MORE ON "SOLUTIONS TO TWO UNSOLVED QUESTIONS ON THE BEST UPPER BOUND FOR THE RANDIĆ INDEX R_{-1} OF TREES"

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Abstract

The Randić index $R_{-1}(G)$ of a graph G is defined as the sum of the $(d(u)d(v))^{-1}$ of all edges (uv) of G, where d(u) denotes the degree of a vertex u in G. In this paper we correct the errors of the proof of the paper [8], i.e., we prove that $R_{-1}(T) \leq \frac{15n+C}{56}$ for all trees of order $n \geq 103$, where C = -1. The structure of the Max Tree - the tree with maximum Randić index R_{-1} , is as it was predicted by Clark and Moon. The Max Tree has only one vertex of the maximum degree and all adjacent vertices are of degree 4. Every vertex of degree 4 has 3 suspended paths of length 2 centered at it.

1. INTRODUCTION

In 1975 Randić [11] proposed two topological indices $R_{-1/2}(G)$ and $R_{-1}(G)$, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The general Randić index $R_{\alpha}(G)$ of a graph G is defined [4] by $R_{\alpha}(G) = \sum_{(uv) \in E(G)} (d(u)d(v))^{\alpha}$, where the summation extends over all edges (uv) of G and d(u) denotes the degree of a vertex u. Randić himself demonstrated [11] that his indices are well correlated with a variety of physico-chemical properties. They have attracted considerable attention of chemists and mathematicians ([1-10]).

In [4] Clark and Moon gave a lower and upper bound for $R_{-1}(T)$ for trees, $1 \le R_{-1}(T) \le \frac{15n+8}{18}$, where the lower bound can be attained by the star, but the upper bound is not best possible. They constructed an infinite sequence T_{7n+1} of trees which are obtained from the star S_{n+1} by appending three internally disjoint paths of length 2 to each leaf of S_{n+1} . Then T_{7n+1} has order $|V(T_{7n+1})| = 7n+1$ and weight $R_{-1}(T_{7n+1}) = \frac{15n+2}{8}$ and $\lim_{n\to\infty} \frac{R_{-1}(T_{7n+1})}{|V(T_{7n+1})|} = \frac{15}{56}$. At the end of their paper [4] they proposed two unsolved questions on the upper bound.

Question 1: Find $K = \lim_{n\to\infty} \frac{f(n)}{n}$, where f(n) is the maximum value of $R_{-1}(T)$ among all trees of order n. We know that $\frac{15}{56} \leq K \leq \frac{5}{18}$ and suspect that the lower bound is closer to K than the upper bound.

Question 2: Refine the upper bound for $R_{-1}(T)$ so that it is sharp for infinitely many values of n.

Rautenbach [12] gave an upper bound for $R_{-1}(T)$ of trees with maximum degree 3. Li and Yang [9] used linear programming to determine the sharp upper bound for $R_{-1}(T)$ of chemical trees (i.e., trees with maximum degree at most 4). Hu, Li and Yuan [7] investigated trees with maximum general Randić index $R_{\alpha}(T)$ among all trees of order n. They distinguished α in several different intervals and for most of the intervals characterized trees with maximum $R_{\alpha}(T)$. Only the interval $-2 < \alpha < -\frac{1}{2}$ (including the point $\alpha = -1$) is left undetermined, but they obtained some properties of Max Tree in this case. The same authors Hu, Li and Yuan [8] tried to give positive answers to the above two questions proposed by Clark and Moon and to find sharp upper bound for $R_{-1}(T)$ of trees. The idea of their proof is similar to the one used in [4], but they made some errors which have been found in [10]. Hu, Jin, Li and Wang [5] determined the maximum value for R_{-1} of all trees of order $n \leq 102$ and gave one of the trees with maximum value of this index. Trees with maximum Randić index R_{-1} – the Max Tree need not be unique. This paper [5] gave us enough information to describe the structure of the Max Tree for $n \geq 103$. In this paper we prove that

 $R_{-1}(T) \leq \frac{15n+C}{56}$ for all trees of order $n \geq 103$, where C=-1 and describe the structure of the Max Tree - it has only one vertex of the maximum degree and all adjacent vertices are of degree 4. Every vertex of degree 4 has 3 suspended paths of length 2 centered at it.

Let T=(V,E) be a tree with order n=|V(T)|. The degree $d_T(u)$ of a vertex u is the number of vertices in T adjacent to u, and we omit the letter T if only one tree is under consideration. A vertex of degree 1 in a tree is called a *leaf*. A suspended path from x to z is a path x, y, z with d(x) = 1, d(y) = 2 and $d(z) \geq 3$. Let x_1y_1z, \dots, x_sy_sz be s distinct suspended paths adjacent to z, and w_1, \dots, w_{d-s} be the vertices of T, other than y_1, \dots, y_s , adjacent to z, then we call such system an (s, d) system centered at z. The Max Tree is a tree with maximum value of the Randić index R_{-1} for a given order n.

All notations, terminology and presumed results can be found in [8].

2. MAIN IMPROVEMENT

We will complete the proof of the next Theorem 1 from [8], which is not complete because of the errors found in [10]. It is likely evident that this Theorem 1 is true, but the first predicted Max Tree appears when n = 92, which causes the difficulties of its proof.

Theorem 1. For a tree T of order n > 103,

$$R_{-1}(T) \le \frac{15n + C}{56}$$

where C = -1.

We will prove this theorem at the end of this paper. At first we will describe some properties of the Max Tree. In [8] Hu, Li and Yuan showed that the "suspected" Max Tree can have the systems: (2,3),(3,4),(1,d) for $3 \le d \le 13$, (2,d) for $4 \le d \le 12$ and (3,d) for $5 \le d \le 11$. We will show that the Max Tree has only (3,4) systems when $n \ge 103$. From now on $n = |V(T)| \ge 103$. We use mathematical induction throughout this paper, i.e., we suppose that Theorem 1 holds for all trees of order less than n. We know that $R_{-1}(T) \le \frac{15n-1}{56}$ for $91 \le n \le 102$ [5].

At first we prove two useful lemmas.

Lemma 1. Every vertex of degree 3 is the center of a (2,3) system of the Max Tree, i.e., it appears only in a (2,3) system.

