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Discrete Applied Mathematics



journal homepage: www.elsevier.com/locate/dam

More on "Connected (n, m)-graphs with minimum and maximum zeroth-order general Randić index"

Ljiljana Pavlović*, Mirjana Lazić, Tatjana Aleksić

Faculty of Science and Mathematics, Department of Mathematics, Radoja Domanovića 12, Kragujevac, Serbia

ARTICLE INFO

Article history: Received 25 May 2008 Received in revised form 12 February 2009 Accepted 13 February 2009 Available online 27 March 2009

Keywords: Zeroth-order general Randić index Extremal (*n*, *m*)-graphs

ABSTRACT

Let *G* be a graph and d(u) denote the degree of a vertex *u* in *G*. The zeroth-order general Randić index ${}^{0}R_{\alpha}(G)$ of the graph *G* is defined as $\sum_{u \in V(G)} d(u)^{\alpha}$, where the summation goes over all vertices of *G* and α is an arbitrary real number. In this paper we correct the proof of the main Theorem 3.5 of the paper by Hu et al. [Y. Hu, X. Li, Y. Shi, T. Xu, Connected (n, m)-graphs with minimum and maximum zeroth-order general Randić index, Discrete Appl. Math. 155 (8) (2007) 1044–1054] and give a more general Theorem. We finally characterize¹ for $\alpha < 0$ the connected G(n, m)-graphs with maximum value ${}^{0}R_{\alpha}(G(n, m))$, where G(n, m) is a simple connected graph with *n* vertices and *m* edges.

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1. Introduction

Let G(n, m) be a simple connected graph with n vertices and m edges. Denote by u its vertex and by d(u) the degree of this vertex. In 1975 Randić proposed a topological index, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The Randić index defined in [13] is: $R(G) = R_{-1/2}(G) = \sum_{(uv)} (d(u)d(v))^{-1/2}$, where the summation goes over all edges uv of G. This index $R_{-1/2}(G)$ became one of the most popular molecular descriptors to which two books are devoted [8,9]. The general Randić index $R_{\alpha}(G)$ of graph G = (V, E) is defined as

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

where α is an arbitrary real number. It has been extensively studied by both mathematicians and theoretical chemists [2–5]. For a survey of results, we refer to the new book written by Li and Gutman [10].

The zeroth-order Randić index ${}^{0}R(G)$ defined by Kier and Hall [9] is:

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

where the summation goes over all vertices of *G*. Pavlović [12] gave a graph with the maximum value of ${}^{0}R(G(n, m))$ for given *n* and *m*. Li and Zheng [11] defined the zeroth-order general Randić index

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

* Corresponding author. Tel.: +381 034 363 780; fax: +381 034 335 040. *E-mail address:* pavlovic@kg,ac.rs (L. Pavlović).

¹ Note added in proof: We have learned in the meantime that correction of the main error and proof for $\alpha \in (-1, 0)$ have been obtained in "(n, m)-Graphs with maximum zeroth-order general Randić index for $\alpha \in (-1, 0)$ " by X. Li, Y. Shi, MATCH, 62 (1) (2009).



Fig. 1. *FPA*₁(12, 6, 2).

where α is an arbitrary real number. In [7], Hu et al. investigated the zeroth-order general Randić index for molecular (n, m)-graphs, i.e. simple connected graphs with n vertices, m edges and maximum degree at most 4. In [6], Hu et al. characterized the simple connected (n, m)-graphs with extremal zeroth-order general Randić index, but they failed to prove correctly the main **Theorem 3.5.** This theorem is a generalization for $\alpha \le -1$ of **Theorem** from [12] given for $\alpha = -\frac{1}{2}$. In this paper we correct the proof of the main Theorem 3.5. of [6] and prove that this Theorem holds for $\alpha < 0$. We characterize for $\alpha < 0$ the connected G(n, m)-graphs with maximum value ${}^{0}R_{\alpha}(G(n, m))$.

2. Main error

.

At first we want to point out the error in the proof of **Theorem 3.5** from [6]. All notations, terminology and presumed results can be found in [6], but we give some important notions.

