MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **83** (2020) 189-203

ISSN 0340 - 6253

On the Maximal *RRR* Index of Trees with Many Leaves

Vladimir Božović[a], Žana Kovijanić Vukićević[a], Goran Popivoda[a], Riste Škrekovski[b,c], Aleksandra Tepeh[c,d]

[a] *Faculty of Science and Mathematics, University of Montenegro, 81000 Podgorica, Montenegro,*
vladimirb@ac.me, zanak@rc.pmf.ac.me, goranp@ac.me

[b] *FMF, University of Ljubljana, 1000 Ljubljana, Slovenia*
[c] *Faculty of Information Studies, 8000 Novo Mesto, Slovenia,*
skrekovski@gmail.com
[d] *University of Maribor, FERI Studies, 2000 Maribor, Slovenia,*
aleksandra.tepeh@gmail.com

(Received June 26, 2019)

Abstract

The reduced reciprocal Randić (RRR) index of the graph $G = (V, E)$ is defined as $\mathrm{RRR}(G) = \sum_{uv \in E} \sqrt{(d_u - 1)(d_v - 1)}$, where d_u and d_v denote the degrees of vertices u and v, respectively. We characterize the trees of order n with p pendant vertices that maximize RRR index for every $p \geq \lfloor n/2 \rfloor$, which has been identified as an open problem by Ren, Hu and Zhao (2016). The main observations which leads to the characterization is that the extremal tree is of height 2.

1 Introduction

Topological indices are numerical quantities of a graph, which are invariant under graph isomorphisms. They have been shown to correlate well with numerous physico-chemical and biological properties, thus they are useful descriptors in QSAR and QSPR studies that are used for predictive purposes. Generally they can be quickly and readily calculated. Calculation of some of them depends on vertex degrees, such topological indices are known as vertex-degree-based topological indices.

One of the most studied and most applied such index is the *Randić index*, defined in [11] as

$$R(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u d_v}},$$

where d_u and d_v denote the degrees of vertices u and v, respectively. It was introduced for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Determining the graphs with extremal values of a certain index if often the topic of interest for many researchers. Results of this type for Randić index can be found in [4, 5, 13], and surveys [6, 9].

Based on successful applications of Randić index, Manso et al. [10] introduced the Fi index to predict the normal boiling point temperatures of hydrocarbons. In the mathematical definition Fi index is comprised of two summands. In [7] Gutman et al. focused on one of the summands and they called it the *reduced reciprocal Randić* (RRR) index, which also belongs to vertex-degree-based topological indices as it is for a graph G defined as

$$\mathrm{RRR}(G) = \sum_{uv \in E} \sqrt{(d_u - 1)(d_v - 1)}.$$

The RRR index was compared in [7] with several well-known topological indices for predicting the standard heats (enthalpy) of formation and normal boiling points of octane isomers and it was concluded that RRR index deserves further attention of researchers. The RRR index of some dendrimer and nanotube structures was computed in [3,8] . Finding extremal values of RRR index under special conditions became the topic of subsequent studies.

The authors of [7] proved that the star graph and the complete graph have the minimum and maximum value, respectively, among all n-vertex graphs. The problem of finding graphs with minimum RRR value among all n-vertex connected unicyclic graphs (n-vertex connected graphs with n edges) was solved in [1]. Recently in [2], graphs having minimum RRR index were identified among all n–vertex connected bicyclic graphs (n-vertex connected graphs with $n + 1$ edges), for $n \geq 5$.

In [7] a conjecture related to the maximum value of RRR index of trees was posed, which was settled by Ren et al. [12] who characterized trees of order n with the maximal value of RRR index. In order to derive the mentioned result, Ren et al. characterized trees that have maximum RRR index among all trees from the class

$$\bigcup_{\lfloor n/2\rfloor \le p < n} \mathcal{T}_{n,p},$$

where $\mathcal{T}_{n,p}$ denotes the class of trees of order n with a fixed number of leaves p. They found that the tree with maximal value of RRR index in the mentioned class has $\lfloor n/2\rfloor$ leaves. Especially, Ren et al. [12] have also identified the trees from $\mathcal{T}_{n,p}$ that attain the maximum value of RRR index if $p < \lfloor n/2\rfloor$. However, the following problem from [12] remained open.

Problem 1. *Characterize trees from $\mathcal{T}_{n,p}$ that have maximal value of RRR index if $\lfloor n/2\rfloor < p \le n-1$.*

In this paper we solve this problem and show that extremal trees are trees of height 2, rooted in (the unique) vertex of maximal degree.