Proof. Let the Max Tree T has the vertex z of degree 3 with the neighbors y_1, y_2 and w and $d = d(w) \ge d(y_i), i = 1, 2$. We distinguish two cases.

Case 1. $d(y_1) \geq 3$ and $d(y_2) \geq 3$. By deleting the vertex z (and edges zy_1, zy_2 and zw) and adding new edges wy_1 and wy_2 we get a new tree T'. Let v_j denote the neighbors of w other than z. Then |V(T')| = n - 1, $d_{T'}(w) = d + 1$, $d(v_j) \geq 2$ and

$$R_{-1}(T) = R_{-1}(T') + \left(\frac{1}{3} - \frac{1}{d+1}\right) \sum_{i=1}^{2} \frac{1}{d(y_i)} + \frac{1}{3d} + \left(\frac{1}{d} - \frac{1}{d+1}\right) \sum_{j=1}^{d-1} \frac{1}{d(v_j)}$$

$$\leq \frac{15(n-1) + C}{56} + \frac{1}{3d} + \frac{d-2}{3(d+1)} \sum_{i=1}^{2} \frac{1}{d(y_i)} + \frac{1}{d(d+1)} \sum_{j=1}^{d-1} \frac{1}{d(v_j)}$$

$$\leq \frac{15n + C}{56} - \frac{15}{56} + \frac{1}{3d} + \frac{d-2}{3(d+1)} \cdot \frac{2}{3} + \frac{1}{d(d+1)} \cdot \frac{d-1}{2}$$

$$= \frac{15n + C}{56} + \frac{-23d^2 + 61d - 84}{504d(d+1)} < \frac{15n + C}{56}$$

The last inequality holds for every d.

Case 2. $d(y_1) = 2$ and $d(y_2) \ge 3$. By deleting the vertices z, y_1 and x_1 ($d(x_1) = 1$) and adding new edge wy_2 we get a new tree T'. Then |V(T')| = n - 3 and

$$\begin{split} R_{-1}(T) &= R_{-1}(T') + \frac{1}{2} + \frac{1}{6} + \frac{1}{3d} + \frac{1}{3d(y_2)} - \frac{1}{dd(y_2)} \\ &\leq \frac{15(n-3) + C}{56} + \frac{2}{3} + \frac{1}{3d} + \frac{1}{3d(y_2)} - \frac{1}{dd(y_2)} \\ &\leq \frac{15n + C}{56} - \frac{23}{168} + \frac{1}{9} + \frac{1}{3d(y_2)} - \frac{1}{3d(y_2)} \\ &= \frac{15n + C}{56} - \frac{13}{504} < \frac{15n + C}{56} \end{split}$$

The remaining case is $d(y_1) = d(y_2) = 2$.

In the same time we have proved that the Max Tree can not have (1,3) systems.

Lemma 2. Every vertex of degree 4 is the center of a (3,4) system of the Max Tree, i.e., it appears only in a (3,4) system.

Proof. Let the Max Tree T has the vertex z of degree 4 with the neighbors y_1, y_2, y_3 and w and d = d(w). We distinguish several cases.

Case 1. $d(y_i) \ge 3$, i = 1, 2, $d(y_3) \ge 4$ and $d = d(w) \ge 3$. By deleting the vertex z (and edges zy_i , i = 1, 2, 3 and zw) and adding new edges wy_i , i = 1, 2, 3, we get a

new tree T'. Let v_j denote the neighbors of w other than z. Then |V(T')| = n - 1, $d_{T'}(w) = d + 2$, $d(v_j) \ge 2$ and

$$R_{-1}(T) = R_{-1}(T') + \left(\frac{1}{4} - \frac{1}{d+2}\right) \sum_{i=1}^{3} \frac{1}{d(y_i)} + \frac{1}{4d} + \left(\frac{1}{d} - \frac{1}{d+2}\right) \sum_{j=1}^{d-1} \frac{1}{d(v_j)}$$

$$\leq \frac{15(n-1) + C}{56} + \frac{1}{4d} + \frac{d-2}{4(d+2)} \sum_{i=1}^{3} \frac{1}{d(y_i)} + \frac{2}{d(d+2)} \sum_{j=1}^{d-1} \frac{1}{d(v_j)}$$

$$\leq \frac{15n + C}{56} - \frac{15}{56} + \frac{1}{4d} + \frac{(d-2)}{4(d+2)} \left(\frac{2}{3} + \frac{1}{4}\right) + \frac{2}{d(d+2)} \left(\frac{d-1}{2}\right)$$

$$= \frac{15n + C}{56} + \frac{-13d^2 + 86d - 168}{336d(d+2)} < \frac{15n + C}{56}$$

The last inequality holds for every d.

Case 2. $d(y_1) = 2$, $d(y_i) \ge 3$, i = 2, 3 and $d(w) \ge 3$. By deleting vertices z, y_1, x_1 and adding new edges wy_2 and wy_3 we get a new tree T'. Then |V(T')| = n - 3, $d_{T'}(w) = d + 1$, $d(v_j) \ge 2$ and

$$R_{-1}(T) = R_{-1}(T') + \frac{1}{2} + \frac{1}{8} + (\frac{1}{4} - \frac{1}{d+1}) \sum_{i=2}^{3} \frac{1}{d(y_i)} + \frac{1}{4d} + (\frac{1}{d} - \frac{1}{d+1}) \sum_{j=1}^{d-1} \frac{1}{d(v_j)}$$

$$\leq \frac{15(n-3) + C}{56} + \frac{5}{8} + \frac{d-3}{4(d+1)} \sum_{i=2}^{3} \frac{1}{d(y_i)} + \frac{1}{4d} + \frac{1}{d(d+1)} \sum_{j=1}^{d-1} \frac{1}{d(v_j)}$$

$$\leq \frac{15n + C}{56} - \frac{5}{28} + \frac{d-3}{6(d+1)} + \frac{1}{4d} + \frac{d-1}{2d(d+1)}$$

$$= \frac{15n + C}{56} - \frac{d^2 - 6d + 21}{84d(d+1)} < \frac{15n + C}{56}$$

Case 3. $d(y_1)=d(y_2)=2, d(y_3)\geq 3$ and $d(w)\geq 3$. By deleting vertices z,y_1,x_1,y_2,x_2 and adding new edge wy_3 we get a new tree T'. Then |V(T')|=n-5 and

$$R_{-1}(T) = R_{-1}(T') + 2(\frac{1}{2} + \frac{1}{8}) + \frac{1}{4d(y_3)} + \frac{1}{4d} - \frac{1}{dd(y_3)}$$

$$\leq \frac{15(n-5) + C}{56} + \frac{5}{4} + \frac{1}{4d(y_3)} + \frac{1}{4d} - \frac{1}{dd(y_3)}$$

$$= \frac{15n + C}{56} - \frac{5}{56} + \frac{1}{4d(y_3)} + \frac{1}{4d} - \frac{1}{dd(y_3)}$$

$$\leq \frac{15n + C}{56} - \frac{5}{56} + \frac{1}{12} < \frac{15n + C}{56}$$

The remaining case is $d(y_1) = d(y_2) = d(y_3) = 2$.

