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Proving a Conjecture Concerning Trees with Maximal Reduced Reciprocal Randić Index

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Abstract

Gutman et al. [MATCH Commun. Math. Comput. Chem. **72** (2014) 617–632] presented three vertex-degree-based graph invariants, among which the reduced reciprocal Randić (RRR) index was defined as

$$RRR(G) = \sum_{ij \in E(G)} \sqrt{(d_i - 1)(d_j - 1)}.$$

They characterized the trees of order n with maximal RRR, but an exact proof has not been given. In this paper, we show that their conjecture is true.

1 Introduction

Let $G = (V(G), E(G))$ be a graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. The degree of a vertex $i \in V(G)$ is defined by d_i. The set of first neighbors of the vertex i is denoted by $N(i)$. Evidently, $|N(i)| = d_i$. In certain cases, we also use $d(i)$ to denote the degree of vertex i. A vertex i is said to be pendent, if $d_i = 1$. And, an edge of a graph is said to be pendent if one of its end-vertices is pendent. The edge connecting two vertices i and j is denoted by ij.

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If $uv \in E(G)$, then $G - uv$ denotes the graph obtained by deleting the edge uv from G. If, in return, $uv \notin E(G)$, then $G + uv$ denotes the graph obtained from G by adding the edge uv to graph G.

A positive non-increasing integer sequence $\pi = (d_1, d_2, \ldots, d_n)$ is called degree sequence, if there exists a connected graph G with $\pi(G) = \pi$. For a tree T, the degree sequence of T is the sequence of the degrees of the non-leaf vertices in descending order. Let $T(\pi)$ be the set of the trees with degree sequence π.

If $V(G)$ is the disjoint union of two nonempty sets $V_1(G)$ and $V_2(G)$ such that every vertex in $V_1(G)$ has degree r and every vertex in $V_2(G)$ has degree s $(r \leq s)$, then G is (r, s)-semiregular. If $r = s$, then G is said to be regular. Analogously, (r, s, q)-regular graph has the vertex set $V(G)$ which can be divided into three disjoint nonempty sets $V_1(G)$, $V_2(G)$ and $V_3(G)$, every vertex in $V_1(G)$ has degree r, every vertex in $V_2(G)$ has degree s and every vertex in $V_3(G)$ has degree q.

A graphical invariant is a number related to a graph which is a structural invariant, in which other words, it is a fixed number under graph automorphisms. In chemical graph theory, these invariants are also known as the topological indices. Topological indices play a significant role in chemistry, pharmacology, etc.

Two oldest and well-known graph invariants are Zagreb indices (M_1 and M_2) first introduced in 1972 [4,5], where Gutman and Trinajstić examined the dependence of total π-electron energy on molecular structure. The Randić (R) index is introduced for the effect of molecular branching [7]. These are defined as

$$M_1(G) = \sum_{i \in V(G)} d_i^2 \tag{1}$$

$$M_2(G) = \sum_{ij \in E(G)} d_i d_j \tag{2}$$

$$R(G) = \sum_{ij \in E(G)} \frac{1}{\sqrt{d_i d_j}} \tag{3}$$

respectively.

In order to consider other factors except for branching, the so-called atom–bond connectivity (ABC) index was proposed by Estrada et al. [6]. Since the atom–bond connectivity index performs very well in QSPR/QSAR studies, numerous mathematical and chemical studies on it have been published.

Recently, Gutman et al. [2] considered three new vertex–degree–based graph invariants, among which the reduced reciprocal Randić index (RRR) was defined as

$$RRR(G) = \sum_{ij \in E(G)} \sqrt{(d_i - 1)(d_j - 1)}. \tag{4}$$

For convenience, we call it RRR index in the subsequent parts of the paper. In some experiments, RRR index has a better correlation with chemical properties than the ABC index. More details can be found in [2].

At the same time, Furtula et al. [3] studied the difference of Zagreb indices on trees. They introduced a new vertex–degree–based invariant which was defined as

$$RM_2(G) = \sum_{ij \in E(G)} (d_i - 1)(d_j - 1). \tag{5}$$

It was called reduced second Zagreb index.

We can observe that RRR index is based on Eq. (5) and Eq. (3). Although, it is a pity that RM_2 is poorly correlated with chemical properties, it can give us a lot of mathematical thoughts in the following proof.

