A Note on the Zeroth–Order General Randić Index of Cacti and Polyomino Chains

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ABSTRACT. The present note is devoted to establish some extremal results for the zeroth–order general Randić index of cacti, characterize the extremal polyomino chains with respect to the aforementioned index, and hence to generalize two already reported results.

Keywords: Topological index, zeroth–order general Randić index, polyomino chain, cacti.

1. INTRODUCTION

Throughout this study, we consider only simple, finite and undirected graphs. For undefined notations and terminologies from (chemical) graph theory, see for example [16, 30]. Topological indices are numerical parameters of a molecular graph, which are invariant under graph isomorphism and reflect certain structural features of the corresponding molecule [30]. In 1975, Randić [28] introduced a topological index (and named it *branching index*, but nowadays this topological index is also known as *connectivity index* and the Randić *index*) for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. This index is defined as

$$R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-\frac{1}{2}}$$

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Received: October 13, 2014; Accepted: November 7, 2014.

where uv is the edge connecting the vertices u and v, d_u is the degree of the vertex u, and $E(G)$ is the edge set of the graph G. The Randić index is the most investigated, most often applied, and most popular among all topological indices. Hundreds of papers and a few books have been devoted to this topological index [13].

The Randić index has been modified in several ways. For instance, general Randić indices [5], higher-order Randić indices [20, 21], edge connectivity index [12], zeroth–order general Randić index [17, 18, 23, 29], and modified Randić index [11, 24] are some of the variants of the Randić index. Details about the Randić index and its modifications can be found in the recent papers [3, 4, 9, 24, 29], recent review [13], and related references cited therein. In the current study, we are concerned with the zeroth–order general Randić index which is defined as

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

where α is any real number different from 0 and 1. Li and Zheng [23] proposed this index and named it *first general Zagreb index*. But nowadays, most authors refer to it as to the zeroth–order general Randić index. At this point it is worth mentioning that R_2^0 and $R_{-0.5}^0$ correspond to the first Zagreb index [14] and zeroth–order Randić index [22] respectively.

A polyomino system (sometimes referred as a lattice animal of squares [10]) is a finite 2-connected plane graph such that each interior face (also known as "cell") is surrounded by a regular square of length one. Such system can be considered as an edge-connected union of cells in the planar square lattice. Details about the polyomino systems can be found in [2, 15, 19]. A polyomino system in which every square has only one or two neighboring squares is called a polyomino chain.

A connected graph G is a cactus if and only if every edge of G lies on at most one cycle. The problem of characterizing the extremal polyomino chains (respectively extremal cacti) with respect to the topological indices over the set of all polyomino chains (respectively cacti) with some fixed parameters has attracted substantial attention from researchers in recent years. For instance, the extremal results about polyomino chains (respectively about cacti) for several topological indices can be found in the recent papers [1, 3, 8, 27, 32] (respectively [6, 7, 25, 26, 31]) and related references cited therein. In this short note, we have attempted the aforementioned problems for the case of R_α^0 index. The second section is devoted to derive some extremal results for the R_α^0 index of cacti. In the third section, we have considered the set of all polyomino chains with fixed number of squares and characterized polyomino chains with the extremal R_α^0 index. Concluding remarks are given in the fourth section.

2. ZEROTH–ORDER GENERAL RANDIĆ INDEX OF CACTI

As usual, the star and cycle with n vertices are denoted by S_n and C_n respectively. Let $C_{n,k}$ be the class of all cacti with k cycles and $n \geq 5$ vertices. Let $G^0(n,k)$ be the cactus obtained from S_n by adding k mutually independent edges (see the Figure 1). Let us assume that $\psi(n,k) = (n-1)\,[(n-1)^{\alpha-1} + 1] + 2k(2^{\alpha}-1)$. To prove the main theorem of this section, we need some auxiliary results.

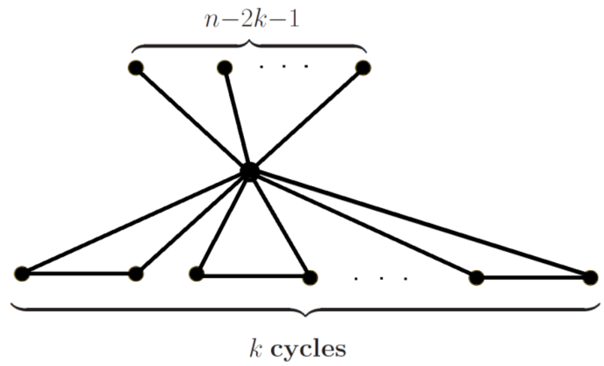

Figure 1. The Cactus $G^0(n,k)$.