We have also proved that the Max Tree can not have (1,4) and (2,4) systems (Cases 2 and 3 of Lemma 2).

Note that the Max Tree can not have $d(y_1) = d(y_2) = d(y_3) = d(w) = 3$.

Lemma 3. The Max Tree T can not have (3, d) systems for $5 \le d \le 11$.

Proof. Let $x_1, y_1, x_2, y_2, x_3, y_3, z, w_1, \dots, w_{d-4}, \tilde{w}$ be the (3, d) system centered at z, where $d(x_i) = 1$, i = 1, 2, 3, $d(y_i) = 2$, i = 1, 2, 3, d(z) = d, $d(w_i) \geq 3$, $i = 1, \dots, d-4$ and $d(\tilde{w}) = \tilde{d} \geq 5$. It is not possible that $d(w_i) = 4$, $i = 1, \dots, d-4$ and $d(\tilde{w}) < 5$ because $|V(T)| \geq 103$ and because of Lemmas 1 and 2. By deleting the vertex z (and edges zy_i , i = 1, 2, 3, zw_i , $i = 1, \dots, d-4$ and $z\tilde{w}$) and adding new edges $\tilde{w}w_i$, $i = 1, \dots, d-4$ and $\tilde{w}\tilde{z}$, where \tilde{z} is the center of the (3, 4) system we get a new tree T'. Let v_j denote the neighbors of \tilde{w} other than z in T. Then |V(T')| = |V(T)|, $d_{T'}(\tilde{w}) = \tilde{d} + d - 4$, $d(\tilde{z}) = 4$, $d(v_j) \geq 2$ and

$$R_{-1}(T) = R_{-1}(T') + 3\left(\frac{1}{2} + \frac{1}{2d}\right) + \frac{1}{d\tilde{d}} + \left(\frac{1}{d} - \frac{1}{\tilde{d} + d - 4}\right) \sum_{i=1}^{d-4} \frac{1}{d(w_i)}$$

$$+ \left(\frac{1}{\tilde{d}} - \frac{1}{\tilde{d} + d - 4}\right) \sum_{j=1}^{\tilde{d} - 1} \frac{1}{d(v_j)} - 3\left(\frac{1}{2} + \frac{1}{8}\right) - \frac{1}{4(\tilde{d} + d - 4)}$$

$$= R_{-1}(T') - \frac{3}{8} + \frac{3}{2d} + \frac{4(\tilde{d} + d - 4) - \tilde{d}d}{4d\tilde{d}(\tilde{d} + d - 4)}$$

$$+ \frac{\tilde{d} - 4}{d(\tilde{d} + d - 4)} \sum_{i=1}^{d-4} \frac{1}{d(w_i)} + \frac{d - 4}{\tilde{d}(\tilde{d} + d - 4)} \sum_{j=1}^{\tilde{d} - 1} \frac{1}{d(v_j)}$$

Since the Max Tree can have only the systems $(1, \bar{d}), (2, \bar{d})$ and $(3, \bar{d})$, the vertex \tilde{w} can have at most 3 suspended path (i.e., $d(v_j) = 2$ for at most three j). Then $\sum_{j=1}^{\bar{d}-1} \frac{1}{d(v_j)} \leq \frac{3}{2} + \frac{\bar{d}-4}{3} = \frac{2\bar{d}+1}{6}$ and

$$\begin{array}{ll} R_{-1}(T) & \leq & R_{-1}(T') - \frac{3}{8} + \frac{3}{2d} + \frac{4(\tilde{d}+d-4) - \tilde{d}d}{4d\tilde{d}(\tilde{d}+d-4)} + \frac{\tilde{d}-4}{d(\tilde{d}+d-4)} \cdot \frac{d-4}{3} \\ \\ & + \frac{d-4}{\tilde{d}(\tilde{d}+d-4)} \cdot \frac{2\tilde{d}+1}{6} \\ \\ & = & R_{-1}(T') - \frac{(d-4)(\tilde{d}-4)(\tilde{d}+d+6)}{24d\tilde{d}(\tilde{d}+d-4)} < R_{-1}(T') \end{array} \qquad \Box$$

Lemma 4. The Max Tree T can not have (2, d) systems for $5 \le d \le 12$.

Proof. Let $x_1, y_1, x_2, y_2, z, w_1, \dots, w_{d-3}, \tilde{w}$ be the (2, d) system centered at z, where $d(x_i) = 1$, i = 1, 2, $d(y_i) = 2$, i = 1, 2, d(z) = d, $d(w_i) \ge 3$, $i = 1, \dots, d-3$

and $d(\tilde{w}) = \tilde{d} \geq 5$. It is not possible that $d(w_i) = 4$, $i = 1, \cdots, d-3$ and $d(\tilde{w}) < 5$ because $\mid V(T) \mid \geq 103$. By deleting the vertex z (and edges zy_i , $i = 1, 2, zw_i$, $i = 1, \cdots, d-3$ and $z\tilde{w}$) and adding new edges $\tilde{w}w_i$, $i = 1, \cdots, d-3$ and $\tilde{w}\tilde{z}$, where \tilde{z} is the center of the (2,3) system we get a new tree T'. Let v_j denote the neighbors of \tilde{w} other than z in T. Then $\mid V(T') \mid = \mid V(T) \mid$, $d_{T'}(\tilde{w}) = \tilde{d} + d - 3$, $d(\tilde{z}) = 3$, $d(v_j) \geq 2$ and