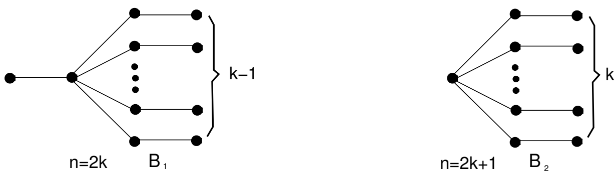

Fig. 1. The trees $T_{RRR}(n)$ which by Conjecture 1.1 have greatest reduced reciprocal Randić index.

Conjecture 1. ([2]) *The trees of order 6 with maximal RRR-value is p_6. The tree of order 8 with maximal RRR-value is the tree obtained by attaching a pendent vertex to a pendent vertex of $T_{RRR}(7)$. For $n \geq 3$, $n \neq 6, 8$, the trees of order n with maximal RRR-value is $T_{RRR}(n)$.*

In order to prove Conjecture 1.1, which is given by Gutman et al. [2], we need to show the following results.

Theorem 2. *Let T is a tree of order n with $p \geq \lfloor \frac{n}{2} \rfloor$ pendent vertices, then the tree T with the maximal RRR-value is $T_{RRR}(n)$.*

The paths $P_{l_1}, P_{l_2}, \ldots, P_{l_k}$ are said to have almost equal lengths if and only if $l_1, \ldots, l_k$ satisfy $|l_i - l_j| \leq 1$ for $1 \leq i \leq j \leq k$.

Theorem 3. *Let T is a tree of order n with $p < \lfloor \frac{n}{2} \rfloor$ pendent vertices, $n \geq 6$, then $RRR(T) \leq RRR(F_n(k))$, where $F_n(k)$ is the tree on n vertices obtained by attaching k paths of almost equal lengths to one common vertex.*

2 Proof of Theorem 1.1

In this section, we use the results in the work of Furtula et al. [3] and the classical, the (*Cauchy–Schwarz inequality*) to prove Theorem 1.1.

Definition 4. ([3]) *Let D be a positive integer, $D \geq 2$. Let S_{D+1} be the star on $D+1$ vertices, and let $v_1, v_2, \ldots, v_D$ be its pendent vertices. For $i = 1, 2, \ldots, D$, let r_i be non-negative integers, labeled so that $r_1 \geq r_2 \geq \cdots \geq r_D$. Construct the tree $T(r_1, r_2, \ldots, r_D)$ by attaching r_i pendent vertices to the vertex v_i of S_{D+1}, and by doing this for $i = 1, 2, \ldots, D$. The tree $T(r_1, r_2, \ldots, r)$ has thus $n = 1 + D + \sum_{i=1}^{D} r_i$ vertices. For given values of $D \geq 2$ and $n \geq D+1$, the set of all trees $T(r_1, r_2, \ldots, r_D)$ constructed in the above described manner is denoted by $T(n, D)$.*

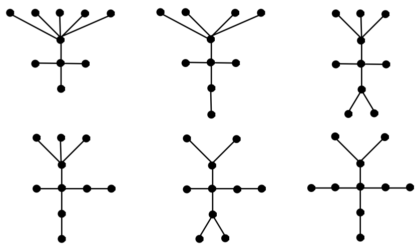

Fig. 2. Trees belonging to the set $T(10, 4)$: T(5,0,0,0), T(4,1,0,0), T(3,2,0,0), T(2,2,1,0), and T(2,1,1,1).

Lemma 5. ([3]) *Let n be a fixed integer, $n \geq 3$.*
(a) If n is even, then the elements of $T(n)$ with maximal reduced second Zagreb index are the elements of $T(n, n/2)$. For all trees $T \in T(n, n/2)$, this maximal value is $RM_2(T) = \frac{1}{4}(n-2)^2$.
(b) If n is odd, then the elements of $T(n)$ with maximal reduced second Zagreb index are the elements of $T(n, \lceil n/2 \rceil) \cup \tau(n, \lfloor n/2 \rfloor)$. For all trees $T \in T(n, \lceil n/2 \rceil) \cup \tau(n, \lfloor n/2 \rfloor)$, this maximal value is $RM_2(T) = \frac{1}{4}(n-1)(n-3)$.

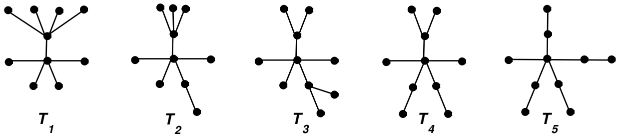

Fig. 3. The trees of order $n = 10$ with maximal RM_2-value, equal to 16. For $i = 1, 2, \ldots, 5, T_i \in T(10, 5)$.

