Sandwiching the (generalized) Randić index

Martin Knor*, **Borut Lužar**†, **Riste Škrekovski**‡

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Abstract

The well-known Randić index of a graph G is defined as $R(G) = \sum \big(d_u \cdot d_v\big)^{-1/2}$, where the sum is taken over all edges $uv \in E(G)$ and d_u and d_v denote the degrees of u and v, respectively. Recently, it was found useful to use its simplified modification: $R'(G) = \sum \big(\max\{d_u, d_v\}\big)^{-1}$, which represents a lower bound for the Randić index. In this paper we introduce generalizations of R' and its counterpart, R'', defined as $R'_\alpha(G) = \sum \min\{{d_u}^\alpha, {d_v}^\alpha\}$ and $R''_\alpha(G) = \sum \max\{{d_u}^\alpha, {d_v}^\alpha\}$, for any real number α. Clearly, the former is a lower bound for the generalized Randić index, and the latter is its upper bound. We study extremal values of R'_α and R''_α, and present extremal graphs within the classes of connected graphs and trees. We conclude the paper with several problems.

Keywords: Randić index, connectivity index, branching index, index R', index R"

1 Introduction

All graphs considered in this paper are connected and simple. Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$, respectively. The degree of any vertex $u \in V(G)$ is denoted by d_u. For the other notation and notions refer to [3].

*Slovak University of Technology in Bratislava, Faculty of Civil Engineering, Department of Mathematics, Bratislava, Slovakia. E-Mail: knor@math.sk

†Faculty of Information Studies, Novo mesto & Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia. E-Mail: borut.luzar@gmail.com

‡Faculty of Information Studies, Novo mesto & Department of Mathematics, University of Ljubljana & Institute of Mathematics, Physics and Mechanics, Ljubljana & University of Primorska, FAMNIT, Koper, Slovenia. E-Mail: skrekovski@gmail.com

In 1975, Randić [18] introduced a parameter to evaluate the branching of molecules whose molecular graphs are trees. Later, Bollobás and Erdős [2] generalized this parameter to

$$R_\alpha(G) = \sum_{uv \in E(G)} \left(d_u d_v\right)^\alpha,$$

for every graph G and an arbitrary value of α. In the case when $\alpha = -\frac{1}{2}$, R_α is called the ***Randić index*** (also the *connectivity* or *branching* index) of G, otherwise it is referred to as the ***generalized Randić index***. An interested reader is referred to the monographs of Kier and Hall [8, 9] for details on chemical properties of Randić index. A comprehensive study of its mathematical properties is done in the monograph of Li and Gutman [11] and in the survey of Li and Shi [13]. For more results regarding the Randić index of various classes of graphs and its generalized variations see e.g. [5, 6, 10, 12, 14, 15, 16, 17, 19].

In order to simplify arguments on various problems related to Randić index, Dvořák, Lidický and Škrekovski [7] introduced a modified version, called ***R' index***, and defined it as

$$R'(G) = \sum_{uv \in E(G)} \Big(\max\{d_u, d_v\}\Big)^{-1} = \sum_{uv \in E(G)} \min\{{d_u}^{-1}, {d_v}^{-1}\}.$$

Clearly, $R'(G)$ is a lower bound for the Randić index of a graph G, i.e. $R'(G) \leq R(G)$. One can naturally introduce a counterpart of R', the index R'', defined as

$$R''(G) = \sum_{uv \in E(G)} \max\{{d_u}^{-1}, {d_v}^{-1}\},$$

which is an upper bound for $R(G)$. Hence, $R'(G) \leq R(G) \leq R''(G)$. The purpose of this paper is to generalize both parameters above as follows:

$$R'_\alpha(G) = \sum_{uv \in E(G)} \min\{{d_u}^\alpha, {d_v}^\alpha\} \qquad \text{and} \qquad R''_\alpha(G) = \sum_{uv \in E(G)} \max\{{d_u}^\alpha, {d_v}^\alpha\}.$$

Since for every pair of vertices u and v it holds that

$$\min\{{d_u}^{2\alpha}, {d_v}^{2\alpha}\} \leq (d_u d_v)^\alpha \leq \max\{{d_u}^{2\alpha}, {d_v}^{2\alpha}\},$$

we can bound the generalized Randić index by R'_α and R''_α:

Observation 1. *For every graph G and $\alpha \in \mathbb{R}$,*

$$R'_{2\alpha}(G) \leq R_\alpha(G) \leq R''_{2\alpha}(G).$$

In the sequel we study extremal properties of both indices and introduce the classes of graphs for which extremal values are achieved. First, observe the following:

$$\begin{aligned} R'_\alpha(G) + R''_\alpha(G) &= \sum_{uv\in E(G)} \min\{{d_u}^\alpha, {d_v}^\alpha\} + \sum_{uv\in E(G)} \max\{{d_u}^\alpha, {d_v}^\alpha\} \\ &= \sum_{uv\in E(G)} ({d_u}^\alpha + {d_v}^\alpha) = \sum_{u\in V(G)} d_u\, {d_u}^\alpha, \end{aligned}$$

which yields:

Observation 2. *For every graph G and $\alpha \in \mathbb{R}$,*

$$R'_\alpha(G) + R''_\alpha(G) = \sum_{u\in V(G)} {d_u}^{1+\alpha}.$$

For $\alpha = -1$, when $R'_\alpha = R'$, we thus infer:

Observation 3. *For a graph G on n vertices,*

$$R'_{-1}(G) + R''_{-1}(G) = n\,.$$

For a function f on graphs and a class of graphs $\mathcal{G}$, we define the ***maximum value of f on $\mathcal{G}$*** and the ***minimum value of f on $\mathcal{G}$*** as

$$\mathrm{Max}\,(f, \mathcal{G}) = \max_{G\in\mathcal{G}} f(G) \qquad \text{and} \qquad \mathrm{Min}\,(f, \mathcal{G}) = \min_{G\in\mathcal{G}} f(G).$$

In the following sections, the classes of all connected graphs, trees, and connected regular graphs on n vertices are denoted by $\mathcal{C}_n$, $\mathcal{T}_n$, and $\mathcal{R}_n$, respectively. As usually, a complete graph, a cycle, a star, and a path on n vertices is denoted by K_n, C_n, S_n, and P_n, respectively.

In Section 2 we determine the extremal values and the corresponding extremal graphs for R' and R'' within the class of connected graphs, whereas trees are investigated in Section 3.

2 Extremal values for connected graphs

In this section we present the extremal values of both indices in the class of connected graphs, and introduce the corresponding extremal graphs. We start with R'_α.

Theorem 4. *The minimum values of R'_α for connected graphs on n vertices and the graphs achieving these values are presented in Table 1.*

α	$(-\infty,0)$	0	$(0,\infty)$
$\mathrm{Min}\,(R'_\alpha,\mathcal{C}_n)$	$(n-1)^{1+\alpha}$	$n-1$	$n-1$
Extremal graphs	S_n	$\mathcal{T}_n$	S_n

Table 1: The minimum values of R'_α for connected graphs on n vertices and the corresponding extremal graphs.

Proof. If $\alpha = 0$, then $R'_0(G) = |E(G)|$, and so $R'_0(G)$ is minimum when G is a tree.

Let $\alpha \in (0,\infty)$. Since $R'_\alpha(G) = \sum_{uv\in E(G)} \min\{{d_u}^\alpha, {d_v}^\alpha\}$, the minimum value of R'_α is attained when G has the smallest possible number of edges, that is $n-1$, and each contributes the smallest possible value, which is 1. Consequently, G is a tree with only pendant edges, so G is isomorphic to S_n and $\mathrm{Min}\,(R'_\alpha,\mathcal{C}_n) = R'_\alpha(S_n) = n-1$.