2 Preliminaries

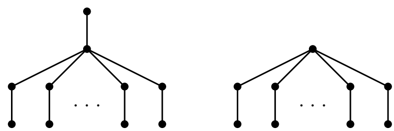
Let $G = (V, E)$ be a simple connected graph with n vertices. For a vertex $v \in V$, let d_v denote the degree of v in G. A *rooted tree* is a pair (T, r) where T is a tree and $r \in V(T)$ is a vertex that is called the *root*. Let (T, r) be a rooted tree and $v \in V(T)\backslash\{r\}$. Let u be the next vertex, neighbor of v, on the unique path towards the root r. Then u is called the *father* of v, and v is a *child* of u. The *height of a vertex* v, $\mathrm{ht}(v)$, in a rooted tree is the number of edges on a longest path between v and a leaf from the descendant of v. The *height of a rooted tree* T is denoted by $\mathrm{ht}(T)$ and defined as

$$\mathrm{ht}(T) = \mathrm{ht}(r),$$

which is the length of a longest path from the root r to a leaf in T. If a vertex v does not have children, then $\mathrm{ht}(v) = 0$.

In [7] a family of n-vertex trees $T_{\mathrm{RRR}}(n)$ was constructed as follows. Let n be a fixed integer, $n \ge 3$. If $n = 2k$, then $T_{\mathrm{RRR}}(n)$ is obtained by attaching one pendant vertex to each of the $k-1$ pendant vertices of the star S_{k+1}, and if $n = 2k+1$, we construct the tree $T_{\mathrm{RRR}}(n)$ by attaching one pendant vertex to each of the k pendant vertices of the star S_{k+1}, see Figure 1. In [12, Theorem 2] it has been proved that the trees $T_{\mathrm{RRR}}(n)$ have maximum RRR index among all trees from $\bigcup_{\lfloor n/2\rfloor \le p < n} \mathcal{T}_{n,p}$.

In both cases, when $n = 2k$ or $n = 2k+1$, $T_{\mathrm{RRR}}(n)$ has $p = k$ leaves. Recall that we are interested to find maximal RRR index among trees from $\mathcal{T}_{n,p}$, for fixed numbers n and p which satisfy $p \geq \lfloor n/2 \rfloor$. Thus according to the mentioned result from [12], the problem for two cases, when $n = 2p$ or $n = 2p+1$, has been resolved. Therefore in the rest of the paper we will assume that $p > \lfloor n/2 \rfloor$, which means that that we will only consider trees from $\mathcal{T}_{n,p}$ that have at least one leaf more than the half of the total number of vertices.



B_{2k} B_{2k+1}

Figure 1. The trees $T_{\mathrm{RRR}}(n)$ that have the maximal RRR value for $p \geq \lfloor n/2 \rfloor$.

In order to simplify the notation, we will denote by $\mathcal{M}_{n,p}$ the graphs from $\mathcal{T}_{n,p}$ with maximal RRR index, where $p > \lfloor n/2 \rfloor$ is fixed. Also, we can skip trivial cases $n = 1, 2, 3, 4$, so assume that $n \geq 5$ for the rest of the paper. Since we consider trees T with $n \geq 5$ and $p > \lfloor n/2 \rfloor$, it also follows that the for the maximal degree $\Delta(T)$ of T it will always hold $\Delta(T) \geq 3$.

3 Properties of optimal trees

When we mention a tree T from $\mathcal{M}_{n,p}$ in this section, we usually regard it as a rooted tree, where the root is a vertex of maximal degree $\Delta(T)$. As already mentioned, we assume that $\Delta(T) \geq 3$.

The next lemma formalizes a straightforward observation that exchanging any two neighbors of two vertices with equal degrees does not affect RRR index. In it the notation $T' = T - \{xy, st\} + \{xt, sy\}$ stands for a tree T' obtained from a tree T by deleting edges xy, st and adding edges xt and sy instead.

Lemma 2. *Let xy and st be two edges in a tree T such that $d_x = d_s$. Let $T' = T - \{xy, st\} + \{xt, sy\}$. Then* $\mathrm{RRR}(T') = \mathrm{RRR}(T)$.

By S_n we denote a star on $n+1$ vertices, i.e. a tree with a vertex adjacent to all other vertices. A *double star* $D_{a,b}$ is a tree consisting of $a+b+2$ vertices (where $a, b \geq 1$), two of which have degrees $a+1$ and $b+1$, respectively, while the remaining ones have degree 1. The number of leaves p in $D_{a,b}$ is thus $a+b$. We may assume that $a \geq b$.

Proposition 3. *Let $T \in \mathcal{M}_{n,p}$.*

1. *If $p = n-1$, then $T = S_n$.*
2. *If $p = n-2$, then T is a double star $D_{a,b}$, where $a - b \leq 1$.*

Proof. Let $T \in \mathcal{M}_{n,p}$. The first claim is obvious since the star on n vertices is the only tree with $n-1$ leaves. It is also clear that if a tree has $n-2$ leaves, then it must be a double star, i.e., $T = D_{a,b}$. Suppose that $a - b \geq 2$. Let x and y be non-leaf vertices with degrees $a+1$ and $b+1$, respectively, in $D_{a,b}$ and z a neighbor of x. Then $D_{a,b} - \{xz\} + \{yz\} = D_{a-1,b+1}$, and

$$\mathrm{RRR}(D_{a-1,b+1}) - \mathrm{RRR}(D_{a,b}) = \sqrt{a-1}\sqrt{b+1} - \sqrt{a}\sqrt{b}.$$

To obtain a contradiction with $T \in \mathcal{M}_{n,p}$ we need to prove that this difference is positive, which can easily be seen, since squaring the inequality $\sqrt{a-1}\sqrt{b+1} > \sqrt{a}\sqrt{b}$ and simplifying the obtained expression we get $a - b > 1$, which holds by the assumption. ■

We next show that in an optimal tree the degree of a father is always at least the degree of its children.