Lemma 2.1. [17] *If T is a tree with n vertices, then*

$$R_{\alpha}^{0}(T)\begin{cases}\leq \psi(n,0) & if\ \alpha < 0\ or\ \alpha > 1\\ \geq \psi(n,0) & if\quad 0 < \alpha < 1,\end{cases}$$

with equalities if and only if $T \cong G^0(n,0)$.

Let us denote by (G_1,u) and (G_2,v) the graphs rooted at the vertices u and v, respectively. Let $G = (G_1,u) \bowtie (G_2,v)$ be the graph obtained from (G_1,u) and (G_2,v) by identifying u with v.

Theorem 2.2. [18] *If G is the unicyclic graph with n vertices and contains the cycle of length l, then*

$$R_{\alpha}^{0}(T)\begin{cases}\leq (n-l+2)^{\alpha} + (l-1)2^{\alpha} + n-l & if\ \ \alpha < 0\ or\ \alpha > 1\\ \geq (n-l+2)^{\alpha} + (l-1)2^{\alpha} + n-l & if\quad 0 < \alpha < 1,\end{cases}$$

with equalities if and only if $G \cong (C_l, u) \bowtie (S_{n-l+1}, v)$.

The following corollary is an immediate consequence of the Theorem 2.2.

Corollary 2.3. *Let G be any unicyclic graph with n vertices. Then*

$$R_\alpha^0(G)\begin{cases}\leq \psi(n,1) & if\ \alpha < 0\ or\ \alpha > 1\\ \geq \psi(n,1) & if\quad 0 < \alpha < 1,\end{cases}$$

with equalities if and only if $G \cong G^0(n,1)$.

Proof. Let us take $f(l) = (n - l + 2)^\alpha + (l-1)2^\alpha + n - l$, where $3 \leq l \leq n$. Then the Lagrange's mean-value theorem guarantees that there exist numbers $\Theta_1 \in (1,2)$ and $\Theta_2 \in (\Theta_1, n - l + 2)$ such that $f'(l) = \alpha(1-\alpha)(n - l + 2 - \Theta_1){\Theta_2}^{\alpha-2}$. Note that $f'(l)$ is positive (respectively negative) for $0 < \alpha < 1$ (respectively for $\alpha < 0$ or $\alpha > 1$). Hence the function $f(l)$ attains its minimum (respectively maximum) value at $l = 3$, for $0 < \alpha < 1$ (respectively for $\alpha < 0$ or $\alpha > 1$). Therefore, from the Theorem 2.2, desired result follows. ■

Lemma 2.4. *Let* $f(x) = x^\alpha - (x-p)^\alpha$, *where* $x > p \geq 1$. *Then* $f(x)$ *is decreasing (respectively increasing) for* $0 < \alpha < 1$ (*respectively for* $\alpha < 0$ *or* $\alpha > 1$).

Proof. Note that $f'(x) = p\alpha(\alpha-1)\Theta^{\alpha-2}$ where $x - p < \Theta < x$. It can be easily seen that $f'(x)$ is negative (respectively positive) for $0 < \alpha < 1$ (respectively for $\alpha < 0$ or $\alpha > 1$). ■

Now, we are ready to prove the main result of this section.

Theorem 2.5. *Let* G *be any cactus belongs to the collection* $C_{n,k}$. *Then*

$$R_\alpha^0(G)\begin{cases}\leq \psi(n,k) & if\ \alpha < 0\ or\ \alpha > 1\\ \geq \psi(n,k) & if\quad 0 < \alpha < 1,\end{cases}$$

with equalities if and only if $G \cong G^0(n,k)$.

Proof. We will use induction on $n + k$. For $k = 0,1$, the theorem directly follows from the Lemma 2.1 and Corollary 2.3. If $k = 2$, then for $n = 5$ there is only one cactus which is isomorphic to $G^0(5,2)$. So, let us assume that $G \in C_{n,k}$, where $k \geq 2$ and $n \geq 6$. We consider two cases:

Case 1. If G has at least one pendent vertex. Let u_0 be the pendent vertex adjacent with the vertex v and $d_v = x$. Let $N_G(v) = \{u_0, u_1, u_2, \dots, u_{x-1}\}$. Without loss of generality, one can assume that $d_{u_i} = 1$ for $0 \leq i \leq p-1$ and $d_{u_i} \geq 2$ for $p \leq i \leq x-1$. Let G' be the graph obtained from G by removing the pendent vertices $u_0, u_1, u_2, \dots, u_{p-1}$, then $G' \in C_{n-p,k}$ and

$$R_\alpha^0(G) = R_\alpha^0(G') + p + x^\alpha - (x-p)^\alpha.$$

From inductive hypothesis, it follows that

$$R_\alpha^0(G) - \psi(n,k) \begin{cases} \leq (n-p-1)^\alpha - (n-1)^\alpha + x^\alpha - (x-p)^\alpha & if\ \alpha < 0\ or\ \alpha > 1 \\ \geq (n-p-1)^\alpha - (n-1)^\alpha + x^\alpha - (x-p)^\alpha & if\ \ 0 < \alpha < 1, \end{cases}$$

with equalities if and only if $G' \cong G^0(n-p,k)$. By using the Lemma 2.4, one have

$$R_\alpha^0(G) - \psi(n,k) \begin{cases} \leq 0 & if\ \alpha < 0\ or\ \alpha > 1 \\ \geq 0 & if\ \ 0 < \alpha < 1, \end{cases}$$

with equalities if and only if $G' \cong G^0(n-p,k)$ and $x = n-1$.