The set of vertices and edges of a simple graph *G* are denoted by V(G) and E(G), respectively. The order of *G* is defined by |V(G)| and the size by |E(G)|. Let G(n, m) be a simple connected graph with *n* vertices and *m* edges. Denote by d(u) the degree of a vertex *u* and by n_i the number of vertices of degree *i*. Then:

$${}^{0}R_{\alpha}(G) = \sum_{u \in V(G)} d(u)^{\alpha} = 1^{\alpha}n_{1} + 2^{\alpha}n_{2} + \dots + (n-1)^{\alpha}n_{n-1}.$$

We give definitions from [1] of some specific graphs.

A pineapple with parameters n, k ($k \le n$), denoted by PA(n, k), is a graph on n vertices consisting of a clique on k vertices and a stable set on the remaining n - k vertices in which each vertex of the stable set is adjacent to a unique and the same vertex of the clique.

A fanned pineapple of type 1 with parameters n, k, p ($n \ge k \ge p$), denoted by $FPA_1(n, k, p)$, is a graph (on n vertices) obtained from a pineapple PA(n, k) by connecting a vertex from the stable set by edges to p vertices of the clique, with $0 \le p \le k - 2$. $FPA_1(12, 6, 2)$ is represented in Fig. 1.

We will prove that the function ${}^{0}R_{\alpha}(G(n, m))$ attains its maximum for $\alpha < 0$ on the fanned pineapple of type 1 graphs. For $\alpha = -1/2$ holds:

Theorem ([12]). Let G(n, m) be a connected graph without loops and multiple edges with n vertices and m edges. If $m = n + \frac{k(k-3)}{2} + p$, where $2 \le k \le n - 1$ and $0 \le p \le k - 2$, then:

$${}^{0}R_{-\frac{1}{2}}(G(n,m)) \leq {}^{0}R_{-\frac{1}{2}}(FPA_{1}(n,k,p)) = \frac{n-k-1}{\sqrt{1}} + \frac{1}{\sqrt{p+1}} + \frac{k-1-p}{\sqrt{k-1}} + \frac{p}{\sqrt{k}} + \frac{1}{\sqrt{n-1}}.$$

In paper [6] the authors failed to prove **Theorem 1** (corresponding Theorem 3.5):

Theorem 1. Let G(n, m) be a simple connected graph with n vertices and m edges. If $m = n + \frac{k(k-3)}{2} + p$, where $2 \le k \le n-1$ and $0 \le p \le k-2$, then for $\alpha \le -1$,

$${}^{0}R_{\alpha}(G(n,m)) \le {}^{0}R_{\alpha}(FPA_{1}(n,k,p)) = (n-k-1) \cdot 1^{\alpha} + (p+1)^{\alpha} + (k-p-1)(k-1)^{\alpha} + p \cdot k^{\alpha} + (n-1)^{\alpha}.$$
 (1)

As we mentioned, this theorem is a generalization of **Theorem** [12]. They used the same technique to prove **Theorem 1** as in [12], except the proof of inequality (4.5). Actually, the authors failed to prove inequality (4.5) on page 1050, line 14–15:

$$f(j) = (n - p - j - 3)(p + 1)^{\alpha} - (n - p + j - 3)(p + j + 1)^{\alpha} + j(n - p - j - 1)(n - 2)^{\alpha} - j(n - p - j - 3)(n - 1)^{\alpha} \ge 0.$$
(4.5)

They wrote (page 1050, line 16–27):

"Since f(0) = f(n - p - 3) = 0, we only need to prove $\frac{\partial^2 f}{\partial j^2} \le 0$. We have:

$$\frac{\partial^2 f}{\partial j^2} = -\alpha (p+j+1)^{\alpha-2} (2(p+j+1) + (\alpha-1)(n-p+j-3)) - 2((n-2)^{\alpha} - (n-1)^{\alpha}),$$

and since $-2((n-2)^{\alpha} - (n-1)^{\alpha}) \le 0$, we have to prove

$$2(p+j+1) + (\alpha - 1)(n-p+j-3) = (n-p+j-3)\alpha - n + 3p+j+5 \le 0.$$
(4.6)

Since $0 \le p \le n - 4$ and $0 \le j \le n - p - 4$, we have $0 \le p + j \le n - 4$ and:

$$\begin{array}{l} n-3p-j-5 \ = \ n-2p-(p+j)-5 \geq n-2p-(n-4)-5 \\ = \ -2p-1 \geq -2(n-4)-1 = -2n+7, \\ n-p+j-3 \leq n-p+(n-p-4)-3 = 2n-7-2p \leq 2n-7. \end{array}$$

So we have

$$\frac{n-3p-j-5}{n-p+j-3} \ge \frac{-2n+7}{2n-7} = -1 \ge \alpha.$$

Then inequality (4.6) holds for $\alpha \leq -1$."