$$\begin{split} R_{-1}(T) &= R_{-1}(T') + 2(\frac{1}{2} + \frac{1}{2d}) + \frac{1}{d\tilde{d}} + (\frac{1}{d} - \frac{1}{\tilde{d} + d - 3}) \sum_{i=1}^{d-3} \frac{1}{d(w_i)} \\ &+ (\frac{1}{\tilde{d}} - \frac{1}{\tilde{d} + d - 3}) \sum_{j=1}^{\tilde{d} - 1} \frac{1}{d(v_j)} - 2(\frac{1}{2} + \frac{1}{6}) - \frac{1}{3(\tilde{d} + d - 3)} \\ &= R_{-1}(T') + \frac{3 - d}{3d} + \frac{3(\tilde{d} + d - 3) - \tilde{d}d}{3d\tilde{d}(\tilde{d} + d - 3)} + \frac{\tilde{d} - 3}{d(\tilde{d} + d - 3)} \sum_{i=1}^{d-3} \frac{1}{d(w_i)} \\ &+ \frac{d - 3}{\tilde{d}(\tilde{d} + d - 3)} \sum_{i=1}^{\tilde{d} - 1} \frac{1}{d(v_j)} \end{split}$$

Since the Max Tree can have only the systems $(1, \bar{d})$ and $(2, \bar{d})$, the vertex \tilde{w} can have at most 2 suspended path (i.e., $d(v_j) = 2$ for at most two j). Then $\sum_{j=1}^{\tilde{d}-1} \frac{1}{d(v_j)} \le \frac{2}{2} + \frac{\tilde{d}-3}{3} = \frac{\tilde{d}}{3}$ and

$$\begin{array}{ll} R_{-1}(T) & \leq & R_{-1}(T') + \frac{3-d}{3d} + \frac{3(\tilde{d}+d-3)-\tilde{d}d}{3d\tilde{d}(\tilde{d}+d-3)} + \frac{\tilde{d}-3}{d(\tilde{d}+d-3)} \cdot \frac{d-3}{3} \\ & + \frac{d-3}{\tilde{d}(\tilde{d}+d-3)} \cdot \frac{\tilde{d}}{3} = R_{-1}(T') - \frac{(d-3)(\tilde{d}-3)}{3d\tilde{d}(\tilde{d}+d-3)} < R_{-1}(T') \end{array} \quad \Box$$

Lemma 5. The Max Tree T can not have (1,d) systems for $5 \le d \le 13$.

Proof. Let $x_1, y_1, z, w_1, \dots, w_{d-2}, \tilde{w}$ be the (1, d) system centered at z, where $d(x_1) = 1$, $d(y_1) = 2$, d(z) = d, $d(w_i) \geq 3$, $i = 1, \dots, d-2$ and $d(\tilde{w}) = \tilde{d} \geq 5$. It is not possible that $d(w_i) = 4$, $i = 1, \dots, d-2$ and $d(\tilde{w}) < 5$ because $|V(T)| \geq 103$. Let v_i denote the neighbors of \tilde{w} other than z. We distinguish several cases.

Case 1. $d(w_i) \geq 4, i = 1, \dots, d-2$. By deleting the vertex z (and edges $zy_1, y_1x_1, zw_i, i = 1, \dots, d-2$ and $z\tilde{w}$) and adding new edges $\tilde{w}w_i, i = 1, \dots, d-2$ we get a new tree T'. Then $|V(T')| = |V(T)| -3, d_{T'}(\tilde{w}) = \tilde{d} + d - 3, d(v_j) \geq 2$ and

$$R_{-1}(T) = R_{-1}(T') + \frac{1}{2} + \frac{1}{2d} + \frac{1}{d\tilde{d}} + (\frac{1}{d} - \frac{1}{\tilde{d} + d - 3}) \sum_{i=1}^{d-2} \frac{1}{d(w_i)}$$

$$\begin{split} &+(\frac{1}{\tilde{d}}-\frac{1}{\tilde{d}+d-3})\sum_{j=1}^{\tilde{d}-1}\frac{1}{d(v_j)}\leq \frac{15(n-3)+C}{56}+\frac{1}{2}+\frac{\tilde{d}+2}{2d\tilde{d}}\\ &+\frac{\tilde{d}-3}{d(\tilde{d}+d-3)}\sum_{i=1}^{d-2}\frac{1}{d(w_i)}+\frac{d-3}{\tilde{d}(\tilde{d}+d-3)}\sum_{j=1}^{\tilde{d}-1}\frac{1}{d(v_j)} \end{split}$$

Since the Max Tree can have only the systems $(1, \bar{d})$, the vertex \tilde{w} can have at most one suspended path (i.e., $d(v_j) = 2$ for at most one j). Then $\sum_{j=1}^{\bar{d}-1} \frac{1}{d(v_j)} \leq \frac{1}{2} + \frac{\bar{d}-2}{3} = \frac{2\bar{d}-1}{6}$ and

$$R_{-1}(T) \leq \frac{15n+C}{56} - \frac{17}{56} + \frac{\tilde{d}+2}{2d\tilde{d}} + \frac{\tilde{d}-3}{d(\tilde{d}+d-3)} \cdot \frac{d-2}{4}$$

$$+ \frac{d-3}{\tilde{d}(\tilde{d}+d-3)} \cdot \frac{2\tilde{d}-1}{6} = \frac{15n+C}{56} + \frac{-9d\tilde{d}^2 + 5d^2\tilde{d} - 57d\tilde{d} + 168\tilde{d} - 28d^2 + 252d - 504}{168d\tilde{d}(\tilde{d}+d-3)}$$

$$< \frac{15n+C}{56}$$

The last inequality holds for $5 \le d \le 13$.