Case 2. If G has no pendent vertex. Then there exist three vertices u, v and w on some cycle of G such that u is adjacent with both the vertices v, w and $d_u = d_v = 2, d_w = x \geq 3$. Then there are two further possibilities:

Subcase 2.1. If v and w are non-adjacent. Then, the graph $G' = G - u + vw$ belongs to the collection $C_{n-1,k}$ and $R_\alpha^0(G) = R_\alpha^0(G') + 2^\alpha$. By using inductive hypothesis, one have

$$R_\alpha^0(G) - \psi(n,k) \begin{cases} \leq 2^\alpha - 1 - [(n-1)^\alpha - (n-2)^\alpha] & if\ \alpha < 0\ or\ \alpha > 1 \\ \geq 2^\alpha - 1 - [(n-1)^\alpha - (n-2)^\alpha] & if\ \ 0 < \alpha < 1, \end{cases}$$

with equalities if and only if $G' \cong G^0(n-1,k)$. But, on the other hand one have

$$2^\alpha - 1 - [(n-1)^\alpha - (n-2)^\alpha] = \alpha({\Theta_1}^{\alpha-1} - {\Theta_2}^{\alpha-1}) \begin{cases} < 0 & if\ \alpha < 0\ or\ \alpha > 1 \\ > 0 & if\ \ 0 < \alpha < 1, \end{cases}$$

where $1 < \Theta_1 < 2$ and $n-2 < \Theta_2 < n-1$.

Subcase 2.2. If v and w are adjacent. Let G' be the graph obtained from G by removing the vertices u, v. Note that the graph G' belongs to the collection $C_{n-2,k-1}$ and

$$R_\alpha^0(G) = R_\alpha^0(G') + 2^{\alpha+1} + x^\alpha - (x-2)^\alpha.$$

From inductive hypothesis, it follows that

$$R_\alpha^0(G) - \psi(n,k) \begin{cases} \leq (n-3)^\alpha - (n-1)^\alpha + x^\alpha - (x-2)^\alpha & if\ \alpha < 0\ or\ \alpha > 1 \\ \geq (n-3)^\alpha - (n-1)^\alpha + x^\alpha - (x-2)^\alpha & if\ \ 0 < \alpha < 1, \end{cases}$$

with equalities if and only if $G' \cong G^0(n-2,k-1)$. By using the Lemma 2.4, one have

$$R_\alpha^0(G) - \psi(n,k) \begin{cases} \leq 0 & if\ \alpha < 0\ or\ \alpha > 1 \\ \geq 0 & if\ \ 0 < \alpha < 1, \end{cases}$$

with equalities if and only if $G' \cong G^0(n-2,k-1)$ and $x = n-1$. This completes the proof. ■

3. EXTREMAL POLYOMINO CHAINS WITH RESPECT TO THE ZEROTH–ORDER GENERAL RANDIĆ INDEX

To establish the main results of this section, we need some preparation. In a polyomino chain, a square having one (respectively two) neighboring square(s) is called *terminal* (respectively non-terminal). A non-terminal square having a vertex of degree 2 is a *kink*. A polyomino chain without kinks is known as *linear chain* (see the Figure 2).

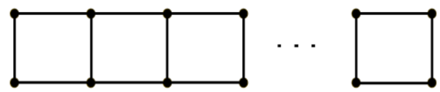

Figure 2. A Linear Chain [1].

A polyomino chain consisting of only kinks and terminal squares is called *zigzag chain* (see the Figure 3).

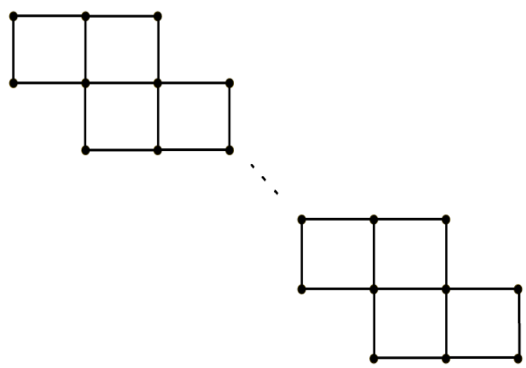

Figure 3. A Zigzag Chain [1].