But, this is not true for $0 \le p \le n - 4$ and $0 \le j \le n - p - 4$ and $\alpha \le -1$. For example, when $\alpha = -1$, we have:

$$(n - p + j - 3)\alpha - n + 3p + j + 5 = -n + p - j + 3 - n + 3p + j + 5 = -2n + 4p + 8 \le 0$$

only when $p \le \frac{n}{2} - 2$. We give a numerical example. Let $\alpha = -1$, n = 100, $p = 60 \le n - 4$, $j = 10 \le n - p - 4$, we have: (4.6) = $(n - n + i, -2)\alpha - n + 2n + i + 5 = -200 + 60 + 180 + 8 = 48 > 0$

$$(4.6) = (n - p + j - 3)\alpha - n + 3p + j + 5 = -200 + 60 + 180 + 8 = 48 \ge 0.$$

We leave to the reader to see what kind of error they made in this conclusion. But, they failed to prove (4.6) and also inequality (4.5). When $\alpha = -\frac{1}{2}$ [12] this inequality is proved using the property of square root.

3. Main improvement

At first we will correct the proof of Theorem 1. Before this, we give one lemma and corollary which hold for $\alpha < 0$.

Lemma 1. Let *r*, *s*, and *t* be real numbers such that: $0 < r \le s \le t$ and $\alpha < 0$. Then:

 $(t-r)s^{\alpha} \le (t-s)r^{\alpha} + (s-r)t^{\alpha}$

and the equality holds only for s = r and s = t.

It is easy to see that the proof of the corresponding Lemma 4.3. from [6] (corresponding Lemma 2 from [12]) holds for $\alpha < 0$.

Corollary 1. For real number s > 1 and $\alpha < 0$, the following holds:

$$2s^{\alpha} < (s-1)^{\alpha} + (s+1)^{\alpha}$$
.

Here we prove inequality (4.5) for $\alpha < 0$.

Lemma 2. Inequality (4.5)

$$f(p,j) = (n-p-j-3)(p+1)^{\alpha} - (n-p+j-3)(p+j+1)^{\alpha} + j(n-p-j-1)(n-2)^{\alpha} - j(n-p-j-3)(n-1)^{\alpha} \ge 0$$
(4.5)

where $n \ge 5$, p and j are integers holds for $0 \le p \le n - 4$, $0 \le j \le n - p - 4$ and $\alpha < 0$.

Proof. It is easy to see that f(p, 0) = f(p, n - p - 3) = 0. It remains to prove (4.5) for $1 \le j \le n - p - 4$. At first we will prove that $f(0, j) \ge 0$, for $0 \le j \le n - 3$. Note that

$$f(0,j) = (n-j-3)(1)^{\alpha} - (n+j-3)(j+1)^{\alpha} + j(n-j-1)(n-2)^{\alpha} - j(n-j-3)(n-1)^{\alpha}.$$
(2)

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Let us denote f(0, j) by $f_0(j)$. Then

$$\begin{aligned} \frac{\partial f_0}{\partial j} &= -1 - (j+1)^{\alpha} - \alpha (n+j-3)(j+1)^{\alpha-1} + (n-2j-1)(n-2)^{\alpha} - (n-2j-3)(n-1)^{\alpha} \\ \frac{\partial^2 f_0}{\partial j^2} &= -2\alpha (j+1)^{\alpha-1} - \alpha (\alpha-1)(n+j-3)(j+1)^{\alpha-2} - 2(n-2)^{\alpha} + 2(n-1)^{\alpha} \\ \frac{\partial^3 f_0}{\partial j^3} &= \alpha (\alpha-1)(j+1)^{\alpha-3}(2n-j-9 - \alpha (n+j-3)) \\ &\geq \alpha (\alpha-1)(j+1)^{\alpha-3}(2n-j-9) \geq \alpha (\alpha-1)(j+1)^{\alpha-3}(n-6) \geq 0 \end{aligned}$$

for $n \ge 6$ and because $j \le n - 3$. Then

$$\frac{\partial^2 f_0}{\partial j^2} \le \left. \frac{\partial^2 f_0}{\partial j^2} \right|_{j=n-3} = 2(-\alpha(n-2)^{\alpha-1} - \alpha(\alpha-1)(n-3)(n-2)^{\alpha-2} - (n-2)^{\alpha} + (n-1)^{\alpha}).$$