Case 2. There is at least one vertex w_j such that $d(w_j) = 3$. Denote this vertex w_{d-2} . By deleting the vertex z (and edges $zy_1, y_1x_1, zw_i, i = 1, \dots, d-2$ and $z\tilde{w}$) and adding new edges $\tilde{w}w_i, i = 1, \dots, d-3$ and one (3,4) system adjacent to \tilde{w} we get a new tree T'. Then $|V(T')| = |V(T)| -1, d_{T'}(\tilde{w}) = \tilde{d} + d - 3, d(v_j) \ge 2$ and

$$\begin{split} R_{-1}(T) &= R_{-1}(T') + \frac{1}{2} + \frac{1}{2d} + \frac{1}{3d} + 2(\frac{1}{2} + \frac{1}{6}) + \frac{1}{d\tilde{d}} - \frac{1}{4(\tilde{d} + d - 3)} + \\ &\qquad (\frac{1}{d} - \frac{1}{\tilde{d} + d - 3}) \sum_{i=1}^{d-3} \frac{1}{d(w_i)} + (\frac{1}{\tilde{d}} - \frac{1}{\tilde{d} + d - 3}) \sum_{j=1}^{\tilde{d} - 1} \frac{1}{d(v_j)} - 3(\frac{1}{2} + \frac{1}{8}) \\ &\leq \frac{15(n-1) + C}{56} - \frac{1}{24} + \frac{5}{6d} + \frac{4(\tilde{d} + d - 3) - d\tilde{d}}{4d\tilde{d}(\tilde{d} + d - 3)} \\ &\qquad + \frac{\tilde{d} - 3}{d(\tilde{d} + d - 3)} \sum_{i=1}^{d-3} \frac{1}{d(w_i)} + \frac{d - 3}{\tilde{d}(\tilde{d} + d - 3)} \sum_{j=1}^{\tilde{d} - 1} \frac{1}{d(v_j)} \end{split}$$

Since the Max Tree can have only the systems $(1, \bar{d})$, the vertex \tilde{w} can have at most one suspended path (i.e., $d(v_j) = 2$ for at most one j). Then $\sum_{j=1}^{\tilde{d}-1} \frac{1}{d(v_j)} \leq \frac{1}{2} + \frac{\tilde{d}-2}{3} = \frac{2\tilde{d}-1}{6}$.

Case 2'. $d(w_i) \ge 3, i = 1, \dots, d - 3$. We have

$$\begin{array}{ll} R_{-1}(T) & \leq & \frac{15n+C}{56} - \frac{13}{42} + \frac{5}{6d} + \frac{4(\tilde{d}+d-3)-d\tilde{d}}{4d\tilde{d}(\tilde{d}+d-3)} + \frac{\tilde{d}-3}{d(\tilde{d}+d-3)} \cdot \frac{d-3}{3} \\ & + \frac{d-3}{\tilde{d}(\tilde{d}+d-3)} \cdot \frac{2\tilde{d}-1}{6} < \frac{15n+C}{56} \end{array}$$

The last inequality holds for d = 5, 6, 7 and every \tilde{d} .

Case 2". $d(w_i) = 3$ for not more than four *i*'s. Then $\sum_{i=1}^{d-3} \frac{1}{d(w_i)} \le \frac{4}{3} + \frac{d-7}{4} = \frac{3d-5}{12}$ and

$$\begin{split} R_{-1}(T) & \leq \frac{15n+C}{56} - \frac{13}{42} + \frac{5}{6d} + \frac{4(\tilde{d}+d-3)-d\tilde{d}}{4d\tilde{d}(\tilde{d}+d-3)} + \frac{\tilde{d}-3}{d(\tilde{d}+d-3)} \cdot \\ \frac{3d-5}{12} + \frac{d-3}{\tilde{d}(\tilde{d}+d-3)} \cdot \frac{2\tilde{d}-1}{6} & = \frac{15n+C}{56} + \\ \frac{35\tilde{d}^2 - 5d\tilde{d}^2 + 2d^2\tilde{d} - 20d\tilde{d} - 21\tilde{d} - 14d^2 + 126d - 252}{84d\tilde{d}(\tilde{d}+d-3)} < \frac{15n+C}{56} \end{split}$$

The last inequality holds for $7 \le d \le 13$ and every \tilde{d} .

Case 2"'. $d(w_i) = 3$ for at least five i's (for $i = d - 2, d - 3, \dots, d - 6$). By deleting the vertex z (and edges $zy_1, y_1x_1, zw_i, i = 1, \dots, d - 2$ and $z\tilde{w}$) and adding new edges $\tilde{w}w_i, i = 1, \dots, d - 7$ and four (3, 4) systems adjacent to \tilde{w} , we get a new tree T'. Then $|V(T')| = |V(T)|, d_{T'}(\tilde{w}) = \tilde{d} + d - 4$ and

$$\begin{split} R_{-1}(T) &= R_{-1}(T') + \frac{1}{2} + \frac{1}{2d} + 10(\frac{1}{2} + \frac{1}{6}) + \frac{5}{3d} + (\frac{1}{d} - \frac{1}{\tilde{d} + d - 4}) \sum_{i=1}^{d-7} \frac{1}{d(w_i)} \\ &+ \frac{1}{d\tilde{d}} + (\frac{1}{\tilde{d}} - \frac{1}{\tilde{d} + d - 4}) \sum_{j=1}^{\tilde{d}-1} \frac{1}{d(v_j)} - \frac{4}{4(\tilde{d} + d - 4)} - 12(\frac{1}{2} + \frac{1}{8}) \\ &= R_{-1}(T') - \frac{1}{3} + \frac{13}{6d} + \frac{\tilde{d} + d - 4 - d\tilde{d}}{d\tilde{d}(\tilde{d} + d - 4)} + \frac{\tilde{d} - 4}{d(\tilde{d} + d - 4)} \sum_{i=1}^{d-7} \frac{1}{d(w_i)} + \frac{d - 4}{\tilde{d}(\tilde{d} + d - 4)} \sum_{i=1}^{\tilde{d}-1} \frac{1}{d(v_j)} \end{split}$$

Since the Max Tree can have only the systems $(1, \bar{d})$, the vertex \tilde{w} can have at most one suspended path (i.e., $d(v_j) = 2$ for at most one j). Then $\sum_{j=1}^{\tilde{d}-1} \frac{1}{d(v_j)} \leq \frac{1}{2} + \frac{\tilde{d}-2}{3} = \frac{2\tilde{d}-1}{6}$, $\sum_{i=1}^{d-7} \frac{1}{d(w_i)} \leq \frac{d-7}{3}$ and

$$R_{-1}(T) \ \leq \ R_{-1}(T') - \frac{1}{3} + \frac{13}{6d} + \frac{\tilde{d} + d - 4 - d\tilde{d}}{d\tilde{d}(\tilde{d} + d - 4)} + \frac{\tilde{d} - 4}{d(\tilde{d} + d - 4)} \cdot \frac{d - 7}{3}$$

$$+\frac{d-4}{\tilde{d}(\tilde{d}+d-4)} \frac{2\tilde{d}-1}{6}$$

$$= R_{-1}(T') + \frac{-\tilde{d}^2 - d\tilde{d} + 10\tilde{d} - d^2 + 10d - 24}{6d\tilde{d}(\tilde{d}+d-4)} < R_{-1}(T')$$

The last inequality holds for $7 \le d \le 13$ and every \tilde{d} . In such a way, the degree of the vertex which eventually has one suspended path has augmented and the number of (2,3) systems has diminished.