Finally, let $\alpha \in (-\infty,0)$. Then $\min\{{d_u}^\alpha, {d_v}^\alpha\} = \max\{d_u, d_v\}^\alpha$. Again, $R'_\alpha(G)$ is minimum if G has the smallest possible number of edges and each contributes the smallest possible value. Since G has n vertices, the smallest possible contribution of an edge is $(n-1)^\alpha$ (recall that $\alpha < 0$). Hence, $R'_\alpha(G)$ is minimum if G is isomorphic to S_n in which case $\mathrm{Min}\,(R'_\alpha,\mathcal{C}_n) = R'_\alpha(S_n) = (n-1)(n-1)^\alpha$. □

Theorem 5. *The maximum values of R'_α for connected graphs on $n \geq 3$ vertices and the graphs achieving these values are presented in Table 2.*

α	$(-\infty,-1)$	-1	$(-1,0)$	0	$(0,\infty)$
$\mathrm{Max}\,(R'_\alpha,\mathcal{C}_n)$	$n2^\alpha$	$\frac{n}{2}$	$\binom{n}{2}(n-1)^\alpha$	$\binom{n}{2}$	$\binom{n}{2}(n-1)^\alpha$
Extremal graphs	C_n	$\mathcal{R}_n$	K_n	K_n	K_n

Table 2: The maximum values of R'_α for connected graphs on n vertices and the corresponding extremal graphs.

Proof. If $\alpha = -1$, then $R'_{-1}(G) = R'(G)$, and for this case it is proved in [1] that $R'(G) \leq \frac{n}{2}$ and only regular graphs attain the value $\frac{n}{2}$, see also [4]. If $\alpha = 0$, then $R'_0(G) = |E(G)|$, and so $R'_0(G)$ is maximum when G is a complete graph.

If $\alpha \in (0,\infty)$, then $\min\{{d_u}^\alpha, {d_v}^\alpha\} = \min\{d_u, d_v\}^\alpha$. So R'_α is maximum if G has maximum possible number of edges and each edge contributes the maximum possible value, that is $(n-1)^\alpha$. Hence $R'_\alpha(G)$ is maximum if G is a complete graph and $\mathrm{Max}\,(R'_\alpha,\mathcal{C}_n) = \binom{n}{2}(n-1)^\alpha$.

Now let $\alpha \in (-1,0)$. Observe that

$$2R'_\alpha(G) = 2\sum_{uv\in E(G)} \min\{{d_u}^\alpha, {d_v}^\alpha\} \leq \sum_{uv\in E(G)} ({d_u}^\alpha + {d_v}^\alpha) = \sum_{u\in V(G)} {d_u}^{1+\alpha}\,, \tag{1}$$

and so

$$R'_\alpha(G) \leq \frac{1}{2}\sum_{u\in V(G)} {d_u}^{1+\alpha}\,.$$

Since $\alpha \in (-1,0)$, we have that $1+\alpha > 0$ and hence ${d_u}^{1+\alpha}$ is maximum if $d_u = n-1$. So $2R'_\alpha(G) \le n(n-1)^{1+\alpha}$, which means that $R'_\alpha(G) \le \binom{n}{2}(n-1)^\alpha$. The equality is attained only if G has $\binom{n}{2}$ edges, each contributing $(n-1)^\alpha$, i.e. if G is isomorphic to K_n.

Finally, let $\alpha \in (-\infty,-1)$. Analogously as above, we have $2R'_\alpha(G) \le \sum_{u\in V(G)} d_u {d_u}^\alpha$. Since G is connected and $n \ge 3$, there is no edge with both endvertices of degree 1. Thus, every edge contributes to $R'_\alpha(G)$ by at most 2^α. This means that we can improve (1) to

$$2R'_\alpha(G) \le \sum_{uv\in E(G)} ({\hat{d}_u}^{\ \alpha} + {\hat{d}_v}^{\ \alpha}) = \sum_{u\in V(G)} d_u {\hat{d}_u}^{\ \alpha} \le \sum_{u\in V(G)} \hat{d}_u {\hat{d}_u}^{\ \alpha}, \tag{2}$$

where $\hat{d}_u = \max\{2, d_u\}$. Since $\alpha < -1$, ${\hat{d}_u}^{\ \alpha+1}$ is maximum if $\hat{d}_u = 2$. Then, $2R'_\alpha(G)$ is maximum if all the inequalities in (2) are equalities, which means that $d_u = 2$ for every $u \in V(G)$. Consequently, $R'_\alpha(G)$ is maximum if G is the cycle C_n, in which case $\mathrm{Max}\,(R'_\alpha, \mathcal{C}_n) = R'_\alpha(C_n) = n2^\alpha$. $\square$

Now we turn our attention to the index R''_α.