Lemma 4. *Let $\lfloor n/2 \rfloor < p \leq n-3$, $T \in \mathcal{M}_{n,p}$ and $a, b \in V(T)$. If a is the father of b, then $d_a \geq d_b$.*

Proof. Let $T \in \mathcal{M}_{n,p}$ be a tree rooted in a vertex r of maximal degree and let a be the father of b. Suppose to the contrary that $d_a < d_b$. Consider a path P from r to a leaf w, which does not contain vertices a and b (such a path exists since $d_r > 1$). Since r is of maximal degree in T, w has degree 1 and $d_b > 1$ by the assumption, there exists an edge xy on P such that x is the father of y, and $d_y < d_b \leq d_x$. Let $T' = T - \{ab, xy\} + \{ay, xb\}$.

To end the proof consider the difference $\mathrm{RRR}(T') - \mathrm{RRR}(T)$:

$$\begin{aligned}
\mathrm{RRR}(T') - \mathrm{RRR}(T) &= \sqrt{d_a-1}\sqrt{d_y-1} + \sqrt{d_b-1}\sqrt{d_x-1} \\
&\quad -\sqrt{d_a-1}\sqrt{d_b-1} - \sqrt{d_y-1}\sqrt{d_x-1} \\
&= (\sqrt{d_b-1} - \sqrt{d_y-1})(\sqrt{d_x-1} - \sqrt{d_a-1}) \\
&\geq (\sqrt{d_b-1} - \sqrt{d_y-1})(\sqrt{d_b-1} - \sqrt{d_a-1}).
\end{aligned}$$

Since $d_a < d_b$ and $d_y < d_b$ we infer that $\mathrm{RRR}(T') - \mathrm{RRR}(T) > 0$, which is in a contradiction with the assumption that $T \in \mathcal{M}_{n,p}$. ■

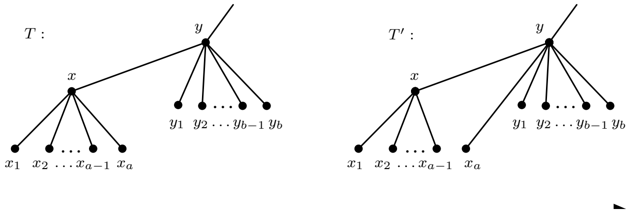


Figure 2. An illustration of trees T and T'.

In what follows we consider trees from $\mathcal{M}_{n,p}$ where the number of leaves p is at most $n-3$, and show that under this condition the inequality in Lemma 4 becomes strict.

Lemma 5. *Let $\lfloor n/2 \rfloor < p \leq n-3$ and $T \in \mathcal{M}_{n,p}$. If x is the father of y, then $d_x > d_y$.*

Proof. By Lemma 4 we already know that $d_x \geq d_y$. We will show that the assumption $d_x = d_y$ leads to a contradiction.

First suppose that $d_x = d_y = 2$. Note that by Lemma 4 there exists exactly one path P from x to a leaf in T such that $y \in V(P)$. Denote by c this leaf, let b be its unique neighbor and let a be the father of b (a and b may coincide with x and y, respectively). Let t be a vertex of degree $d \geq 3$ in T with a leaf neighbor u (such vertices t and u exist since $p > \lfloor n/2 \rfloor$). Let $T' = T - \{bc\} + \{uc\}$. It is easy to see that $\mathrm{RRR}(T') - \mathrm{RRR}(T) = \sqrt{d-1} - 1 > 0$, a contradiction with T being in $\mathcal{M}_{n,p}$.

Now assume $d_x = d_y = a \geq 3$. Let $x_1, x_2, \dots, x_{a-1}$ be degrees of neighbors of x, different from y, and let $y_1, y_2, \dots, y_{a-1}$ be degrees of neighbors of y, different from x. By Lemma 2 we may assume that $x_1 \leq x_2 \leq \cdots \leq x_{a-1} \leq y_1 \leq y_2 \leq \cdots \leq y_{a-1}$. Let z be the neighbor of x whose degree is x_{a-1} and let $T' = T - \{xz\} + \{yz\}$. For the sake of simplicity we will write b instead of x_{a-1} in what follows. Then