A *segment* is the maximal linear chain in a polyomino chain, including the kinks and/or terminal squares at its end. Denote by $n_i(G)$ the number of vertices of degree i in a graph G. Now, we are in position to derive the main results of this section. The following theorem provides a general expression for evaluating the R_α^0 index.

Theorem 3.1. *Let B_n be a polyomino chain with $n \geq 3$ squares and k kinks. Then*

$$R_\alpha^0(B_n) = 2 \times 3^\alpha n + (2^\alpha + 4^\alpha - 2 \times 3^\alpha)k + 4 \times 2^\alpha - 2 \times 3^\alpha.$$

Proof. By simple reasoning one have, $n_2(B_n) = k + 4$, $n_4(B_n) = k, n_3(B_n) = 2n - 2k - 2$. By using these values in the definition of the R_α^0 index, one arrives at the desired result. ■

If s denotes the number of segments in a polyomino chain, then it is easy to see that $k = s - 1$. Hence, as the direct consequences of the Theorem 3.1, one have the following corollaries:

Corollary 3.2. [32] *Let B_n be a polyomino chain with $n \geq 3$ squares and s segments.Then*

$$R_2^0(B_n) = 18n + 2s - 4.$$

Corollary 3.3. *Let L_n ,Z_n and B_n be linear, zigzag and any polyomino chain respectively with $n \geq 3$ squares.*

1. *If $\alpha < 0$ or $\alpha > 1$, then*

$$2 \times 3^\alpha n + 4 \times 2^\alpha - 2 \times 3^\alpha \leq R_\alpha^0(B_n) \leq (2^\alpha + 4^\alpha)n + 2(2^\alpha + 3^\alpha - 4^\alpha),$$

the lower bound is attained if and only if $B_n \cong L_n$ and the upper bound is attained if and only if $B_n \cong Z_n$.

2. *If $0 < \alpha < 1$, then*

$$(2^\alpha + 4^\alpha)n + 2(2^\alpha + 3^\alpha - 4^\alpha) \leq R_\alpha^0(B_n) \leq 2 \times 3^\alpha n + 4 \times 2^\alpha - 2 \times 3^\alpha,$$

with left equality if and only if $B_n \cong Z_n$ and the right equality holds if and only if $B_n \cong L_n$.

Proof. Suppose that B_n has k kinks. Then from Theorem 3.1, it follows that

$$R_\alpha^0(B_n) = 2 \times 3^\alpha n + (2^\alpha + 4^\alpha - 2 \times 3^\alpha)k + 4 \times 2^\alpha - 2 \times 3^\alpha.$$

Now, let us take $F(\alpha) = 2^\alpha + 4^\alpha - 2 \times 3^\alpha$. It can be easily seen that

- for $F(\alpha) > 0$, $R_\alpha^0(B_n)$ is the maximum (respectively minimum) if and only if k is the maximum (respectively minimum),
- if $F(\alpha) < 0$ then $R_\alpha^0(B_n)$ is the maximum (respectively minimum) if and only if k is the minimum (respectively maximum) and
- for $F(\alpha) = 0$, $R_\alpha^0(B_n)$ is constant.

On the other hand, there exist real numbers Θ_1, Θ_2 such that $2 < \Theta_1 < 3 < \Theta_2 < 4$ and

$$F(\alpha) = 4^\alpha - 3^\alpha - (3^\alpha - 2^\alpha) = \alpha({\Theta_2}^{\alpha-1} - {\Theta_1}^{\alpha-1}) \begin{cases} > 0 & if\ \alpha < 0\ or\ \alpha > 1 \\ < 0 & if\ \ 0 < \alpha < 1. \end{cases}$$

This completes the proof. ■

Corollary 3.4. [32] *If B_n is a polyomino chain with $n \geq 3$ squares. Then*

$$18n - 2 \leq R_2^0(B_n) \leq 20n - 6,$$

the lower bound is attained if and only if $B_n \cong L_n$ and the upper bound is attained if and only if $B_n \cong Z_n$.

4. CONCLUSION

In the present study, we have proved the following two results.

- If $0 < \alpha < 1$ (respectively $\alpha < 0$ or $\alpha > 1$) then the cactus $G^0(n,k)$ attains the minimum (respectively maximum) R_α^0 value over the class of all cacti with n vertices and k cycles.
- If $\alpha < 0$ or $\alpha > 1$ then the linear chain L_n (respectively the zigzag chain Z_n) attains the minimum (respectively maximum) R_α^0 value over the set of all polyomino chains with n squares and if $0 < \alpha < 1$ then the situation is reversed.

ACKNOWLEDGMENT. The authors would like to express their sincere gratitude to the Editor-in-Chief (Professor Ali Reza Ashrafi) for his insightful comments and valuable suggestions, which led to a number of improvements in the earlier version of this manuscript.

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