Theorem 6. *The minimum values of R''_α for connected graphs on $n \ge 3$ vertices and the graphs achieving these values are presented in Table 3.*

α	$(-\infty,-1)$	-1	$(-1,0)$	0	$(0,\infty)$
$\mathrm{Min}\,(R''_\alpha, \mathcal{C}_n)$	$\binom{n}{2}(n-1)^\alpha$	$\frac{n}{2}$	?	$n-1$	$(n-1)2^\alpha$
Extremal graphs	K_n	$\mathcal{R}_n$	?	$\mathcal{T}_n$	P_n

Table 3: The minimum values of R''_α for connected graphs on n vertices and the corresponding extremal graphs. The case when $\alpha \in (-1,0)$ is open (see Conjecture 11).

Proof. If $\alpha = -1$, then the result follows from Theorem 5 and Observation 3. If $\alpha = 0$, then $R''_0(G) = |E(G)|$ and so $R''_0(G)$ is minimum when G is a tree.

Let $\alpha \in (0,\infty)$. Since $R''_\alpha(G) = \sum_{uv\in E(G)} \max\{{d_u}^\alpha, {d_v}^\alpha\}$, the minimum value of $R''_\alpha(G)$ is attained when G has the smallest possible number of edges, that is $n-1$, and each contributes the smallest possible value. Since G is connected and $n \ge 3$, every edge has a vertex of degree at least 2. Consequently, $R''_\alpha(G)$ is minimum if G is a tree with maximum degree 2, that is G is isomorphic to the path P_n. So $\mathrm{Min}\,(R''_\alpha, \mathcal{C}_n) = R''_\alpha(P_n) = (n-1)2^\alpha$.

Let $\alpha \in (-\infty,-1)$. Observe that

$$2R''_\alpha(G) = 2\sum_{uv\in E(G)} \max\{{d_u}^\alpha, {d_v}^\alpha\} \ge \sum_{uv\in E(G)} ({d_u}^\alpha + {d_v}^\alpha) = \sum_{u\in V(G)} {d_u}^{1+\alpha},$$

and hence

$$R''_\alpha(G) \ge \frac{1}{2}\sum_{u\in V(G)} {d_u}^{1+\alpha}. \tag{3}$$

Since $\alpha \in (-\infty, -1)$, we have $1 + \alpha < 0$ and so ${d_u}^{1+\alpha}$ is minimum if $d_u = n - 1$. By (3), $R''_\alpha(G) \geq \frac{1}{2}n(n-1)^{1+\alpha} = \binom{n}{2}(n-1)^\alpha$. The equality is attained only if G has $\binom{n}{2}$ edges, each contributing by $(n-1)^\alpha$, i.e. if G is isomorphic to K_n. $\square$

Theorem 7. *The maximum values of R''_α for connected graphs on n vertices and the graphs achieving these values are presented in Table 4.*

α	$(-\infty, -1)$	-1	$(-1, 0)$	0	$(0, \infty)$
$\mathrm{Max}\,(R''_\alpha, \mathcal{C}_n)$	$n-1$	$n-1$	?	$\binom{n}{2}$	$\binom{n}{2}(n-1)^\alpha$
Extremal graphs	S_n	S_n	?	K_n	K_n

Table 4: The maximum values of R''_α for connected graphs on n vertices and the corresponding extremal graphs. The case of $\alpha \in (-1, 0)$ remains open (see Problem 12).

Proof. If $\alpha = -1$, then the result follows from Theorem 4 and Observation 3. If $\alpha = 0$, then $R''_0(G) = |E(G)|$ for every graph G and so $R''_0(G)$ is maximum when G is the complete graph.

Let $\alpha \in (0, \infty)$. Then R''_α attains its maximum if it has the maximum possible number of edges, each of which contributes the maximum possible value. Since the maximum contribution of an edge is $(n-1)^\alpha$, $R''_\alpha(G)$ is maximum if G is the complete graph K_n, and hence $\mathrm{Max}\,(R''_\alpha, \mathcal{C}_n) = R''_\alpha(K_n) = \binom{n}{2}(n-1)^\alpha$.