We have shown that the "suspected" Max Tree can have only the systems (2,3) and (3,4) when $n \geq 103$. Now we will show that all systems (2,3) and (3,4) are centered at only one vertex. At first, we prove the next useful lemma, which will be sharpened up later.

Lemma 6. The Max Tree can not have the vertex with more than 12 (2,3) systems centered at it.

Proof. Let 13 (2,3) systems be centered at vertex z, at least, where d(z) = d, $d \ge 13$ and w_i , $i = 1, \dots, d-13$ are the other neighbors of z. By deleting 7 (2,3) systems and adding 5 (3,4) systems centered at z, we get a new tree T'. Then |V(T')| = |V(T)|, $d_{T'}(z) = d-2$ and

$$\begin{split} R_{-1}(T) &= R_{-1}(T') + 14(\frac{1}{2} + \frac{1}{6}) + \frac{13}{3d} - 15(\frac{1}{2} + \frac{1}{8}) - \frac{5}{4(d-2)} - \frac{6}{3(d-2)} \\ &+ (\frac{1}{d} - \frac{1}{d-2}) \sum_{i=1}^{d-13} \frac{1}{d(w_i)} = R_{-1}(T') - \frac{d^2 - 28d + 208}{24d(d-2)} - \\ &\frac{2}{d(d-2)} \sum_{i=1}^{d-13} \frac{1}{d(w_i)} \le R_{-1}(T') - \frac{d^2 - 28d + 208}{24d(d-2)} < R_{-1}(T') \end{split}$$

because $d^2 - 28d + 208 > 0$ for every d.

Theorem 2. The Max Tree can have only one vertex with maximum degree and all (2,3) systems and (3,4) systems can be centered at it.

Proof. Let z and y be two adjacent vertices of the Max Tree T such that $d(z) = d \ge 5$ and $d(y) = \tilde{d} \ge 5$. We differ several cases depending on the number of (2,3) systems centered at z and y. We take that the number of (2,3) systems centered at z is greater than or equal to the number of (2,3) systems centered at y.

Case 1. The number of (2,3) systems centered at z is less than or equal to 4

(and the same is for y). Let w_1, \dots, w_{d-1} be the vertices of T, other than y, adjacent to z and let $v_1, \dots, v_{\tilde{d}-1}$ be the vertices of T, other than z, adjacent to y. By deleting the vertex y and connecting zv_j , $j=1,\dots,\tilde{d}-1$, we get a new tree T'. Then |V(T')|=|V(T)|-1, $d_{T'}(z)=d+\tilde{d}-2$ and

$$\begin{split} R_{-1}(T) &= R_{-1}(T') + \frac{1}{d\tilde{d}} + (\frac{1}{d} - \frac{1}{d + \tilde{d} - 2}) \sum_{i=1}^{d-1} \frac{1}{d(w_i)} + (\frac{1}{\tilde{d}} - \frac{1}{d + \tilde{d} - 2}) \\ & \sum_{j=1}^{\tilde{d}-1} \frac{1}{d(v_j)} \leq \frac{15(n-1) + C}{56} + \frac{1}{d\tilde{d}} + \frac{\tilde{d} - 2}{d(d + \tilde{d} - 2)} \sum_{i=1}^{d-1} \frac{1}{d(w_i)} + \\ & \frac{d - 2}{\tilde{d}(d + \tilde{d} - 2)} \sum_{j=1}^{\tilde{d}-1} \frac{1}{d(v_j)} \end{split}$$

Hold:
$$\sum_{i=1}^{d-1} \frac{1}{d(w_i)} \le \frac{4}{3} + \frac{d-5}{4} = \frac{3d+1}{12}$$
 and $\sum_{j=1}^{\tilde{d}-1} \frac{1}{d(v_j)} \le \frac{4}{3} + \frac{\tilde{d}-5}{4} = \frac{3\tilde{d}+1}{12}$ and
$$R_{-1}(T) \le \frac{15n+C}{56} - \frac{15}{56} + \frac{1}{d\tilde{d}} + \frac{\tilde{d}-2}{d(d+\tilde{d}-2)} \cdot \frac{3d+1}{12} + \frac{d-2}{\tilde{d}(d+\tilde{d}-2)} \cdot \frac{3\tilde{d}+1}{12} = \frac{15n+C}{56} - \frac{d^2(3\tilde{d}-14) + d(3\tilde{d}^2 + 78\tilde{d}-140) - 14\tilde{d}^2 - 140\tilde{d} + 336}{168d\tilde{d}(d+\tilde{d}-2)}$$

$$< \frac{15n+C}{56}$$

because $d^2(3\tilde{d}-14)+d(3\tilde{d}^2+78\tilde{d}-140)-14\tilde{d}^2-140\tilde{d}+336>0$ for $d\geq 5$ and $\tilde{d}\geq 5$.

Case 2. The number of (2,3) systems centered at z is 5 (m=0), 6 (m=1) and 7 (m=2), where m is the difference between this number and 5. Let 5 (2,3) systems be centered at z, at least, and let w_1, \dots, w_{d-6} be the vertices of T, other than y and 5 (2,3) systems, adjacent to z and let $v_1, \dots, v_{\tilde{d}-1}$ be the vertices of T, other than z, adjacent to y. By deleting the vertex y and connecting zv_j , $j=1,\dots,\tilde{d}-1$, deleting 4 (2,3) systems centered at z and adding 3 (3,4) systems centered at z we get a new tree T'. Then |V(T')| = |V(T)|, $d_{T'}(z) = d + \tilde{d} - 3$ and