$$\begin{aligned}
\mathrm{RRR}(T') - \mathrm{RRR}(T) &= \sqrt{a-2}(\sqrt{x_1-1} + \cdots + \sqrt{x_{a-2}-1}) + \sqrt{a(b-1)} \\
&\quad + \sqrt{a(a-2)} + \sqrt{a}(\sqrt{y_1-1} + \cdots + \sqrt{y_{a-1}-1}) \\
&\quad - \sqrt{a-1}(\sqrt{x_1-1} + \cdots + \sqrt{x_{a-2}-1}) - \sqrt{(a-1)(b-1)} \\
&\quad - (a-1) - \sqrt{a-1}(\sqrt{y_1-1} + \cdots + \sqrt{y_{a-1}-1}) \\
&= (\sqrt{a-2} - \sqrt{a-1})(\sqrt{x_1-1} + \cdots + \sqrt{x_{a-2}-1}) \\
&\quad + (\sqrt{a} - \sqrt{a-1})(\sqrt{y_1-1} + \cdots + \sqrt{y_{a-1}-1} + \sqrt{b-1}) \\
&\quad - (a-1) + \sqrt{a(a-2)}.
\end{aligned} \tag{1}$$

Now we consider two cases with respect to the value of b.

Case 1. Let $b = 1$. Then $x_1 = x_2 = \cdots = x_{a-2} = 1$. Note that $y_{a-1} \geq 2$, otherwise T is a double star, which implies $p = n-2$, a contradiction to our assumption. Thus $\mathrm{RRR}(T') - \mathrm{RRR}(T) \geq (\sqrt{a} - \sqrt{a-1}) - (a-1) + \sqrt{a(a-2)}$ in this case. However, it turns out that the right side of this inequality is positive. Namely, by squaring both sides of the inequality $\sqrt{a} + \sqrt{a(a-2)} > (a-1) + \sqrt{a-1}$ we obtain that $a\sqrt{a-2} > (a-1)\sqrt{a-1}$, or equivalently

$$\frac{a}{\sqrt{a-1}} > \frac{a-1}{\sqrt{a-2}}, \tag{2}$$

where the inequality (2) can be seen as $g(a) > g(a-1)$ where g is the function defined as $g(x) = \frac{x}{\sqrt{x-1}}$ for $x \in [1, \infty)$. Since $g'(x) = \frac{x-2}{2(x-1)\sqrt{x-1}}$ and clearly $g'(x) > 0$ for $x > 2$, we conclude that the function g is strictly increasing for $x > 2$. Consequently, the inequality (2) holds for $a \geq 3$. With this we have shown that $\mathrm{RRR}(T') - \mathrm{RRR}(T) > 0$, which is in contradiction with $T \in \mathcal{M}_{n,p}$.

Case 2. Now let $b \geq 2$. Since $x_1 \leq x_2 \leq \cdots \leq x_{a-2} \leq b \leq y_1 \leq y_2 \leq \cdots \leq y_{a-1}$, we infer from (1) that

$$\begin{aligned} \mathrm{RRR}(T') - \mathrm{RRR}(T) \;\; \geq \;\; & (\sqrt{a} - \sqrt{a-1})a\sqrt{b-1} - (\sqrt{a-1} - \sqrt{a-2})(a-2)\sqrt{b-1} \\ & -(a-1) + \sqrt{a(a-2)}. \end{aligned} \tag{3}$$

The expression on the right side of inequality (3) achieves the smallest value when $b = 2$, thus

$$\begin{aligned} \mathrm{RRR}(T') - \mathrm{RRR}(T) \;\; \geq \;\; & (\sqrt{a} - \sqrt{a-1})a - (\sqrt{a-1} - \sqrt{a-2})(a-2) \\ & -(a-1) + \sqrt{a(a-2)}. \end{aligned} \tag{4}$$

Our goal is to prove that for $a \geq 3$ the right side of inequality (4) is positive, i.e.

$$(\sqrt{a} - \sqrt{a-1})a - (\sqrt{a-1} - \sqrt{a-2})(a-2) - (a-1) + \sqrt{a(a-2)} > 0,$$

or equivalently,

$$(\sqrt{a} - \sqrt{a-1}) + (\sqrt{a} - \sqrt{a-1})(a-1) - (\sqrt{a-1} - \sqrt{a-2})(a-2) - (a-1) + \sqrt{a(a-2)} > 0.$$

To this end it suffices to prove that $(\sqrt{a} - \sqrt{a-1})(a-1) - (\sqrt{a-1} - \sqrt{a-2})(a-2) > 0$, as we have already seen in Case 1 that $\sqrt{a} - \sqrt{a-1} - (a-1) + \sqrt{a(a-2)} > 0$. To show this it is enough to see that the function $f(x) = x(\sqrt{x+1} - \sqrt{x})$ is strictly increasing, since from this it will follow that $f(a-1) > f(a-2)$. Since $f'(x) = \frac{3x - 3\sqrt{x(x+1)} + 2}{2\sqrt{x+1}}$, and $3x - 3\sqrt{x(x+1)} + 2 > 0$ for $x \geq 0$, the proof is complete as this implies a contradiction with T being in $\mathcal{M}_{n,p}$ again. ■

In the beginning of this section we assumed that $T \in \mathcal{M}_{n,p}$ is rooted in a vertex r such that $d_r = \Delta(T)$. Lemma 5 implies the following.