Lemma 6. *Let G be a connected graph with m edges and $p > 0$ pendent vertices, then we have $RRR(G) \le \sqrt{(m-p)RM_2(G)}$, with equality if and only if G is a $(r, 1)$-semiregular graph or a tripartite $(r, s, 1)$-regular graph.*

Recall that for $r \neq s$, a graph G is said to be (r, s)-semiregular graph if its vertex degrees assume only the values r and s, and if there is at least one vertex of degree r and at least one degree of s. If every vertex of degree r is adjacent to vertices of degree s and vice versa, then G is bipartite $(r, 1)$-semiregular graph. Similarly, tripartite (r, s, q)-regular graph means its vertex degrees assume only the values r,s and q, and vertices of same degree are not adjacent.

Proof. Recall the Eq.(4), we have

$$RRR^2(G) = \Bigg(\sum_{ij \in E(G)} \sqrt{(d_i - 1)(d_j - 1)} \Bigg)^2 = \Bigg(\sum_{\substack{ij \in E(G) \\ d_i \neq 1, d_j \neq 1}} \sqrt{(d_i - 1)(d_j - 1)} \Bigg)^2$$

$$\le \sum_{\substack{ij \in E(G) \\ d_i \neq 1, d_j \neq 1}} 1 \sum_{\substack{ij \in E(G) \\ d_i \neq 1, d_j \neq 1}} (d_i - 1)(d_j - 1) \tag{6}$$

$$= \sum_{\substack{ij \in E(G) \\ d_i \neq 1, d_j \neq 1}} 1 \sum_{ij \in E(G)} (d_i - 1)(d_j - 1) = (m - p)RM_2(G).$$

So we immediately get

$$RRR(G) \le \sqrt{(m-p)RM_2(G)}\,. \tag{7}$$

The above inequality (6) is based on the Cauchy–Schwarz inequality, and the equality holds if and only if $\sqrt{(d_i - 1)(d_j - 1)}$ is a constant number for all edges $v_i v_j \in E(G)$, except for pendent edges. For any two adjacent non-pendent edges $v_i v_j$, $v_i v_k \in E(G)$, we have $\sqrt{(d_i - 1)(d_j - 1)} = \sqrt{(d_i - 1)(d_k - 1)}$, i,e, $d_j = d_k$. Suppose that $d_i = r$, then all vertices, except pendent vertices, adjacent to the vertex v_i are of the same degree (say s). On the other hand, all vertices, except pendent vertices, adjacent to the vertex v_j, $v_i v_j \in E(G)$, are of degree r. Considering the fact that G is connected and it has p pendent vertices, it follows that the vertex set of the degree s, the vertex set of degree r and the pendent vertex set are independent sets. Then, G should be a tripartite $(r, s, 1)-regular$ graph. If $r = s$, G is a $(r, 1)$-semiregular. □

Proof of Theorem 1.1: Let T is a tree of order n with $p \geq \lfloor \frac{n}{2} \rfloor$ pendent vertices.

Case 1: n is even.

Naturally, by Lemma 2.1 and Lemma 2.2, we have

$$RRR(T) \leq \sqrt{(n-1-p)RM_2(T)} \tag{8}$$

$$\leq \sqrt{(n-1-p)\frac{(n-2)^2}{4}} \tag{9}$$

$$\leq \sqrt{\frac{(n-2)^3}{8}}. \tag{10}$$

The Eq. (8) holds if and only if T is a $(r, 1)$-semiregular tree or a tripartite $(r, s, 1)$-regular tree. The Eq. (9) holds if and only if $T \in T(n, n/2)$. The Eq. (10) holds if and only if $p = n/2$. From $T(n, n/2)$, we can find only one element satisfying Eq. (8) and Eq. (10). That is exactly B_1 showed in Fig. 1.

Case 2: n is odd.

By the same way of case.1, we have

$$RRR(T) \leq \sqrt{\frac{n-1}{2} \cdot \frac{n-3}{2}}. \tag{11}$$

The Eq. (11) holds if and only if $T \cong B_2$ (showed in Fig. 1). Hence, the proof of Theorem 1.2 is completed.

3 Proof of Theorem 1.2

In this section, we use the techniques from [8] to characterize the extremal trees with given degree sequence that has the maximal RRR-value and provide an algorithm to construct such trees. Then inspired by the thoughts of Liu et al. [9], we use a modified operation to prove Theorem 1.2.