$$\begin{array}{ll} R_{-1}(T) & = & R_{-1}(T') + 8(\frac{1}{2} + \frac{1}{6}) + \frac{5}{3d} + \frac{1}{d\tilde{d}} + (\frac{1}{d} - \frac{1}{d + \tilde{d} - 3}) \sum_{i=1}^{d-6} \frac{1}{d(w_i)} + \\ & & (\frac{1}{\tilde{d}} - \frac{1}{d + \tilde{d} - 3}) \sum_{j=1}^{\tilde{d}-1} \frac{1}{d(v_j)} - \frac{3}{4(d + \tilde{d} - 3)} - \frac{1}{3(d + \tilde{d} - 3)} \end{array}$$

$$\begin{split} -9(\frac{1}{2}+\frac{1}{8}) &= R_{-1}(T') - \frac{7}{24} + \frac{5\tilde{d}+3}{3d\tilde{d}} - \frac{13}{12(d+\tilde{d}-3)} \\ &+ \frac{\tilde{d}-3}{d(d+\tilde{d}-3)} \sum_{i=1}^{d-6} \frac{1}{d(w_i)} + \frac{d-3}{\tilde{d}(d+\tilde{d}-3)} \sum_{j=1}^{\tilde{d}-1} \frac{1}{d(v_j)} \end{split}$$

Hold: $\sum_{i=1}^{d-6} \frac{1}{d(w_i)} \le \frac{m}{3} + \frac{d-6-m}{4} = \frac{3d+m-18}{12}, \ m=0,1,2, \ d \ge 6+m \ \text{and} \ \sum_{j=1}^{\tilde{d}-1} \frac{1}{d(v_j)} \le \frac{k}{3} + \frac{\tilde{d}-k-1}{4} = \frac{3\tilde{d}+k-3}{12}, \ k=4,\cdots,5+m, \ \tilde{d} \ge k+1 \ \text{and}$

$$\begin{split} R_{-1}(T) &\leq R_{-1}(T') - \frac{7}{24} + \frac{5\tilde{d}+3}{3d\tilde{d}} - \frac{13}{12(d+\tilde{d}-3)} + \\ &\frac{\tilde{d}-3}{d(d+\tilde{d}-3)} \cdot \frac{3d+m-18}{12} + \frac{d-3}{\tilde{d}(d+\tilde{d}-3)} \cdot \frac{3\tilde{d}+k-3}{12} = R_{-1}(T') - \\ &\frac{d^2(\tilde{d}-2(k-3)) + d(\tilde{d}^2+\tilde{d}-6(7-k)) - 2(2+m)\tilde{d}^2 - 6(2-m)\tilde{d}+72}{24d\tilde{d}(d+\tilde{d}-3)} \\ &< R_{-1}(T') \end{split}$$

because $d^2(\tilde{d}-2(k-3))+d(\tilde{d}^2+\tilde{d}-6(7-k))-2(2+m)\tilde{d}^2-6(2-m)\tilde{d}+72>0$ for $m=0,\ d\geq 6,\ k=4,5,\ \tilde{d}\geq k+1;\ m=1,\ d\geq 7,\ k=4,5,6,\ \tilde{d}\geq k+1$ and $m=2,\ d\geq 8,\ k=4,5,6,7,\ \tilde{d}\geq k+1.$

Case 3. The number of (2,3) systems centered at z is 8 (m=0), 9 (m=1), 10 (m=2), 11 (m=3) and 12 (m=4), where m is the difference between this number and 8. Let 8 (2,3) systems be centered at z, at least, and let w_1, \dots, w_{d-9} be the vertices of T, other than y and 8 (2,3) systems, adjacent to z and let $v_1, \dots, v_{\tilde{d}-1}$ be the vertices of T, other than z, adjacent to y. By deleting the vertex y and connecting zv_j , $j=1,\dots,\tilde{d}-1$, deleting 7 (2,3) systems centered at z and adding 5 (3,4) systems centered at z we get a new tree T'. Then |V(T')| = |V(T)| -1, $d_{T'}(z) = d + \tilde{d} - 4$ and

$$R_{-1}(T) = R_{-1}(T') + 14\left(\frac{1}{2} + \frac{1}{6}\right) + \frac{8}{3d} + \frac{1}{d\tilde{d}} + \left(\frac{1}{d} - \frac{1}{d + \tilde{d} - 4}\right) \sum_{i=1}^{d-9} \frac{1}{d(w_i)} + \left(\frac{1}{\tilde{d}} - \frac{1}{d + \tilde{d} - 4}\right) \sum_{j=1}^{\tilde{d} - 1} \frac{1}{d(v_j)} - \frac{5}{4(d + \tilde{d} - 4)} - \frac{1}{3(d + \tilde{d} - 4)} + \frac{1}{3(d + \tilde{d} - 4)} + \frac{\tilde{d} - 4}{d(d + \tilde{d} - 4)} + \frac{\tilde{d} - 4}{d(d + \tilde{d} - 4)} + \frac{\tilde{d} - 4}{d(d + \tilde{d} - 4)} + \frac{\tilde{d} - 4}{\tilde{d}(d + \tilde{d} - 4)} + \frac$$

Hold:
$$\sum_{i=1}^{d-9} \frac{1}{d(w_i)} \le \frac{m}{3} + \frac{d-9-m}{4} = \frac{3d+m-27}{12}, \ m=0,1,2,3,4, d \ge 9+m \text{ and } \sum_{j=1}^{\tilde{d}-1} \frac{1}{d(v_j)} \le \frac{k}{3} + \frac{\tilde{d}-k-1}{4} = \frac{3\tilde{d}+k-3}{12}, \ k=4,5,\cdots,8+m, \ \tilde{d} \ge k+1 \text{ and}$$

$$\begin{split} R_{-1}(T) & \leq \frac{15n+C}{56} - \frac{13}{42} + \frac{8\tilde{d}+3}{3d\tilde{d}} - \frac{19}{12(d+\tilde{d}-4)} + \frac{\tilde{d}-4}{d(d+\tilde{d}-4)} \cdot \\ & \frac{3d+m-27}{12} + \frac{d-4}{\tilde{d}(d+\tilde{d}-4)} \cdot \frac{3\tilde{d}+k-3}{12} = \frac{15n+C}{56} - \\ & \frac{d^2(5\tilde{d}-7(k-3)) + d(5\tilde{d}^2 - 27\tilde{d} - 28(6-k)) - 7(m+5)\tilde{d}^2 + 28(2+m)\tilde{d} + 336}{84d\tilde{d}(d+\tilde{d}-4)} \\ & \leq \frac{15n+C}{56} \end{split}$$

because $d^2(5\tilde{d}-7(k-3))+d(5\tilde{d}^2-27\tilde{d}-28(6-k))-7(m+5)\tilde{d}^2+28(2+m)\tilde{d}+336>0$ for $m=0,\ d\geq 9,\ k=4,5,6,7,8,\ \tilde{d}\geq k+1;\ m=1,\ d\geq 10,\ k=4,5,6,7,8,9,\ \tilde{d}\geq k+1;\ m=2,\ d\geq 11,\ k=4,5,6,7,8,9,10,\ \tilde{d}\geq k+1;\ m=3,\ d\geq 12,\ k=4,5,6,7,8,9,10,11,\ \tilde{d}\geq k+1$ and $m=4,\ d\geq 13,\ k=4,5,6,7,8,9,10,11,12,\ \tilde{d}\geq k+1.$

Now we can sharpen up Lemma 6 using Theorem 2.