Since $(n-1)^{\alpha} - (n-2)^{\alpha} = \alpha(n-2)^{\alpha-1} + \frac{\alpha(\alpha-1)}{2}(n-2+\theta)^{\alpha-2}$, $0 < \theta < 1$, we have

$$\begin{split} \frac{\partial^2 f_0}{\partial j^2} &\leq 2\alpha (\alpha - 1) \left(-(n-3)(n-2)^{\alpha - 2} + \frac{1}{2}(n-2+\theta)^{\alpha - 2} \right) \\ &\leq 2\alpha (\alpha - 1) \left(-(n-3)(n-2)^{\alpha - 2} + \frac{1}{2}(n-2)^{\alpha - 2} \right) \\ &= 2\alpha (\alpha - 1)(n-2)^{\alpha - 2} \left(-n + \frac{7}{2} \right) \leq 0 \end{split}$$

for $n \ge 4$ and because $(n - 2 + \theta)^{\alpha - 2} \le (n - 2)^{\alpha - 2}$. Since $f_0(0) = f_0(n - 3) = 0$, we conclude for $n \ge 6$ that $f_0(j) \ge 0$, for $0 \le j \le n - 3$.

Further, we have

$$\begin{split} \frac{\partial f}{\partial p} &= -(p+1)^{\alpha} + \alpha (n-p-j-3)(p+1)^{\alpha-1} + (p+j+1)^{\alpha} \\ &-\alpha (n-p+j-3)(p+j+1)^{\alpha-1} - j(n-2)^{\alpha} + j(n-1)^{\alpha} \\ \frac{\partial^2 f}{\partial p^2} &= -2\alpha (p+1)^{\alpha-1} + \alpha (\alpha-1)(n-p-j-3)(p+1)^{\alpha-2} \\ &+ 2\alpha (p+j+1)^{\alpha-1} - \alpha (\alpha-1)(n-p+j-3)(p+j+1)^{\alpha-2} \\ &= -\alpha \left[2((p+1)^{\alpha-1} - (p+j+1)^{\alpha-1}) - (\alpha-1)(n-p-j-3)((p+1)^{\alpha-2} \\ &- (p+j+1)^{\alpha-2} \right) + 2(\alpha-1)j(p+j+1)^{\alpha-2} \right] \\ &\geq -\alpha \left[-2(\alpha-1)j(p+1+\theta j)^{\alpha-2} + 2(\alpha-1)j(p+j+1)^{\alpha-2} \right] \\ &= 2\alpha (\alpha-1)j \left[(p+1+\theta j)^{\alpha-2} - (p+1+j)^{\alpha-2} \right] \geq 0 \end{split}$$

because $(p+j+1)^{\alpha-1} - (p+1)^{\alpha-1} = (\alpha-1)j(p+1+\theta j)^{\alpha-2}$, $0 < \theta < 1$, $(p+1)^{\alpha-2} - (p+j+1)^{\alpha-2} \ge 0$ and $(p+1+\theta j)^{\alpha-2} \ge (p+1+j)^{\alpha-2}$. Then

$$\frac{\partial f}{\partial p} \leq \left. \frac{\partial f}{\partial p} \right|_{p=n-j-3} = (n-2)^{\alpha} - (n-j-2)^{\alpha} - 2\alpha j(n-2)^{\alpha-1} - j(n-2)^{\alpha} + j(n-1)^{\alpha}.$$

Let us denote $\left. \frac{\partial f}{\partial p} \right|_{p=n-j-3} = g(j)$. We have

$$\begin{aligned} \frac{\partial g}{\partial j} &= \alpha (n-j-2)^{\alpha-1} - 2\alpha (n-2)^{\alpha-1} - (n-2)^{\alpha} + (n-1)^{\alpha} \\ \frac{\partial^2 g}{\partial j^2} &= -\alpha (\alpha-1)(n-j-2)^{\alpha-2} \le 0. \end{aligned}$$