In recent years, an efficient algorithm (the greedy algorithm) on some extremal trees with given degree sequence is widely used in many index studies. For instance, Xing et al. [11] and Gan et al. [10], respectively, used it to characterize the trees with minimal ABC index. And Liu et al. [9] used it to characterize the trees with maximal second Zagreb index. All the above-mentioned trees are connected and all have a fixed degree sequence.

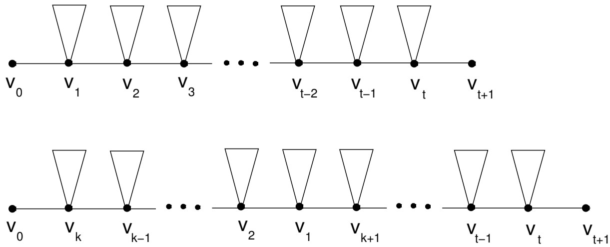

Fig. 4. A new tree T' obtained by the transformation $T - \{v_0v_1, v_kv_{k+1}\} + \{v_0v_k, v_1v_{k+1}\}$.

Lemma 7. *Let T be a tree with maximal RRR index, every path $v_0v_1v_2\ldots v_tv_{t+1} \in T$, where v_0 and v_{t+1} are leaves, has the properties:*

(a) If t is odd, then

$d(v_1) \le d(v_t) \le d(v_2) \le d(v_{t-1}) \ldots \le d(v_{\frac{t-1}{2}}) \le d(v_{\frac{t+3}{2}}) \le d(v_{\frac{t+1}{2}})$.

(b) If t is even, then

$d(v_1) \le d(v_t) \le d(v_2) \le d(v_{t-1}) \cdots \le d(v_{\frac{t+4}{2}}) \le d(v_{\frac{t}{2}}) \le d(v_{\frac{t+2}{2}})$.

Proof. It suffices to prove that $d(v_i) \le d(v_{t+1-i}) \le d(v_k), (i+1 \le k \le t+1-i, i = 1, 2, \ldots, \lceil \frac{t+1}{2} \rceil)$.

By induction on i. For $i = 1$, suppose for contradiction that $d(v_k) < d(v_1)$ for some $2 \le k \le t-1$. Then we can construct a new tree T' (with the same degree sequence) obtained from T by deleting edges v_0v_1 and v_kv_{k+1}, adding two new edges v_0v_k and v_1v_{k+1}. We denote the operation by $T' = T - \{v_0v_1, v_kv_{k+1}\} + \{v_0v_k, v_1v_{k+1}\}$. Recall the Eq. (4), we have

$$RRR(T') - RRR(T) = \left(\sqrt{d(v_1)-1} - \sqrt{d(v_k)-1}\right)\sqrt{d(v_{k+1})-1} > 0\,. \qquad (12)$$

Contradiction to the maximal optimality of T, hence we must have $d(v_1) \le d(v_k)$. Similarly, $d(v_t) \le d(v_k)$, then we have

$$d(v_1) \le d(v_t) \le d(v_k) \qquad \text{for any } 2 \le k \le t.$$

We now assume Lemma 3.1 holds for any $l \le i-1$, which means that $d(v_l) \le d(v_{t+1-l}) \le d(v_k)$,$(l+1 \le k \le t+1-l, l = 1, 2, \ldots, \lfloor (t+1)/2 \rfloor)$. Suppose for contradiction that $d(v_i) > d(v_k)$ for some $i+1 \le k \le t+1-i$. We construct a new tree $T' = T - \{v_{i-1}v_i, v_kv_{k+1}\} + \{v_{i-1}v_k, v_iv_{k+1}\}$. By then inductive hypothesis,

$$RRR(T') - RRR(T) = \left(\sqrt{d(v_i)-1} - \sqrt{d(v_k)-1}\right)\left(\sqrt{d(v_{k+1})-1} - \sqrt{d(v_{i-1})-1}\right) > 0\,. \quad (13)$$

It contradicts to the maximal optimality of T. Thus we have $d(v_i) \leq d(v_k)$ for $i+1 \leq k \leq t+1-i$. Similarly, we can verify that $d(v_{t+1-i}) \leq d(v_k)$ for $i+1 \leq k \leq t+1-i$. Therefore, we have $d(v_i) \leq d(v_{t+1-i}) \leq d(v_k)$, $i \leq k \leq t+1-i$, which completes the proof of Lemma 3.1. □

Corollary 8. *Let T be a tree of order n with maximal RRR index among the trees with fixed degree sequence. Then there are no two non-adjacent edges v_1v_2 and v_3v_4 such that $d(v_1) < d(v_3) \leq d(v_4) < d(v_2)$.*

Proof. By Lemma 3.1, we can obtain that easily. □

Let $\pi = (d_1, d_2, \ldots, d_m)$ be a tree degree sequence. Delorme et al. [12] discovered that the properties of extremal trees with maximum Randić index for $\alpha = 1$ are the same as the features of Kruskal's classical algorithm for the minimum spanning tree problem. Wang [8] generalized it to be greedy algorithm and Liu et al. [9] generalized it to be BFS-algorithm. Now, we present the greedy algorithm that can construct the trees which satisfy the Lemma 3.1 and corollary 3.2 and has the maximal RRR-value. More details can be found in the above literatures.