For two fixed positive integers, x and y, the function

$$f(\alpha) = \max\{x^\alpha, y^\alpha\}$$

is continuous and non-decreasing. This implies that for a fixed graph G, the function

$$g(\alpha) = R''_\alpha(G) = \sum_{uv \in E(G)} \max\{{d_u}^\alpha, {d_v}^\alpha\} \tag{4}$$

is also continuous and non-decreasing. Since for $\alpha = -1$ there is a unique extremal graph, namely the star S_n, and for $\alpha \in (-\infty, -1]$ the function $R''_\alpha(S_n)$ is constantly equal to $n-1$, it follows that $\mathrm{Max}\,(R''_\alpha, \mathcal{C}_n) = n - 1$ and the unique extremal graph is S_n. $\square$

3 Extremal values for trees

In this section we present the extremal values of R'_α and R''_α in the class of trees and introduce the corresponding extremal graphs.

First, we introduce a procedure, called *debranching*, which transforms a tree T on n vertices into the path P_n. A *ray* is a (directed) path with the initial vertex of degree at least 3, the terminal vertex of degree 1, and all internal vertices (if

any) of degree 2. The *length* of a ray is the number of its edges. Note that if T is not isomorphic to P_n, then there are at least three rays in T. Denote by R one of these rays and denote by r the first vertex of R. In debranching we repeatedly perform the following procedure until we obtain the path P_n.

Debranching procedure. ***Let s be a vertex of degree at least 3 which is at the greatest distance from r. Let S be a longest ray starting at s, $S \neq R$, and let w be the last vertex of S. Delete the last edge of S and add the edge connecting w with the last vertex of R.***

Observe that the debranching procedure extends the ray R by an edge. Now we state the main theorems of this section.

Theorem 8. *The minimum and maximum values of R''_α for trees on $n \geq 3$ vertices and the graphs achieving these values are presented in Table 5.*

α	$(-\infty, 0)$	0	$(0, \infty)$
$\mathrm{Min}\,(R''_\alpha, \mathcal{T}_n)$	$2 + (n-3)2^\alpha$	$n-1$	$(n-1)2^\alpha$
Extremal graphs	P_n	$\mathcal{T}_n$	P_n
$\mathrm{Max}\,(R''_\alpha, \mathcal{T}_n)$	$n-1$	$n-1$	$(n-1)^{1+\alpha}$
Extremal graphs	S_n	$\mathcal{T}_n$	S_n

Table 5: The minimum and maximum values of R''_α for trees on n vertices and the corresponding extremal trees.

Proof. Since $R''_0(T) = |E(T)| = n-1$ for every tree T on n vertices, $\mathrm{Min}\,(R''_0, \mathcal{T}_n) = \mathrm{Max}\,(R''_0, \mathcal{T}_n) = n-1$ and every tree is an extremal graph.

If $\alpha \in (0, \infty)$, then the result for $\mathrm{Min}\,(R''_\alpha, \mathcal{T}_n)$ follows from Theorem 6, so we consider only $\mathrm{Max}\,(R''_\alpha, \mathcal{T}_n)$. The expression $\max\{{d_u}^\alpha, {d_v}^\alpha\}$ is maximal if either $d_u = n-1$ or $d_v = n-1$. Hence, $R''_\alpha(T)$ attains its maximum if T is a tree in which every edge contains a vertex of degree $n-1$, i.e. if T is isomorphic to the star S_n. Hence $\mathrm{Max}\,(R''_\alpha, \mathcal{T}_n) = R''_\alpha(S_n) = (n-1)(n-1)^\alpha$.

Finally, let $\alpha \in (-\infty, 0)$. Then, $\max\{{d_u}^\alpha, {d_v}^\alpha\}$ is maximal if either $d_u = 1$ or $d_v = 1$. Hence, $R''_\alpha(T)$ attains its maximum if T is a tree in which every edge contains a vertex of degree 1, i.e. if T is isomorphic to S_n, and so $\mathrm{Max}\,(R''_\alpha, \mathcal{T}_n) = R''_\alpha(S_n) = n-1$.