Corollary 6. *Let $\lfloor n/2 \rfloor < p \leq n-3$ and $T \in \mathcal{M}_{n,p}$. Then there exists exactly one vertex of maximal degree in T.*

We will also need the following property.

Lemma 7. *Let $\lfloor n/2 \rfloor < p \leq n-3$, $T \in \mathcal{M}_{n,p}$ and $v \in V(T)$.*

(a) If v has a leaf neighbor, then its height is either 1 or 2.

(b) If the degree of every child of v is 2, then $\mathrm{ht}(v) = 2$.

Proof. Suppose that T is a rooted tree and let a leaf ℓ be a neighbor of v. To prove the first statement by contradiction, assume that v has a child a that has a child b with $d_b \geq 2$. By Lemma 5 we know that $d_v > d_a > d_b$. Let $T' = T - \{ab, lv\} + \{al, bv\}$. Then

$$\begin{aligned} \mathrm{RRR}(T') - \mathrm{RRR}(T) &= \sqrt{d_b - 1}\sqrt{d_v - 1} - \sqrt{d_b - 1}\sqrt{d_a - 1} \\ &= \sqrt{d_b - 1}(\sqrt{d_v - 1} - \sqrt{d_a - 1}). \end{aligned}$$

Since this expression is positive, we have a contradiction with $T \in \mathcal{M}_{n,p}$.

The second claim follows by Lemma 5, as the only possible child of a vertex with degree 2 is a leaf. ■

A vertex is called a *fork vertex* if it is of degree at least 3, it has at least one leaf child, and all its children are of degree 1 or 2, see Figure 3. By Lemma 7, every fork vertex in T, where $T \in \mathcal{M}_{n,p}$ and $\lfloor n/2 \rfloor < p \leq n-3$, is of height 1 or 2.

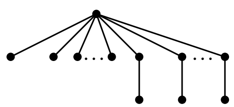


Figure 3. An example of a fork vertex.

Lemma 8. *Let $\lfloor n/2 \rfloor < p \leq n-3$. Then $T \in \mathcal{M}_{n,p}$ contains a fork vertex.*

Proof. Since the number of leaves is bigger than half the number of vertices, there exists a vertex x such that $d_x > 2$ and x has a leaf as a child. By Lemma 7, x is of height at most 2. If x is a not a fork vertex, then it must have a child y of degree greater than 2. As $\mathrm{ht}(y) = 1$, it follows that y is a fork vertex. ■

We have the following property of fork vertices in optimal trees.

Lemma 9. *Let $\lfloor n/2 \rfloor < p \leq n-3$ and $T \in \mathcal{M}_{n,p}$ a tree, rooted in r. If the degree of every child of r is at least 2, then every fork vertex in T has a child of degree 2.*

Proof. Suppose to the contrary that there exists a fork vertex y with only leaf children. Since the degree of every child of r is at least 2, vertices y and r are different. Let x be the father of y (x and r may coincide), and let $d = d_r$. By Lemma 5 and the definition of a fork vertex we have $d \geq d_x > d_y \geq 3$. Denote by C the set of children of r. Let ℓ be a leaf child of y, and let $T' = T - \{y\ell\} + \{r\ell\}$. Consider the difference

$$\begin{aligned}
\mathrm{RRR}(T') - \mathrm{RRR}(T) &= \sqrt{d}\sum_{u\in C}\sqrt{d_u - 1} + \sqrt{d_x - 1}\sqrt{d_y - 2} \\
&\quad -\sqrt{d-1}\sum_{u\in C}\sqrt{d_u - 1} - \sqrt{d_x - 1}\sqrt{d_y - 1} \\
&= (\sqrt{d} - \sqrt{d-1})\sum_{u\in C}\sqrt{d_u - 1} \\
&\quad -\sqrt{d_x - 1}(\sqrt{d_y - 1} - \sqrt{d_y - 2}).
\end{aligned}$$

Since the degree of every vertex in C is at least 2, we have $\sum_{u\in C}\sqrt{d_u - 1} \geq |C| = d > d - 1$, thus

$$\mathrm{RRR}(T') - \mathrm{RRR}(T) > (d-1)(\sqrt{d} - \sqrt{d-1}) - \sqrt{d_x - 1}(\sqrt{d_y - 1} - \sqrt{d_y - 2}).$$

Using straightforward calculations one can check that since $d \geq 4$ it holds

$$(d-1)(\sqrt{d} - \sqrt{d-1}) > \frac{1}{1+\sqrt{2}}\sqrt{d-1},$$

and since $d_y \geq 3$ we have

$$\sqrt{d_y - 1} - \sqrt{d_y - 2} \leq \frac{1}{1+\sqrt{2}}.$$

Since $d \geq d_x$, we obtain

$$\sqrt{d_x - 1}(\sqrt{d_y - 1} - \sqrt{d_y - 2}) \leq \frac{1}{1+\sqrt{2}}\sqrt{d_x - 1} \leq \frac{1}{1+\sqrt{2}}\sqrt{d-1} < (d-1)(\sqrt{d} - \sqrt{d-1}),$$

implying that $\mathrm{RRR}(T') > \mathrm{RRR}(T)$, a contradiction with the assumption that $T \in \mathcal{M}_{n,p}$. ∎

The following lemma will be crucial in the proof that an optimal tree is of height 2.