Definition 9. ([8]) *Suppose the degrees of the non-leaf vertices are given, the greedy tree is achieved by the following greedy algorithm:*

(1) Label the vertex with the largest degree as v (the root).

(2) Label the neighbors of v as $v_1, v_2, \ldots$, assign the largest degrees available to them such that $d(v_1) \geq d(v_2) \geq \cdots$.

(3) Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, \ldots$ such that take all the largest degrees available and that $d(v_{11}) \geq d(v_{12}) \geq \cdots$ then do the same for $v_2, v_3, \ldots$.

(4) Repeat (3) for all newly labeled vertices, always start with neighbors of the labeled vertex with largest whose neighbors are not labeled yet.

For a given tree with degree sequence π, we can get a unique greedy tree which has the maximal RRR index. But the Fig. 5 shows that we cannot deduce that this greedy tree is the unique tree with maximal RRR index. Fortunately, this fact dose not affect our conclusion.

Lemma 10. *Let $f(x,y) = (\sqrt{x+y-3} - \sqrt{x-1})(x-1) + 1 - \sqrt{y-1}$. If $x \geq y \geq 3$, then $f(x,y) > 0$.*

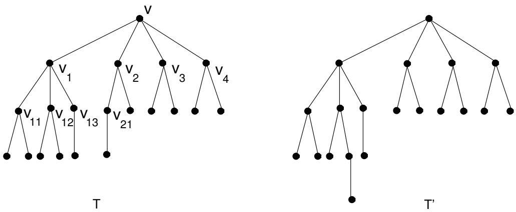

Fig. 5. Two extremal trees T and $T'$of degree sequence $\pi(4,4,3,3,3,3,3,2,2)$ with maximal RRR index. T is a greedy tree, but T' is not.

Proof. Bearing in mind that $x \geq y \geq 3$, we conclude that

$$\frac{\partial f}{\partial y} = \frac{x-1}{2\sqrt{x+y-3}} - \frac{1}{2\sqrt{y-1}} > \frac{\sqrt{(x-1)(y-1)} - \sqrt{x+y-3}}{2\sqrt{(x+y-3)(y-1)}} > 0$$

since $(x-1)(y-1) - (x+y-3) = (x-2)(y-2) > 0$. It is easy to verify that $f(x) = (\sqrt{x} - \sqrt{x-1})(x-1)$ is monotonic increasing. So we get

$$\begin{aligned} f(x,y) &\geq f(x,3) = (\sqrt{x} - \sqrt{x-1})(x-1) + 1 - \sqrt{2} \\ &\geq f(3,3) = (\sqrt{3} - \sqrt{2}) \times 2 + 1 - \sqrt{2} \approx 0.22 > 0\,. \end{aligned}$$

□

Lemma 11. *Let u, v be two non-adjacent vertices of a connected graph G, and w be a vertex of $N(u) \backslash \{N(v) \cup v\}$. Let $G' = G + vw - uw$, where $d_u \geq d_v \geq 3$. If $d_y \geq d_x$ and $d_y \geq 2$ for every $y \in N(v)$ and every $x \in N(u)$, then $RRR(G') > RRR(G)$.*

Proof. By Eq.(4), we set $d_{y'} = \min\limits_{y \in N(v)} \{d_y\}$, $d_{x'} = \max\limits_{x \in N(u) \backslash \{w\}} \{d_x\}$. Then we have