It remains to consider the minimal values of R''_α when $\alpha \in (-\infty, 0)$. We show that $R''_\alpha(T) \geq R''_\alpha(P_n)$ for every tree T on n vertices and that the equality holds only if T is isomorphic to P_n.

Let T be a tree on n vertices. We apply the debranching procedure to T. The value of $R''_\alpha(T)$ does not change if the length of S is greater than 1, since the contribution of the last two edges of S and the last edge of R to $R''_\alpha(T)$ before the procedure is equal to the contribution of the last edge of S and the last two edges of R after the procedure. In both cases it is $1 + 1 + 2^\alpha$. Clearly, the contributions of other edges remain the same.

So suppose that the length of S is 1. By the choice of s in the debranching procedure, there is at most one edge incident to s which is not in a ray. Denote this edge (if it exists) by f. Let e be the last edge of R before the procedure. The contribution of e to $R''_\alpha(T)$ is changed by $2^\alpha - 1$, which is negative. However, there may be one more edge whose contribution changes, namely the edge f. If the other endvertex of f has degree at least d_s, then the contribution of f to $R''_\alpha(T)$ changes by $-{d_s}^\alpha + (d_s - 1)^\alpha$; otherwise its contribution does not change. In what follows, we prove that if $d_s \geq 3$, then the changes in contributions altogether are negative. Indeed,

$$-1 + 2^\alpha - {d_s}^\alpha + (d_s - 1)^\alpha < 0, \tag{5}$$

which implies that if the length of S is 1, then the value of $R''_\alpha(T)$ after the procedure decreases.

Define $f(x) = (x-1)^\alpha - x^\alpha$, where $x \geq 2$ and $\alpha < 0$. Then, $f'(x) = \alpha[(x-1)^{\alpha-1} - x^{\alpha-1}] < 0$, which means that $f(x)$ is a decreasing function, and so $f(2) > f(d_s)$, or equivalently $1 - 2^\alpha > (d_s - 1)^\alpha - {d_s}^\alpha$, which is equivalent to (5).

If $T \neq P_n$, then the last application of debranching procedure yields $R''_\alpha(T) > R''_\alpha(P_n)$, so P_n is the unique extremal graph for $\mathrm{Min}\,(R''_\alpha, \mathcal{T}_n)$ and $\mathrm{Min}\,(R''_\alpha, \mathcal{T}_n) = R''_\alpha(P_n) = 2 + (n-3)2^\alpha$. $\square$

Theorem 9. *The minimum and maximum values of R'_α for trees on $n \geq 3$ vertices and the graphs achieving these values are presented in Table 6.*

α	$(-\infty, 0)$	0	$(0, 1)$	1	$(1, \infty)$
$\mathrm{Min}\,(R'_\alpha, \mathcal{T}_n)$	$(n-1)^{1+\alpha}$	$n-1$	$(n-1)$	$(n-1)$	$(n-1)$
Extremal graphs	S_n	$\mathcal{T}_n$	S_n	S_n	S_n
$\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n)$	$(n-1)2^\alpha$	$n-1$	$2 + (n-3)2^\alpha$	$2n-4$	?
Extremal graphs	P_n	$\mathcal{T}_n$	P_n	P_n	?

Table 6: The minimum and maximum values of R'_α for trees on n vertices and the corresponding extremal trees. The values of $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n)$ for $\alpha \in (1, \infty)$ are not completely determined. We partially consider them in Theorem 10, the remainder is proposed as Problem 13.

Proof. The results for $\mathrm{Min}\,(R'_\alpha, \mathcal{T}_n)$ follow from Theorem 4, so we consider only the extremal values of $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n)$ in the sequel. If $\alpha = 0$, then $R'_0(T) = |E(T)| = n - 1$ for every tree T on n vertices, thus $\mathrm{Max}\,(R'_0, \mathcal{T}_n) = n - 1$ and all trees in $\mathcal{T}_n$ are extremal graphs.

Let $\alpha \in (-\infty, 0)$. Since $n \geq 3$, every edge has a vertex of degree at least 2, and so $\min\{{d_u}^\alpha, {d_v}^\alpha\} \leq 2^\alpha$. Thus, $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n) \leq (n-1)2^\alpha$ and the extremal graph has all vertices of degree at most 2, i.e. it is the path P_n. Hence, $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n) = R'_\alpha(P_n) = (n-1)2^\alpha$.