Lemma 10. *Let $\lfloor n/2 \rfloor < p \leq n-3$ and $T \in \mathcal{M}_{n,p}$ a tree, rooted in r. Then r has a leaf child.*

Proof. Suppose to the contrary that no child of the root r is a leaf. By Lemma 8 there exists a fork vertex y in T, and y has a child of degree 2 by Lemma 9. Note that $y \neq r$, since y has a leaf child by the definition of a fork vertex. Let x be the father of y (which may coincide with r), and let $d = d_r$. Denote by C the set of children of r and let A be the set of children of y whose degree equals 2, and $a = |A|$. As already noted, $a \geq 1$. Let $T' = T - \{yv | v \in A\} + \{rv | v \in A\}$, i.e., T' is obtained from T by deleting every edge between y and a vertex from A, and connecting instead r with every vertex in A.

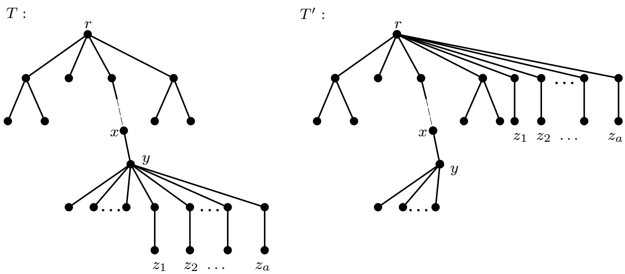


Figure 4. An illustration of trees T and T'.

In the below estimation of $\mathrm{RRR}(T') - \mathrm{RRR}(T)$, we use the fact that $\sum_{u \in C} \sqrt{d_u - 1} \geq |C| = d$ and $d_y < d$ (the latter holds by Lemma 5):

$$
\begin{aligned}
\mathrm{RRR}(T') - \mathrm{RRR}(T) &= \sqrt{d+a-1}\left(\sum_{u \in C} \sqrt{d_u - 1} + a\right) + \sqrt{(d_x-1)(d_y-a-1)} \\
&\quad - \sqrt{d-1}\sum_{u \in C}\sqrt{d_u-1} - a\sqrt{d_y-1} - \sqrt{(d_x-1)(d_y-1)} \\
&> \left(\sum_{u \in C}\sqrt{d_u-1} + a\right)(\sqrt{d+a-1} - \sqrt{d-1}) \\
&\quad + \sqrt{(d_x-1)(d_y-a-1)} - \sqrt{(d_x-1)(d_y-1)} \\
&\geq (d+a)(\sqrt{d+a-1} - \sqrt{d-1}) \\
&\quad - \sqrt{d_x-1}\left(\sqrt{d_y-1} - \sqrt{d_y-a-1}\right).
\end{aligned}
$$

To prove that $\mathrm{RRR}(T') - \mathrm{RRR}(T) > 0$, which will give us a contradiction with $T \in \mathcal{M}_{n,p}$, we need to see that

$$
(d+a)(\sqrt{d+a-1} - \sqrt{d-1}) > \sqrt{d_x-1}\left(\sqrt{d_y-1} - \sqrt{d_y-a-1}\right).
$$

This inequality can be transformed to

$$
(d+a)\frac{d+a-1-(d-1)}{\sqrt{d+a-1}+\sqrt{d-1}} > \sqrt{d_x-1}\frac{d_y-1-(d_y-a-1)}{\sqrt{d_y-1}+\sqrt{d_y-a-1}},
$$

and since $a \geq 1$, further to

$$(d+a)\left(\sqrt{d_y-1}+\sqrt{d_y-a-1}\right) > \sqrt{d_x-1}\left(\sqrt{d+a-1}+\sqrt{d-1}\right), \qquad (5)$$

thus proving inequality (5) is our final goal. Since $a \leq d_y - 2$, we have $\sqrt{d_y-a-1} \geq 1$, and since $d_y \geq 3$, it holds $\sqrt{d_y-1} \geq \sqrt{2}$. Therefore $\sqrt{d_y-1}+\sqrt{d_y-a-1} > 2$. Clearly we have $\sqrt{d_x-1} < \sqrt{d+a}$. Now we derive

$$\begin{aligned}
(d+a)\left(\sqrt{d_y-1}+\sqrt{d_y-a-1}\right) &> 2(d+a) \\
&= 2\sqrt{d+a}\sqrt{d+a} \\
&> \sqrt{d_x-1}\left(\sqrt{d+a-1}+\sqrt{d-1}\right),
\end{aligned}$$

which concludes the proof of inequality (5). ■

Finally we can state the main observation on optimal trees.