$$\begin{aligned} & RRR(G') - RRR(G) \\ &= \sqrt{d_v}\Big(\sum_{y \in N(v)} \sqrt{d_y - 1} + \sqrt{d_w - 1} \Big) + \sqrt{d_u - 2}\Big(\sum_{x \in N(u) \backslash \{w\}} \sqrt{d_x - 1} \Big) \\ &- \sqrt{d_v - 1}\Big(\sum_{y \in N(v)} \sqrt{d_y - 1} \Big) - \sqrt{d_u - 1}\Big(\sum_{x \in N(u) \backslash \{w\}} \sqrt{d_x - 1} + \sqrt{d_w - 1} \Big) \\ &= \Big(\sqrt{d_v} - \sqrt{d_v - 1}\Big)\Big(\sum_{y \in N(v)} \sqrt{d_y - 1}\Big) - \Big(\sqrt{d_u - 1} - \sqrt{d_u - 2}\Big)\Big(\sum_{x \in N(u) \backslash \{w\}} \sqrt{d_x - 1}\Big) \\ &+ \Big(\sqrt{d_v} - \sqrt{d_u - 1} \Big)\sqrt{d_w - 1} \\ &\geq \Big(\sqrt{d_v} - \sqrt{d_v - 1}\Big)\Big(d_v\sqrt{d_{y'} - 1}\Big) - \Big(\sqrt{d_u - 1} - \sqrt{d_u - 2}\Big)\Big(d_u - 1\Big)\sqrt{d_{x'} - 1} \end{aligned}$$

$$+\left(\sqrt{d_v}-\sqrt{d_u-1}\right)\sqrt{d_w-1} \tag{14}$$

$$\geq \left[\left(\sqrt{d_v}-\sqrt{d_v-1}\right)d_v-\left(\sqrt{d_u-1}-\sqrt{d_u-2}\right)\left(d_u-1\right)\right]\sqrt{d_{x'}-1}$$

$$+\left(\sqrt{d_v}-\sqrt{d_u-1}\right)\sqrt{d_w-1} \tag{15}$$

$$\geq 0. \tag{16}$$

The Eq.(14) holds if and only if $d_y = d_{y'}$ for $y \in N(v)$ and $d_x = d_{x'}$ for $x \in N(v)\backslash\{w\}$. The Eq. (15) holds if and only if $d_{y'} = d_{x'}$. The inequality (16) based on the fact that $f(x) = (\sqrt{x}-\sqrt{x-1})x$ is strictly monotonous increasing for $x \geq 2$, and Eq. (16) holds if and only if $d_{x'} = 1$ and $d_w = 1$.

¿From what has been discussed, all above equalities hold if and only if $d_y = d_x = 1$. But recall the fact that $d_y \geq 2$ for $y \in N(v)$, the strict inequality (16) holds. Hence, we have $RRR(G') > RRR(G)$. □

Proof of Theorem 1.2: Assume T is a tree of order n with fixed degree sequence $\pi(d_1, d_2, \ldots, d_m)$. We can construct a new tree T^* by greedy algorithm, then we have $RRR(T^*) \geq RRR(T)$. Since $d_1 \leq p < \lfloor \frac{n}{2} \rfloor$, we can easily get $m - 1 \geq d_1$. For the greedy tree T^*, that means every vertex of $N(v_1)$ is non-pendent. By the definition of the tree degree sequence, we have

$$d_2 \geq d_3 \geq \cdots \geq d_m \geq 2 \tag{17}$$

If all equalities in (17) are attained, we get a graph $F_n(p)$ by greedy algorithm. Otherwise, we can find a largest k, such that $k \leq m$ and $d_2 \geq d_3 \geq \cdots \geq d_k \geq 3$. For the sake of simplicity, we use v_i to denote the vertex of degree d_i.

Case 1: $v_1v_k \notin E(T^*)$.

Assume v_w is a child of v_k, then, we can construct a new tree $T' = T^* + v_1v_w - v_kv_w$. Clearly, T' is also a tree with p pendent vertices. By the Lemma 3.4, we have $RRR(T') > RRR(T^*)$.

Case 2: $v_1v_k \in E(T^*)$.

At this moment, we can find v_s for $2 \leq s \leq k$ such that there is a vertex of degree two in $N(v_s)$. Otherwise, it contradicts to the fact that $p < \lfloor \frac{n}{2} \rfloor$. Assume $N(v_s)\backslash\{v_1\} = \{v_{s_1}, v_{s_2}, \ldots, v_{s_t}\}$ and $d(v_{s_1}) \leq d(v_{s_2}) \leq \cdots \leq d(v_{s_t})$. By the definition of the greedy algorithm, we have $d(v_{s_i}) \leq 2$ for $v_{s_i} \in N(v_s)\backslash\{v_1\}$. Assume there is x vertices of degree two in $N(v_s)\backslash\{v_1, v_{s_1}\}$, then $1 \leq x \leq d(v_s) - 2$. Construct a new tree T' by