Lemma 7. The Max Tree can not have the vertex with more than 6(2,3) systems centered at it.

Proof. Let 7 (2,3) systems be centered at vertex z, at least, where d(z) = d, $d \ge 14$ and w_i , $i = 1, \dots, d-7$ are the other neighbors of z. By deleting 7 (2,3) systems and adding 5 (3,4) systems centered at z, we get a new tree T'. Then |V(T')| = |V(T)|, $d_{T'}(z) = d-2$ and

$$R_{-1}(T) = R_{-1}(T') + 14\left(\frac{1}{2} + \frac{1}{6}\right) + \frac{7}{3d} - 15\left(\frac{1}{2} + \frac{1}{8}\right) - \frac{5}{4(d-2)} + \left(\frac{1}{d} - \frac{1}{d-2}\right) \sum_{i=1}^{d-7} \frac{1}{d(w_i)} = R_{-1}(T') - \frac{d^2 - 28d + 112}{24d(d-2)} - \frac{2}{d(d-2)} \sum_{i=1}^{d-7} \frac{1}{d(w_i)}$$

Since $3 \le d(w_i) \le 4$, holds $\sum_{i=1}^{d-7} \frac{1}{d(w_i)} \ge \frac{d-7}{4}$ and

$$\begin{array}{lcl} R_{-1}(T) & \leq & R_{-1}(T') - \frac{d^2 - 28d + 112}{24d(d-2)} - \frac{2}{d(d-2)} \cdot \frac{d-7}{4} \\ \\ & = & R_{-1}(T') - \frac{d-14}{24d} \leq R_{-1}(T') \end{array}$$

because
$$d - 14 \ge 0$$
, for $d \ge 14$. If $d \le 13$, $|V(T)| \le 78 < 103$.

Now we will finally prove Theorem 1 with Lemma 8.

Lemma 8. The Max Tree has one vertex with maximum degree $d_M = \frac{n-1}{7}$ and all (3,4) systems are centered at it.

Proof. As we have shown, the "suspected" Max Tree has one vertex of the maximum degree and all (3,4) systems and (2,3) systems are centered at it. The maximum number of (2,3) systems is 6. Denote by 5t the number of vertices on t (t=0,1,2,3,4,5,6) (2,3) systems. The maximum degree is $d_M=d_q+t$ where $d_q=\frac{n-1-5t}{7}$ and

$$\begin{array}{ll} R_{-1}(T) & = & (3(\frac{1}{2}+\frac{1}{8})+\frac{1}{4(d_q+t)})d_q+2t(\frac{1}{2}+\frac{1}{6})+\frac{t}{3(d_q+t)} \\ \\ & = & \frac{15d_q}{8}+\frac{16t+3}{12}+\frac{t}{12(d_q+t)}=\frac{15n-1}{56}-\frac{t}{168} \\ \\ & + \frac{7t}{12(n-1+2t)} \leq \frac{15n-1}{56}-\frac{t}{168}+\frac{7t}{12(102+2t)} \leq \\ \\ & = & \frac{15n-1}{56} \end{array}$$

 $R_{-1}(T)=\frac{15n-1}{56}$ when t=0, i.e., the Max Tree has one vertex with maximum degree $d_M=\frac{n-1}{7}$ and all (3,4) systems are centered at it.

The Max Tree is possible only if $n-1 \equiv 0 \pmod{7}$. We will give our conjecture about the structure of the Max Tree when $n-1 \neq 0 \pmod{7}$. We denote by $(1,5)^*$ system which has one suspended path x,y,z and three (2,3) systems adjacent to z, where d(z) = 5. System which has 8 (2,3) systems adjacent to one vertex z, where the d(z) = 9 we denote by $(8_{(2,3)}, 9)$. When $n-1 \neq 0 \pmod{7}$ the Max Tree can have $(2,3), (4,5), (1,5)^*$ and $(8_{(2,3)}, 9)$ system. Denote by p the number of (2,3) systems, by q the number of (3,4) systems, by r the number of (4,5) systems, by r the number of $(3,5)^*$ systems and by r the number of $(8_{(2,3)}, 9)$ systems. In the next table we predict the structure of the Max Tree when $r \geq n_0$.

$n-1 \pmod{7}$	р	q	r	s	v	$R_{-1}(T)$
0	0	$\frac{n-1}{7}$	0	0	0	$\frac{15n-1}{56}$
1	3	$\frac{n-16}{7}$	0	0	0	$\frac{15n-1}{56} - \frac{1}{56} + \frac{7}{4(n+5)}$
2	0	$\frac{n-10}{7}$	1	0	0	$\frac{15n-1}{56} - \frac{3}{5} \cdot \frac{1}{56} - \frac{7}{20(n-3)}$
3	2	$\frac{n-11}{7}$	0	0	0	$\frac{15n-1}{56} - \frac{2}{3} \cdot \frac{1}{56} + \frac{7}{6(n+3)}$
4	0	$\frac{n-19}{7}$	0	1	0	$\frac{15n-1}{56} - \frac{6}{5} \cdot \frac{1}{56} - \frac{7}{20(n-12)}$
5	1	$\frac{n-6}{7}$	0	0	0	$\frac{15n-1}{56} - \frac{1}{3} \cdot \frac{1}{56} + \frac{7}{12(n+1)}$
6	0	$\frac{n-42}{7}$	0	0	1	$\frac{15n-1}{56} - \frac{29}{27} \cdot \frac{1}{56} - \frac{35}{36(n-35)}$

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