Then

$$\begin{aligned} \frac{\partial g}{\partial j} &\leq \left. \frac{\partial g}{\partial j} \right|_{j=1} = \alpha (n-3)^{\alpha-1} - 2\alpha (n-2)^{\alpha-1} - (n-2)^{\alpha} + (n-1)^{\alpha} \\ &= \alpha \left((n-1)^{\alpha-1} + (n-3)^{\alpha-1} - 2(n-2)^{\alpha-1} \right) + (n-1)^{\alpha} - (n-2)^{\alpha} \\ &- \alpha (n-1)^{\alpha-1} \leq \alpha (n-2+\theta)^{\alpha-1} - \alpha (n-1)^{\alpha-1} \leq 0 \end{aligned}$$

because $(n-1)^{\alpha-1} + (n-3)^{\alpha-1} - 2(n-2)^{\alpha-1} \ge 0$ (Corollary 1), $(n-1)^{\alpha} - (n-2)^{\alpha} = \alpha(n-2+\theta)^{\alpha-1}$, $0 < \theta < 1$ and $(n-2+\theta)^{\alpha-1} - (n-1)^{\alpha-1} \ge 0$. Finally, we have $g(j) \le g(1)$.

$$g(1) = (n-1)^{\alpha} - (n-2)^{\alpha} + (n-2)^{\alpha} - (n-3)^{\alpha} - 2\alpha(n-2)^{\alpha-1}.$$

Since $(n-1)^{\alpha} - (n-2)^{\alpha} = \alpha(n-2)^{\alpha-1} + \frac{\alpha(\alpha-1)}{2}(n-2+\theta)^{\alpha-2}$, $0 < \theta < 1$ and $(n-2)^{\alpha} - (n-3)^{\alpha} = -[(n-3)^{\alpha} - (n-2)^{\alpha}] = -[-\alpha(n-2)^{\alpha-1} + \frac{\alpha(\alpha-1)}{2}(-1)^2(n-2-\vartheta)^{\alpha-2}]$, $0 < \vartheta < 1$, we have:

$$g(1) = \alpha (n-2)^{\alpha-1} + \frac{\alpha (\alpha-1)}{2} (n-2+\theta)^{\alpha-2} + \alpha (n-2)^{\alpha-1} - \frac{\alpha (\alpha-1)}{2} (n-2-\vartheta)^{\alpha-2} - 2\alpha (n-2)^{\alpha-2} = \frac{\alpha (\alpha-1)}{2} \left((n-2+\theta)^{\alpha-2} - (n-2-\vartheta)^{\alpha-2} \right) \le 0.$$

This means that $\frac{\partial f}{\partial p} \leq 0$ for $j \geq 1$ and we conclude that $f(p, j) \geq 0$ for $1 \leq j \leq n-3$, $0 \leq p \leq n-j-3$ because $0 = f(n-j-3, j) \leq f(p, j) \leq f(0, j)$. We proved this lemma for $n \geq 6$, but we checked that it holds for n = 5 too. \Box

We proved (4.5) for $\alpha < 0$ and $n \ge 5$. Thus, we corrected the proof of Theorem 1. But, $\alpha \le -1$ appears only in the proof of Lemma 4.8 [6]. We will prove that this Lemma holds for $-1 < \alpha < 0$, too. At first we give one useful Lemma.

Lemma 3. If a maximum graph G^* has $r (r \le n-3)$ vertices of degree n-1, then the minimum degree of G^* is r.

This lemma is actually Lemma 4.7 from [6] and the proof holds for $\alpha < 0$.

Lemma 4. If $m \le (n^2 - 3n + 2)/2$, then $n_1(G^*) \ne 0$, for any maximum graph G^* and for $\alpha < 0$.

Proof. Since this Lemma is proved for $\alpha \le -1$ (Lemma 4.8 [6]) we will prove it only for $-1 < \alpha < 0$. All notations are the same as in the Lemma 4.8 and we will not repeat the whole text. We will focus on ${}^{0}R_{\alpha}(G') - {}^{0}R_{\alpha}(G^*)$, where α appears. Before that we sketch some important steps of the proof.

Suppose the contrary, $n_1(G^*) = 0$. We can suppose that the minimum degree of G^* is r, i.e. $n_1 = n_2 = \cdots = n_{r-1} = 0$ and $n_r \neq 0$ for $r \geq 2$. Then G^* has r vertices of degree n-1. For otherwise, if G^* has $k \neq r$ vertices of degree n-1, we have by Lemma 3 that the minimum degree of G^* is k. Let u be a vertex of degree r, then u is joined with all vertices w_1, w_2, \ldots, w_r of maximum degree n-1.