$T' = T^* + \{v_1v_{s_2}, \dots, v_1v_{s_t}\} - \{v_sv_{s_2}, \dots, v_sv_{s_t}\}$. We have

$$RRR(T') - RRR(T^*)$$

$$= \sqrt{d(v_1)+d(v_s)-3}\Big(\sum_{v_i\in N(v_1)\setminus\{v_s\}} \sqrt{d(v_i)-1} + \sum_{v_j\in N(v_s)\setminus\{v_{s_1},v_1\}} \sqrt{d(v_j)-1}\Big)$$

$$+ \sqrt{d(v_1)+d(v_s)-3} + \sqrt{d(v_{s_1})-1}\Big(1-\sqrt{d(v_s)-1}\Big)$$

$$- \sqrt{(d(v_1)-1)(d(v_s)-1)} - \sqrt{d(v_1)-1}\Big(\sum_{v_i\in N(v_1)\setminus\{v_s\}} \sqrt{d(v_i)-1}\Big)$$

$$- \sqrt{d(v_s)-1}\Big(\sum_{v_j\in N(v_s)\setminus\{v_{s_1},v_1\}} \sqrt{d(v_j)-1}\Big)$$

$$= \sqrt{d(v_1)+d(v_s)-3} - \sqrt{(d(v_1)-1)(d(v_s)-1)} + \sqrt{d(v_{s_1})-1}\Big(1-\sqrt{d(v_s)-1}\Big)$$

$$+ \Big(\sqrt{d(v_1)+d(v_s)-3} - \sqrt{d(v_1)-1}\Big)\Big(\sum_{v_i\in N(v_1)\setminus\{v_s\}} \sqrt{d(v_i)-1}\Big)$$

$$+ \Big(\sqrt{d(v_1)+d(v_s)-3} - \sqrt{d(v_s)-1}\Big)\Big(\sum_{v_j\in N(v_s)\setminus\{v_{s_1},v_1\}} \sqrt{d(v_j)-1}\Big).$$

Subcase 2.1: $d(v_{s_1}) = 1$

$$RRR(T') - RRR(T^*)$$

$$\geq \sqrt{d(v_1)+d(v_s)-3} - \sqrt{(d(v_1)-1)(d(v_s)-1)} + \Big(\sqrt{d(v_1)+d(v_s)-3} - \sqrt{d(v_s)-1}\Big)x$$

$$+ \Big(\sqrt{d(v_1)+d(v_s)-3} - \sqrt{d(v_1)-1}\Big)\Big(d(v_1)-1\Big) \tag{18}$$

$$> \frac{(d(v_s)-2)(d(v_1)-1)}{\sqrt{d(v_1)+d(v_s)-3}+\sqrt{d(v_1)-1}} - \frac{(d(v_s)-2)(d(v_1)-2)}{\sqrt{d(v_1)+d(v_s)-3}+\sqrt{(d(v_1)-1)(d(v_s)-1)}}$$

$$+ \Big(\sqrt{d(v_1)+d(v_s)-3} - \sqrt{d(v_s)-1}\Big)x$$

$$> \frac{d(v_s)-2}{\sqrt{d(v_1)+d(v_s)-3}+\sqrt{d(v_1)-1}} + \Big(\sqrt{d(v_1)+d(v_s)-3} - \sqrt{d(v_s)-1}\Big)x$$

$$> 0\ . \tag{19}$$

Subcase 2.2: $d(v_{s_1}) = 2$ then $x = d(v_s) - 2$

$$RRR(T') - RRR(T^*)$$

$$\geq \sqrt{d(v_1)+d(v_s)-3} - \sqrt{(d(v_1)-1)(d(v_s)-1)} + \Big(1-\sqrt{d(v_s)-1}\Big)$$

$$+\Big(\sqrt{d(v_1)+d(v_s)-3}-\sqrt{d(v_s)-1}\Big)\Big(d(v_s)-2\Big)$$
$$+\Big(\sqrt{d(v_1)+d(v_s)-3}-\sqrt{d(v_1)-1}\Big)\Big(d(v_1)-1\Big) \tag{20}$$
$$>\frac{(d(v_s)-2)(d(v_1)-2)}{\sqrt{d(v_1)+d(v_s)-3}+\sqrt{d(v_s)-1}}-\frac{(d(v_s)-2)(d(v_1)-2)}{\sqrt{d(v_1)+d(v_s)-3}+\sqrt{(d(v_1)-1)(d(v_s)-1)}}$$
$$+\Big(\sqrt{d(v_1)+d(v_s)-3}-\sqrt{d(v_s)-1}\Big)\Big(d(v_s)-2\Big)+\Big(1-\sqrt{d(v_s)-1}\Big)$$
$$>0\,. \tag{21}$$

The Eqs. (18) and (20) hold if and only if $d(v_i)=2$ for $v_i \in N(v_1)\backslash\{v_s\}$. Since $d(v_s)\geq 3$ and $x\geq 1$, the inequality (19) holds immediately. From Lemma 3.3, we can easily obtain the inequality (21). Hence we have $RRR(T')>RRR(T^*)$.