Lemma 11. *Let* $\lfloor n/2 \rfloor < p \leq n-3$ *and* $T \in \mathcal{M}_{n,p}$. *Then* $\mathrm{ht}(T) = 2$.

Proof. By Lemma 10 and Lemma 7 we derive that $\mathrm{ht}(T) \leq 2$. However, $\mathrm{ht}(T)$ cannot be 1, as T is a star in this case, for which $p = n-1$, contradicting our assumption that $p \leq n-3$. ■

4 The structure of optimal trees

Let $T \in \mathcal{M}_{n,p}$ and $p > \lfloor n/2 \rfloor$. Recall that by Proposition 3, in the case when $p = n-1$, T is a star, and in the case when $p = n-2$, T is a double star $D_{a,b}$, where $|a-b| \leq 1$. Further, if $p \leq n-3$ the height of a tree from $T \in \mathcal{M}_{n,p}$ equals 2 by Lemma 11. This implies that in a tree T besides the root r, which is the vertex of maximal degree (recall that such a vertex is unique, by Corollary 6), we have three types of vertices, which we group in three sets:

- A denotes the set of leaf children of r,
- B is the set of non-leaf children of r, and
- C is the set of leaves, not adjacent to r,

see Figure 6. Let a, b, c denote cardinalities of the sets A, B, C, respectively. Since $n = 1 + a + b + c = 1 + b + p$ and we consider trees for given n and p, b is a constant, i.e. $b = n - p - 1$. Further, we have $a = p - c$, thus it remains to find c. To describe its value, we first prove the following lemma.

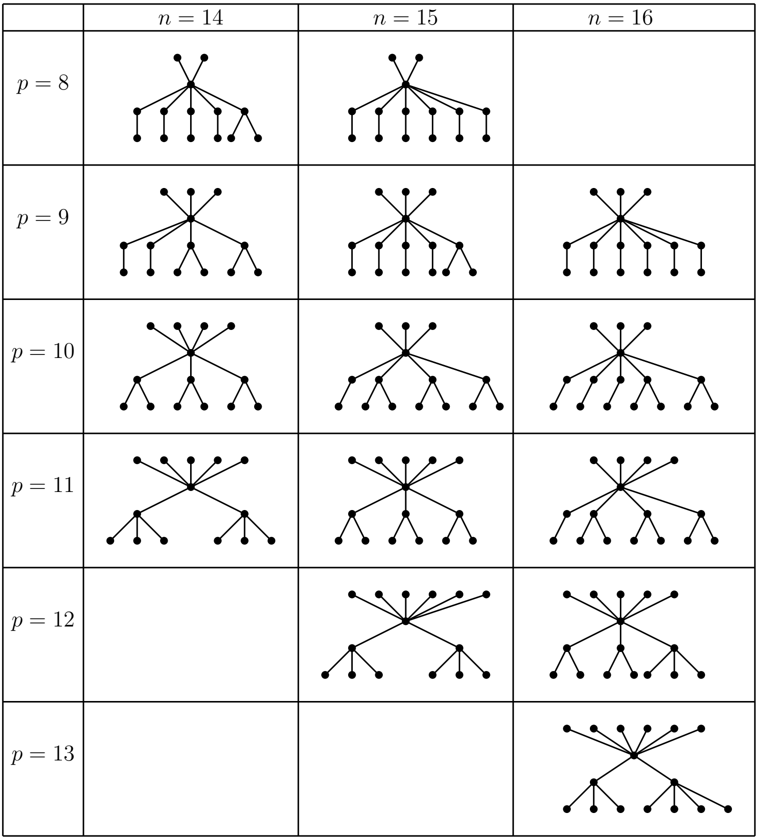


Figure 5. Optimal trees with given n and p such that $\lfloor n/2 \rfloor < p \leq n - 3$.

Lemma 12. *Let $\lfloor n/2 \rfloor < p \leq n - 3$ and $T \in \mathcal{M}_{n,p}$. Then all non-leaf children of the root r of T have almost the same degree, i.e. they either have x or $x + 1$ leaf children, for some $x \geq 1$.*

Proof. Suppose to the contrary that the root r (with degree d) in $T \in \mathcal{M}_{n,p}$ has children a and b with degrees α and β, respectively, such that $\alpha - 1 > \beta > 1$. By Lemma 11, all the children of a and b are leaves. Let v be a child of a. Let $T' = T - \{av\} + \{bv\}$. Then

$$\mathrm{RRR}(T') - \mathrm{RRR}(T) = \sqrt{d-1}(\sqrt{\alpha - 2} + \sqrt{\beta} - \sqrt{\alpha - 1} - \sqrt{\beta - 1}).$$