Denote by $S(G^*)$ the subgraph induced by $G^* \setminus \{u, w_1, w_2, \dots, w_r\}$ and $K(G^*)$ the complete graph on $V(S(G^*))$. Then

$$|E(K(G^*))| - |E(S(G^*))| = \binom{n-r-1}{2} - \binom{m-r(n-r) - \binom{r}{2}}{2}$$
$$\geq \binom{n-r-1}{2} - \frac{n^2 - 3n + 2}{2} + r(n-r) + \binom{r}{2} = r.$$

Then we can add at least r - 1 edges in $S(G^*)$, and after that, these vertices do not still form a complete graph.

For $r \ge 2$, denote by G' a simple connected graph obtained from G^* when we delete r - 1 edges between vertex u and vertices w_2, \ldots, w_r and add r - 1 new edges among n - r - 1 vertices between r - 1 pairs of vertices: v_1 (degree j_1) and v'_1 (degree j'_1), v_2 (degree j_2) and v'_2 (degree j'_2), \ldots, v_{r-1} (degree j_{r-1}) and v'_{r-1} (degree j'_{r-1}). These vertices are not necessarily distinct. If we add several edges to one vertex, we will calculate each time the change of the degree of this vertex. For example $(j_i + x)^{\alpha} - j_i^{\alpha} = \sum_{t=1}^{x} (j_i + t)^{\alpha} - (j_i + t - 1)^{\alpha}$. We have

$${}^{0}R_{\alpha}(G') - {}^{0}R_{\alpha}(G^{*}) = 1 - r^{\alpha} + (r-1)(n-2)^{\alpha} - (r-1)(n-1)^{\alpha} + \sum_{i=1}^{r-1} ((j_{i}+1)^{\alpha} - j_{i}^{\alpha}) + \sum_{i=1}^{r-1} ((j_{i}'+1)^{\alpha} - j_{i}'^{\alpha}) + \sum_{i=1}^{r-1} ((j_{i}'+1)^{\alpha}$$

because $(n-2)^{\alpha} - (n-1)^{\alpha} > 0$ and $(j_i + 1)^{\alpha} - j_i^{\alpha}$ is an increasing function. Then h(0, r) = 0 and $\frac{\partial h}{\partial \alpha} = (2r-2)(r+1)^{\alpha} \ln(r+1) - (2r-1)r^{\alpha} \ln r$. $\frac{\partial h}{\partial \alpha} = 0$ for $\alpha = \alpha^* = \ln \frac{(2r-1)\ln r}{(2r-2)\ln(r+1)} / \ln(1+\frac{1}{r})$. We will show that $\alpha^* \ge 0$ for $r \ge 4$. Since α^* is the point of minimum for $h(\alpha, r)$ we conclude that $h(\alpha, r) \ge h(0, r) = 0 \ge h(\alpha^*, r)$ for $\alpha \in (-1, 0)$. $\alpha^* \ge 0$ if $\frac{(2r-1)\ln r}{(2r-2)\ln(r+1)} \ge 1$, that is if $z(r) = (2r-1)\ln r - (2r-2)\ln(r+1) \ge 0$.

$$z(r) = (2r - 2)\ln r - (2r - 2)\ln(r + 1) + \ln r = \ln \frac{r^{2(r-1)}}{(r+1)^{2(r-1)}} + \ln r$$
$$= -2\ln\left(1 + \frac{1}{r}\right)^{r} + 2\ln\left(1 + \frac{1}{r}\right) + \ln r > -2\ln 3 + \ln r \ge 0$$

for $r \ge 9$ and because $(1 + \frac{1}{r})^r < 3$. By hand we checked that z(r) > 0 for r = 4, 5, ..., 8.

It remains to prove that \dot{G}^* cannot have any vertex of minimum degree r = 2 or r = 3. Let us consider the case r = 3.



Fig. 2. Subcase 1". Graphs G^* and G' for n = 7.



Fig. 3. Subcase 2''. Graphs G^* and G' for n = 8.

1. Case r = 3. Since ${}^{0}R_{\alpha}(G') - {}^{0}R_{\alpha}(G^{*}) \ge 1 - 3^{\alpha} + 2(n-2)^{\alpha} - 2(n-1)^{\alpha} + 4(4^{\alpha} - 3^{\alpha}) > 0$ for $\alpha \in (-1, 0)$ and n = 5, 6, we will take that n is greater than or equal to 7. We will divide this case into two subcases: 1'. among n - 4 vertices (without w_1, w_2, w_3 and u) there is a vertex of degree equal to $4, 5, \ldots, n - 3$; 1". there is no such vertex.