Let $\alpha \in (0, 1)$ and let T be any tree on n vertices. We apply the debranching procedure to T and we show that $R'_\alpha(T) \leq R'_\alpha(P_n)$. We also show that the equality holds only if T is isomorphic to P_n.

Analogously as in the proof of Theorem 8, one can show that the debranching procedure does not change $R'_\alpha(T)$ if the length of S is greater than 1. On the other hand, if the length of S is 1, then $R'_\alpha(T)$ changes by $2^\alpha - 1$, which is positive, or by $2^\alpha - 1 - {d_s}^\alpha + (d_s - 1)^\alpha$, where $d_s \geq 3$. However, if $\alpha < 1$, then $f(x) = (x-1)^\alpha - x^\alpha$ is an increasing function since its derivative is greater than 0. Therefore, $f(2) < f(d_s)$, which implies that $2^\alpha - 1 - {d_s}^\alpha + (d_s - 1)^\alpha > 0$. Consequently, P_n is the unique extremal graph for $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n)$ and $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n) = R'_\alpha(P_n) = 2 + (n-3)2^\alpha$.

If $\alpha = 1$, then we proceed in the same way as in the case $\alpha \in (0,1)$. So, let us start with an arbitrary tree T on n vertices and repeat the debranching procedure until the path P_n is obtained. If the length of S is greater than 1, then the debranching procedure does not change $R'_1(T)$, while if the length of S equals 1, then the debranching procedure does not decrease $R'_1(T)$. However, the very last application of debranching procedure applies on a tree with only three rays, two of which have length 1. In this case $R'_1(T)$ changes by $2^1 - 1$, which means that P_n is the unique extremal graph also in this case. □

It is natural to expect that Theorems 8 and 9 are complementary in a sense that P_n is the unique extremal graph for $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n)$ also for $\alpha \in (1, \infty)$. In fact, since for a fixed G the $R'_\alpha(G)$ is continuous as a function of α, for every n there is a constant c'_n, such that for $\alpha \in (1, c'_n)$ the unique extremal graph for $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n)$ is P_n. However, we show in the next theorem that for $n \geq 4$ the path P_n is not an extremal graph for $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n)$ if α is big enough.

So let $n \geq 4$. Take two stars $S_{\lfloor \frac{n}{2} \rfloor}$ and join their centers by an edge. This yields a *balanced double star*. If n is odd, then subdivide also one of the pendant edges. Denote by D_n the resulting tree, see Figure 1 for D_8 and D_9.

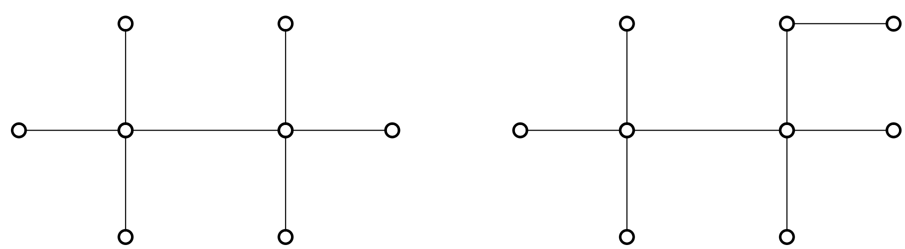

Figure 1: The trees D_8 and D_9.

Theorem 10. *For every $n \geq 4$, there exists a constant $c_n > 1$ such that D_n is the unique extremal graph for $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n)$ whenever $\alpha \in (c_n, \infty)$. If n is even, then $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n) = \lfloor \frac{n}{2} \rfloor^\alpha + n - 2$, while if n is odd, then $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n) = \lfloor \frac{n}{2} \rfloor^\alpha + 2^\alpha + n - 3$.*

Proof. Let $\alpha > 0$. Then $\min\{{d_u}^\alpha, {d_v}^\alpha\}$ attains its maximum in a tree if both $d_u \geq \lfloor \frac{n}{2} \rfloor$ and $d_v \geq \lfloor \frac{n}{2} \rfloor$. We say that a tree is *nice* if it has an edge $e = uv$ such that $d_u \geq \lfloor \frac{n}{2} \rfloor$ and $d_v \geq \lfloor \frac{n}{2} \rfloor$.