It is easy to see that under the condition $\alpha - 1 > \beta$ it holds

$$\sqrt{\alpha - 2} + \sqrt{\beta} > \sqrt{\alpha - 1} + \sqrt{\beta - 1},$$

thus $\mathrm{RRR}(T') - \mathrm{RRR}(T) > 0$, a contradiction. ■

Since every vertex from B has either x or $x+1$ leaf children, we have $x = \lfloor \frac{c}{b} \rfloor$. Thus the extremal tree T is completely determined by the values a, b, c. Let b_0 denote the number of vertices in B that have x leaf children, and let b_1 denote the number of vertices in B that have $x+1$ leaf children. Then $b = b_0 + b_1$. Further, we have $b_1 = c - bx$ and $b_0 = b - b_1 = b + bx - c$. Then

$$\begin{aligned}
\mathrm{RRR}(T) &= \sqrt{d-1} \sum_{u \in B} \sqrt{d_u - 1} \\
&= \sqrt{d-1}(b_0\sqrt{x} + b_1\sqrt{x+1}) \\
&= \sqrt{d-1}\left((b + b\lfloor \tfrac{c}{b} \rfloor - c)\sqrt{\lfloor \tfrac{c}{b} \rfloor} + (c - b\lfloor \tfrac{c}{b} \rfloor)\sqrt{\lfloor \tfrac{c}{b} \rfloor + 1}\right).
\end{aligned}$$

With this we have expressed $\mathrm{RRR}(T)$ as a discrete function with the variable c. Thus the sought-after value of c is the one for which this function attains its maximum. Using a computer program we identified c for some given values of n and p, where $\lfloor n/2 \rfloor < p \leq n-3$, and the corresponding extremal trees are presented in Figure 5.

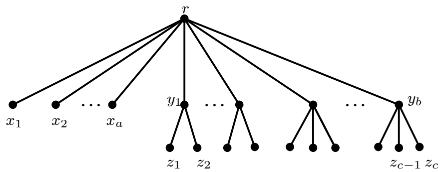


Figure 6. The structure of optimal trees.

We conclude the paper with the outline of the above observations in the following theorem.

Theorem 13. *Let $T \in \mathcal{T}_{n,p}$ with $\lfloor n/2 \rfloor < p \leq n-3$. Let T be rooted in a vertex r of maximal degree d, with a leaves adjacent to r, $b = n - p - 1$ non-leaf neighbors of r, and let $c = n - a - b - 1$. Then $T \in \mathcal{M}_{n,p}$ if and only if the following holds:*

(1) T is of height 2,

(2) the non-leaf children of r have almost the same degree (i.e. $\lfloor \frac{c}{b} \rfloor + 1$ and $\lceil \frac{c}{b} \rceil + 1$), and

(3) the expression

$$\sqrt{d-1}\left((b+b\lfloor\frac{c}{b}\rfloor-c)\sqrt{\lfloor\frac{c}{b}\rfloor}+(c-b\lfloor\frac{c}{b}\rfloor)\sqrt{\lfloor\frac{c}{b}\rfloor+1}\right)$$

attains the maximum value under the assumption that the conditions (1) and (2) hold.

Acknowledgments: The first three authors are partially supported by Ministry of Science of Montenegro, while the last two authors are partially supported by Slovenian research agency ARRS, programs no. P1–0383 and J1–1692.

References

[1] A. Ali, A. A. Bhatti, A note on the minimum reduced reciprocal Randić index of n-vertex unicyclic graphs, *Kuwait J. Sci.* **44** (2017) 27–33.

[2] A. Ali, S. Elumalai, S. Wang, D. Dimitrov, On the bicyclic graphs with minimum reduced reciprocal Randić index, *Iranian J. Math. Chem.* **9** (2018) 227–239.

[3] A. Aslam, Y. Bashir, M. Rafiq, F. Haider, N. Muhammad, N. Bibi, Three new/old vertex–degree–dased dopological indices of some dendrimers structure, *El. J. Biol.* **13** (2017) 94–99.

[4] B. Bollobás, P. Erdős, Graphs of extremal weights, *Ars Comb.* **50** (1998) 225–233.

[5] J. Gao, M. Lu, On the Randić index of unicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 377–384.

[6] I. Gutman, Degree–based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361.

[7] I. Gutman, B. Furtula, C. Elphick, Three new/old vertex–degree–based topological indices, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 617–632.

[8] M. K. Jamil, A. Javed, W. Nazeer, M. R. Farahani, Y. Gao, Four vertex–degree–based topological indices of $VC_5C_7[p;q]$ nanotubes, *Commun. Math. Appl.* **9** (2017) 99–105.

[9] X. Li, Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 127–156.

[10] F. C. G. Manso, H. S. Júnior, R. E. Bruns, A. F. Rubira, E. C. Muniz, Development of a new topological index for the prediction of normal boiling point temperatures of hydrocarbons: The *Fi* index, *J. Mol. Liq.* **165** (2012) 125–132.

[11] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[12] X. Ren, X. Hu, B. Zhao, Proving a conjecture concerning trees with maximal reduced reciprocal Randić index, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 171–184.

[13] Y. Zhu, G. Liu, J. Wang, On the Randić index of bicyclic graphs, in: I. Gutman, B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, Univ. Kragujevac, Kragujevac, 2008, pp. 119–132.