Subcase 1'. We have

$${}^{0}R_{\alpha}(G') - {}^{0}R_{\alpha}(G^{*}) = 1 - 3^{\alpha} + 2(n-2)^{\alpha} - 2(n-1)^{\alpha} + \sum_{i=1}^{2} ((j_{i}+1)^{\alpha} - j_{i}^{\alpha}) + \sum_{i=1}^{2} ((j_{i}'+1)^{\alpha} - j_{i}'^{\alpha}) > 1 - 3^{\alpha} + 5^{\alpha} - 4^{\alpha} + 3(4^{\alpha} - 3^{\alpha}) = 1 - 4 \cdot 3^{\alpha} + 2 \cdot 4^{\alpha} + 5^{\alpha} > 0$$

for $\alpha \in (-1, 0)$, because $2[(n-2)^{\alpha} - (n-1)^{\alpha}] > 0$, $(j_i+1)^{\alpha} - j_i^{\alpha}$ is an increasing function, $t(\alpha) = 1 - 4 \cdot 3^{\alpha} + 2 \cdot 4^{\alpha} + 5^{\alpha} > 0$ because t(0) = 0 and $t'(\alpha) = -4 \ln 3 \cdot 3^{\alpha} + 2 \ln 4 \cdot 4^{\alpha} + \ln 5 \cdot 5^{\alpha} < 2 \ln 4(4^{\alpha} - 3^{\alpha}) + \ln 5(5^{\alpha} - 3^{\alpha}) < 0$.

Subcase 1". In this case all vertices except w_1 , w_2 and w_3 are of degree 3. Let u, v_1 , v_2 and v_3 be vertices of degree 3. We delete 2 edges between vertex u and vertices w_2 , w_3 and add one edge between vertices v_1 and v_2 and one edge between v_1 and v_3 (see Fig. 2). We get again that ${}^{0}R_{\alpha}(G') - {}^{0}R_{\alpha}(G^*) > 1 - 4 \cdot 3^{\alpha} + 2 \cdot 4^{\alpha} + 5^{\alpha} > 0$ for $\alpha \in (-1, 0)$.

2. Case r = 2. We can check that ${}^{0}R_{\alpha}(G') - {}^{0}R_{\alpha}(G^{*}) \ge 1 - 2^{\alpha} + (n-2)^{\alpha} - (n-1)^{\alpha} + 2(3^{\alpha} - 2^{\alpha}) > 0$ for $\alpha \in (-1, 0)$ and n = 5, 6, 7. We assume that n is greater than or equal to 8. We divide this case into two subcases: 2'. among n - 3 vertices (without w_1, w_2 and u) there is a vertex of degree equal to 3, 4, ..., n - 3; 2". there is no such vertex.

Subcase 2'. We have

$${}^{0}R_{\alpha}(G') - {}^{0}R_{\alpha}(G^{*}) = 1 - 2^{\alpha} + (n - 2)^{\alpha} - (n - 1)^{\alpha} + (j_{1} + 1)^{\alpha} - j_{1}^{\alpha} + (j_{1}' + 1)^{\alpha} - j_{1}^{'\alpha} > 1 - 2^{\alpha} + 4^{\alpha} - 3^{\alpha} + 3^{\alpha} - 2^{\alpha} = 1 + 2^{2\alpha} - 2^{\alpha+1} > 0$$

for $\alpha \in (-1, 0)$ because $1 + 2^{2\alpha} - 2^{\alpha+1}$ is a decreasing function in (-1, 0).

Subcase 2". In this case all vertices except w_1 and w_2 are of degree 2. Let u, u_1, \ldots, u_5 be 6 vertices of degree 2. Let us denote by G' a simple connected graph obtained from G^* when we delete one edge between vertices u, u_1, u_2 and vertex w_2 and add one edge between vertices u_3 and u_4 , one edge between u_3 and u_5 and one edge between u_4 and u_5 (see Fig. 3). We have

$${}^{0}R_{\alpha}(G') - {}^{0}R_{\alpha}(G^{*}) = 3(1 - 2^{\alpha}) + (n - 4)^{\alpha} - (n - 1)^{\alpha} + 3(4^{\alpha} - 2^{\alpha})$$

> 3(1 + 2^{2\alpha} - 2^{\alpha+1}) > 0

for $\alpha \in (-1, 0)$. \Box

Now we can prove a more general theorem.