For the greedy tree T^* obtained by the tree degree sequence $\pi(d_1,d_2,\ldots,d_m)$, if there is some k $(2\leq k\leq m)$ such that $d_k\geq 3$, we will find a new tree T' with a bigger RRR-value than T^* which obtained by the operation of case.1 or case.2. And T' has the degree sequence $\pi'(d_1+x,d_2,\ldots,d_k-x,2,\ldots,2)$ $(1\leq x\leq d_k-2)$. Suppose T^{**} is the greedy tree in $T(\pi')$, we have $RRR(T^{**})\geq RRR(T')\geq RRR(T^*)$.

Repeating the transformation $T^*\to T'\to T^{**}$ a sufficient number of times, results in a tree T with degree sequence $\pi(p,2,\ldots,2)$. Clearly T also has p pendent vertices. By the greedy algorithm, we will get $T\cong F_n(p)$.

4 Proof of Conjecture 1.1

Until now, we have characterized the trees of order n with p ($p\geq\lfloor n/2\rfloor$ and every $p<\lfloor n/2\rfloor$) pendent vertices that have the maximal RRR-value. In order to prove Conjecture 1.1, we just need to compare the parameter p.

Proof of Conjecture 1.1: Recall the conclusions of Theorems 1.2 and 1.3, from which we have

(i) $RRR(T)\leq\frac{n-2}{2}\sqrt{\frac{n-2}{2}}$, for $p\geq\lfloor\frac{n}{2}\rfloor$ and p is even.

(ii) $RRR(T)\leq\frac{n-1}{2}\sqrt{\frac{n-3}{2}}$, for $p\geq\lfloor\frac{n}{2}\rfloor$ and p is odd.

(iii) $RRR(T)\leq(n-2p-1)+p\sqrt{p-1}$, for $p<\lfloor\frac{n}{2}\rfloor$.

It is easy to verify that $f(x)=(n-2x-1)+x\sqrt{x-1}$ is a strictly monotonous increasing when $x\in[2,\lfloor\frac{n}{2}\rfloor)$. So we have

(iv) $RRR(T)\leq(n-2\lfloor\frac{n}{2}\rfloor+1)+(\lfloor\frac{n}{2}\rfloor-1)\sqrt{\lfloor\frac{n}{2}\rfloor-2}$

when n is odd and $n\geq 7$, since $p=\lfloor\frac{n}{2}\rfloor-1\geq 2$, we have

$$RRR(B_2)-RRR(F_n(\frac{n-3}{2}))=\frac{n-1}{2}\sqrt{\frac{n-3}{2}}-\frac{n-3}{2}\sqrt{\frac{n-5}{2}}-2>0$$

when n is even and $n \geq 6$, since $p = \lfloor \frac{n}{2} \rfloor - 1 \geq 2$, we have

$$RRR(B_1) - RRR(F_n(\frac{n-2}{2})) = \frac{n-2}{2}\sqrt{\frac{n-2}{2}} - \frac{n-2}{2}\sqrt{\frac{n-4}{2}} - 1 \qquad (22)$$

if $n = 6, 8$, the Eq. (22) is negative . Otherwise, the Eq. (22) is positive.

Assume T is a tree of order $n \geq 6$ with maximal RRR-value, except for $n = 6, 8$, then $T \cong T_{RRR}(n)$. When $n = 6$ or $n = 8$, we have $T \cong F_6(2) \cong P_6$ or $T \cong F_8(3)$, where $F_8(3)$ is the tree obtained by attaching a pendent vertex to a pendent vertex of $T_{RRR}(7)$. Then, the Conjecture 1.1 is proved.

Remark: In this paper, we characterize the trees with p pendent vertices that maximize the RRR index for every $p < \lfloor n/2 \rfloor$. If one reads Theorem 1.2 carefully, it will be seen that we cannot get the same results for every $p \geq \lfloor n/2 \rfloor$. So it is still remains as an open problem.

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