Since $d(u) = 4$, we have $2 < \xi < 3 \leq d(u) - 1 < \eta < d(u)$. Thus when $0 < \alpha < 1$, we have ${}^0R_\alpha(G') > {}^0R_\alpha(G)$ and when $\alpha > 1$ or $\alpha < 0$, we have ${}^0R_\alpha(G') < {}^0R_\alpha(G)$, a contradiction.

If $k \geq r$, then we can show that $|A_4| = 0$ by the same argument.

■

3. Main Results

In the section, we use $G(n, r)$ to denote the set of cacti of order n and with r cycles and $G^0(n, r)$ to denote the cacti obtained from r triangles and $n - 2r - 1$ edges by taking one vertex of each triangle and each edge, and combining them as one vertex. Fig.1 and Fig.2 illustrate the graphs $G^0(n, r)$ with $n = 13$, $r = 3$ and $n = 5$, $r = 2$, respectively.

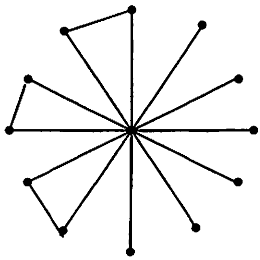

Fig. 1. $G^0(13,3)$

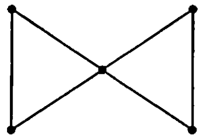

Fig. 2. $G^0(5,2)$

Now we have our main results.

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

$$^0R_\alpha(G) \geq 2^{\alpha+1}r + (n-1)^\alpha + (n-2r-1) \qquad \text{for} \quad 0<\alpha<1$$

and

$$^0R_\alpha(G) \leq 2^{\alpha+1}r + (n-1)^\alpha + (n-2r-1) \qquad \text{for} \quad \alpha>1 \quad \text{or} \quad \alpha<0.$$

The equalities hold if and only if $G \cong G^0(n,r)$.

Proof. Let $G \in G(n,r)$ such that $^0R_\alpha(G)$ is as small as possible for $0 < \alpha < 1$ or $^0R_\alpha(G)$ is as large as possible for $\alpha > 1$ or $\alpha < 0$. By Lemmas 2.1 and 2.2, all cycles and pendent edges of G with a common vertex, say u. So we just need to show that the length of each cycle of G is 3.

Suppose there exists a cycle C_i such that the length of C_i is at least 4. Let $C_i = v_1v_2\cdots v_kv_1$, without loss of generality, let v_1 be the vertex such that $d(v_1) \geq d(v_i)$, for $2 \leq i \leq k$. Then $k \geq 4$ and $d(v_1) \geq 2$. Denote $G' = G - v_2v_3 + v_1v_3$. Then $G' \in G(n,r)$ and

$$\begin{aligned} ^0R_\alpha(G') - ^0R_\alpha(G) &= [(d(v_1)+1)^\alpha + 1] - [d(v_1)^\alpha + 2^\alpha] \\ &= [(d(v_1)+1)^\alpha - d(v_1)^\alpha] - (2^\alpha - 1) \\ &= \alpha(\xi^{\alpha-1} - \eta^{\alpha-1}), \end{aligned}$$

where $d(v_1) < \xi < d(v_1)+1$ and $1 < \eta < 2$. Since $d(v_1) \geq 2$, we have $1 < \eta < 2 \leq d(v_1) < \xi < d(v_1)+1$. Thus we have ${}^0R_\alpha(G') <{}^0R_\alpha(G)$ when $0 < \alpha < 1$ and ${}^0R_\alpha(G') >{}^0R_\alpha(G)$ when $\alpha > 1$ or $\alpha < 0$, a contradiction.

Hence the length of each cycle of G is 3 which implies $G \cong G^0(n,r)$. Note that ${}^0R_\alpha(G^0) = 2^{\alpha+1}r+(n-1)^\alpha+(n-2r-1)$. Thus the conclusions of our theorem hold. ■

Let $G \in G(n,r)$. Denote $A_i(G) = \{u : d(u) = i, u \in V(G)\}$. If $r = 1$, then ${}^0R_\alpha(G) \leq n2^\alpha$ when $0 < \alpha < 1$ or ${}^0R_\alpha(G) \geq n2^\alpha$ when $\alpha > 1$ or $\alpha < 0$ by Lemma 2.3. So we will assume $r \geq 2$ in the next two theorems.

Theorem 3.2. *Let $G \in G(n,r)$ $(r \geq 2)$ and $n = 2r + k$, where $1 \leq k \leq r - 1$. Then*

$$ {}^0R_\alpha(G) \leq (r+2)2^{\alpha+1} + (r-k)4^\alpha + (2k-2)3^\alpha, \quad \text{for} \quad 0<\alpha<1 $$

$$ {}^0R_\alpha(G) \geq (r+2)2^{\alpha+1} + (r-k)4^\alpha + (2k-2)3^\alpha, \quad \text{for} \quad \alpha>1 \quad \text{or} \quad \alpha<0. $$

The equalities hold if and only if $|A_4(G)| = r - k$, $|A_3(G)| = 2k - 2$ and $|A_2(G)| = r + 2$.

Proof. Choose $G' \in G(n,r)$ such that ${}^0R_\alpha(G')$ is as large as possible for $0 < \alpha < 1$ or ${}^0R_\alpha(G')$ is as small as possible for $\alpha > 1$ or $\alpha < 0$. By Lemmas 2.3, 2.4 and 2.5, $2 \leq d(u) \leq 4$ for any $u \in V(G')$ and then $|A_j(G)| = 0$ for $j \geq 5$. By Lemma 2.6, $|A_4(G')| = r - k$. From the definition of cacti, we have $|A_3(G')| = 2k-2$ and $|A_2(G')| = r + 2$. Note that ${}^0R_\alpha(G') = (r+2)2^{\alpha+1} + (r-k)4^\alpha + (2k-2)3^\alpha$. Thus the conclusions of our theorem hold. ■

Theorem 3.3. *Let $G \in G(n,r)$ $(r \geq 2)$ and $n = 2r + k$, where*

$k \geq r$. *Then*

$$^0R_\alpha(G) \leq (2r-2)3^{\alpha+1} + (k+2)2^\alpha, \qquad \text{for} \quad 0 < \alpha < 1$$

$$^0R_\alpha(G) \geq (2r-2)3^{\alpha+1} + (k+2)2^\alpha, \qquad \text{for} \quad \alpha > 1 \quad \text{or} \quad \alpha < 0.$$

The equalities hold if and only if $|A_3(G)| = 2r+2$ *and* $|A_2(G)| = k+2$.

Proof. Choose $G' \in G(n,r)$ $(r \geq 2)$ such that $^0R_\alpha(G')$ is as large as possible for $0 < \alpha < 1$ or $^0R_\alpha(G')$ is as small as possible for $\alpha > 1$ or $\alpha < 0$. By Lemmas 2.3 and 2.6, we have $|A_j(G)| = 0$ for $j \geq 4$ and $2 \leq d(u) \leq 3$ for each $u \in V(G')$. So $|A_3(G')| = 2r+2$ by the definition of cacti and then $|A_2(G')| = k+2$. Since $^0R_\alpha(G') = (2r-2)3^{\alpha+1} + (k+2)2^\alpha$, our conclusion holds. ∎

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