Theorem 2. Let G(n, m) be a simple connected graph with n vertices and m edges. If $m = n + \frac{k(k-3)}{2} + p$, where $2 \le k \le n-1$ and $0 \le p \le k-2$, then for $\alpha < 0$,

 ${}^{0}R_{\alpha}(G(n,m)) \leq {}^{0}R_{\alpha}(FPA_{1}(n,k,p)) = (n-k-1) \cdot 1^{\alpha} + (p+1)^{\alpha} + (k-p-1)(k-1)^{\alpha} + p \cdot k^{\alpha} + (n-1)^{\alpha}.$

The proof of this theorem is omitted because it is similar to the proof of Theorem 3.5 from [6] and is based on Lemmas 1–4. We also checked that this theorem holds for n = 5 and $4 \le m \le 10$.

At the end we will mention another unclear point in [6]. In the proof of Theorem 3.4 they wrote: "The graph $G - \{x_1\}$ consists of a connected graph G_1 with no isolated vertices, together with a set J_1 of isolated vertices". In general, graph $G - \{x_1\}$ consists of some connected components and a set J_1 of isolated vertices. It has to be proved that G_1 is a connected graph. Further they wrote: "In fact, let $d_1, d_2, \ldots, d_{n'}$ be the degree sequence of G_1 , then ${}^0R_{\alpha}(G_1) = \sum_{i=1}^{n'} d_i^{\alpha}$ attains minimum if and only if ${}^0R_{\alpha}(G) = (n-1)^{\alpha} + (n-n'-1)1^{\alpha} + \sum_{i=1}^{n'} (d_i + 1)^{\alpha}$ attains minimum." This also has to be proved because it is not obvious.

Also Theorem 4.5. [6] is a Corollary of Lemma 3.3 [6].

Acknowledgement

This research was supported by Ministry of Science, Technology and Development of Serbia, Grant No. 144015G – "Graph Theory and mathematical Programming with Applications to Chemistry and Technical Sciences".

References

- M. Aouchiche, F.K. Bell, D. Cvetković, P. Hansen, P. Rowlinson, S.K. Simić, D. Stevanović, Variable neighborhood search for extremal graphs. 16. Some conjectures related to the largest eigenvalue of a graph, Eur. J. Oper. Res. 191 (3) (2008) 661–676.
- [2] B. Bollobás, P. Erdős, Graphs of extremal weights, Ars Combin. 50 (1998) 225–233.
- [3] G. Caporossi, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs IV: Chemical trees with extremal connectivity index, Comput. Chem. 23 (1999) 469–477.
- [4] G. Caporossi, I. Gutman, P. Hansen, Lj. Pavlović, Graphs with maximum connectivity index, Comput. Biol. Chem. 27 (2003) 85–90.
- [5] L.H. Clark, J.W. Moon, On the General Randić Index for Certain Families of Trees, Ars Combin. 54 (2000) 223-235.
- [6] Y. Hu, X. Li, Y. Shi, T. Xu, Connected (*n*, *m*)-graphs with minimum and maximum zeroth-order general Randić index, Discrete Appl. Math. 155 (8) (2007) 1044–1054.
- [7] Y. Hu, X. Li, Y. Shi, T. Xu, I. Gutman, On molecular graphs with smallest and greatest zeroth-order general Randić index, MATCH Commun. Math. Comput. Chem. 54 (2) (2005) 425–434.
- [8] L.B. Kier, L.H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, 1976.
- [9] L.B. Kier, L.H. Hall, Molecular Connectivity in Structure-Activity Analysis, Research Studies Press, Wiley, Chichester, UK, 1986.
- [10] X. Li, I. Gutman, Mathematical Aspects of Randić-Type Molecular Structure Descriptors, in: Mathematical Chemistry Monographs, vol. 1, Kragujevac, 2006.
- [11] X. Li, J. Zheng, A unified approach to the extremal trees for different indices, MATCH Commun. Math. Comput. Chem. 54 (1) (2005) 195-208.
- [12] L. Pavlović, Maximal value of the zeroth-order Randić index, Discrete Appl. Math. 127 (2003) 615-626.
- [13] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97 (1975) 6609-6615.