Let T^+ and T^- be trees on n vertices such that T^+ is nice and T^- is not nice. Then $R'_\alpha(T^+) \geq \lfloor \frac{n}{2} \rfloor^\alpha$ while $R'_\alpha(T^-) \leq (n-1)(\lfloor \frac{n}{2} \rfloor - 1)^\alpha$. Obviously, there is $c_n > 0$ such that $\lfloor \frac{n}{2} \rfloor^\alpha > (n-1)(\lfloor \frac{n}{2} \rfloor - 1)^\alpha$ for every $\alpha \geq c_n$, which means that for $\alpha \in (c_n, \infty)$ the tree T^- cannot be extremal for $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n)$.

It remains to find all nice trees. If n is even then the unique nice tree is D_n, while if n is odd there are exactly two nice trees. The first is D_n and the other, T_n, is obtained by taking the stars $S_{\lfloor \frac{n}{2} \rfloor}$ and $S_{\lceil \frac{n}{2} \rceil}$ and connecting their centers by an edge. Then $R'_\alpha(D_n) = \lfloor \frac{n}{2} \rfloor^\alpha + 2^\alpha + n - 3$, while $R'_\alpha(T_n) = \lfloor \frac{n}{2} \rfloor^\alpha + n - 2$. $\square$

4 Discussion and further work

In the paper, we presented the extremal values of generalized indices R'_α and R''_α for most values of α. There are, however, some intervals on which the exact bounds are not determined yet. We discuss them here.

In Theorem 6, the case $\alpha \in (-1, 0)$ remains open. However, due to the continuity of $R''_\alpha(G)$ as a function of α, it is obvious that an extremal graph for α close to -1 must be regular, while an extremal graph for α close to 0 must be a tree. From (3) one can see that the regular graph is the cycle C_n, while the tree is the path P_n, by Theorem 8 below. Since for $\alpha \in (-1, 0)$ we have $R''_\alpha(C_n) = n2^\alpha$ and $R''_\alpha(P_n) = 2 + (n-3)2^\alpha$, and since these values are equal for $\alpha = \log_2(\frac{2}{3})$, we propose the following conjecture.

Conjecture 11. *For $\alpha \in (-1, \log_2(\frac{2}{3}))$, $\mathrm{Min}\,(R''_\alpha, \mathcal{C}_n) = n\,2^\alpha$ and the extremal graph is C_n. For $\alpha \in (\log_2(\frac{2}{3}), 0)$, $\mathrm{Min}\,(R''_\alpha, \mathcal{C}_n) = 2 + (n-3)2^\alpha$ and the extremal graph is P_n.*

In Theorem 7, the extremal values are not established for $\alpha \in (-1, 0)$. By the continuity of $g(\alpha)$ in (4), we can deduce that S_n is an extremal graph also for $\alpha \in (-1, c_1(n)]$ and K_n is an extremal graph for $\alpha \in [c_2(n), 0)$ for some $c_1(n)$ and $c_2(n)$, where $-1 < c_1(n) \leq c_2(n) < 0$. However, here the situation seems to be much more complicated than in the case of $\mathrm{Min}\,(R''_\alpha, \mathcal{C}_n)$. For example, if $n = 4$ then $c_1(4) < c_2(4)$, and for $\alpha \in [c_1(4), c_2(4)]$ the extremal graph is $K_n - e$, i.e. the complete graph without one edge. Obviously, for $n > 4$ the number of extremal graphs for α in the interval $(c_1(n), c_2(n))$ is increasing.

Problem 12. *Determine the constants $c_1(n)$ and $c_2(n)$ for every n and the extremal graphs for R''_α, with $\alpha \in [c_1(n), c_2(n)]$.*

The values of $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n)$ which are left undetermined in Theorem 9 are partially considered in Theorem 10, but not established completely.

Problem 13. *Determine the exact bounds for $\mathrm{Max}\,(R'_\alpha, \mathcal{T}_n)$ for $\alpha \in (1, \infty)$.*

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