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Solutions to Two Unsolved Questions on the Best Upper Bound for the Randić Index R_{-1} of Trees *

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Abstract

The general Randić index $R_\alpha(G)$ of a graph G is defined as the sum of the weights $(d(u)d(v))^\alpha$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G and α is an arbitrary real number. Clark and Moon gave the lower and upper bounds for the Randić index R_{-1} of trees with order n. The lower bound is sharp. However, a sharp upper bound has not been obtained for a long time. Clark and Moon proposed two unsolved questions on the upper bound. In this paper, we give positive answers to the two questions. We show that $lim_{n\to\infty} f(n)/n = 15/56$, and give a sharp upper bound for which there are infinitely many trees of order n whose values of Randić index R_{-1} attain the bound.

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1 Introduction

In 1975, Randić proposed a pair of chemical indices $R(G)$ and $R_{-1}(G)$ for a (chemical) graph G:

$$R(G) = \sum_{uv\in E(G)} (d(u)d(v))^{-\frac{1}{2}}$$

and

$$R_{-1}(G) = \sum_{uv\in E(G)} (d(u)d(v))^{-1},$$

where $d(u)$ denotes the degree of a vertex u in G.

Like other successful chemical indices, these two indices have been closely correlated with many chemical properties, and so have received considerable attention from chemists and mathematicians, see [1,3-12]. Here, we are interested in the latter index for trees. First, we provide a general setting and a survey of some known results.

For all $n \leq 20$, Clark et al. [5] determined all trees of order n with maximum value of R_{-1} among all trees of order n. In 2000, Clark and Moon [6] gave a lower and upper bound for $R_{-1}(T)$, $1 \leq R_{-1}(T) \leq \frac{5n+8}{18}$, where the lower bound can be attained by the star, but the upper bound is not best possible. They constructed an infinite sequence T_r $(r \geq 2)$ of trees which are obtained from the star S_r by appending three internally-disjoint paths of length 2 to each leaf of S_r. Then T_r has order $|V(T_r)| = 7r + 1$ and weight $R_{-1}(T_r) = (15r+2)/8$, and so $lim_{n\to\infty} R_{-1}(T_r)/|V(T_r)| = 15/56$. At the end of their paper [6] they proposed two unsolved questions on the upper bound.

Question 1: Find $K = lim_{n\to\infty} f(n)/n$, where $f(n)$ is the maximum value of R_{-1} among all trees of order n. From above we know that $\frac{15}{56} \leq K \leq \frac{5}{18}$, and Clark and Moon thought 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.

Many researchers tried to solve the above problems, but failed. Rautenbach [12] gave an upper bound for $R_{-1}(T)$ of trees with maximum degree 3. Li and Yang [11] gave a method to determine the sharp upper bound for R_{-1} of chemical trees (i.e., trees with maximum degree at most 4). In [9], we investigated trees with maximum value of general Randić index R_α among all trees of order n. We distinguished α in several different intervals, and for most of the intervals we characterized trees with maximum general Randić index and gave the corresponding values. Only the interval $-2 < \alpha < -\frac{1}{2}$ (including the point $\alpha = -1$) is left undetermined and seems very complicated. The Max Trees (trees with maximum Randić index) could be not unique in this interval. Only some properties of Max Trees were obtained in this case. All the above researches concern the upper bound. In the present paper, we give positive answers to the above two questions proposed by Clark and Moon, and completely solve the sharp upper bound problem for R_{-1} of trees.

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. The path of order n is denoted by P_n, and the star of order n is denoted by S_n. A tree with $2m+1$ vertices is called a *subdivided star* S^*_{2m+1}, if it is obtained from a star S_{m+1} by subdividing each edge of the star exactly once. All notation, terminology and presumed results can be found in Bondy and Murty [2].

2 Solution to Question 1 - an upper bound and the ratio K

We assume that our trees of order n have vertex set $[n] := \{1, 2, \cdots, n\}$.

Theorem 2.1 *For a tree T of order $n \geq 3$,*

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

where C is a constant not larger than 11. Therefore, we have

$$K = lim_{n\to\infty} f(n)/n = \frac{15}{56},$$

which solves the first question in [6].

Proof. By induction on n. Let T be a tree of order n with maximum value of Randić index R_{-1}. If we choose C large enough, it is easy to see that the result holds for all $3 \leq n \leq 71$. Actually, we can employ a good computer to check that C is not larger than 11. So, next we always assume that $n \geq 72$, and the result holds for all smaller values of n.

Since $R_{-1}(S_n) = 1 < \frac{15n+C}{56}$, $R_{-1}(P_n) = \frac{n+1}{4} < \frac{15n+C}{56}$ and $R_{-1}(S^*_{2m+1}) = \frac{m+1}{2} < \frac{15(2m+1)+C}{56}$, we can assume that $T \ncong S_n$, $T \ncong P_n$ nor $T \ncong S^*_{2m+1}$. Let $x_1, \cdots, x_l$ $(l \geq 1)$ be the leaves of T, adjacent to a vertex y and $z_1, \cdots, z_m$ be the other vertices of T adjacent to y, where $l + m$ is as large as possible. Since $T \ncong S_n$, we have $m \geq 1$ and all $d(z_j) \geq 2$. Now $2 \leq n - l \leq n - 1$ and

$$\begin{aligned} R_{-1}(T) &= R_{-1}(T - \{x_1, \cdots, x_l\}) + \frac{l}{m+l} - \frac{l}{m(m+l)} \sum_{j=1}^{m} \frac{1}{d(z_j)} \\ &\leq \frac{15(n-l)+C}{56} + \frac{l}{m+l} - \frac{l}{m(m+l)} \sum_{j=1}^{m} \frac{1}{d(z_j)} \qquad (2.1) \\ &\leq \frac{15n+C}{56}, \end{aligned}$$

provided $m + l \geq 4$, and hence $m + l \leq 3$.

Suppose $l = 2$ and $m = 1$. Then

$$(2.1) = \frac{15(n-2)+C}{56} + \frac{2}{3} - \frac{2}{3d(z)} < \frac{15n+C}{56}$$

holds for $d(z) \leq 5$. Let $w_1 \cdots w_{d(z)-1}$, $(d(z) \geq 6)$ be the vertices of T, other than y, adjacent to z. Now $n-3 \geq 6$ and

$$\begin{aligned} R_{-1}(T) &= R_{-1}(T - \{x_1, x_2, y\}) + \frac{2}{3} + \frac{1}{3d} - \frac{l}{d(z)(d(z)-1)} \sum_{j=1}^{d(z)-1} \frac{1}{d(w_j)} \\ &\leq \frac{15(n-3)+C}{56} + \frac{2}{3} + \frac{1}{3d} - \frac{l}{d(z)(d(z)-1)} \sum_{j=1}^{d(z)-1} \frac{1}{d(w_j)} \\ &< \frac{15n+C}{56} - \frac{45}{56} + \frac{2}{3} + \frac{1}{18} \\ &< \frac{15n+C}{56}. \end{aligned}$$

Suppose $l = 1$ and $m = 2$. Now $n-2 \geq 4$ and

$$\begin{aligned} R_{-1}(T) &= R_{-1}(T - \{x_1, y\} + z_1 z_2) + \frac{1}{3} + \frac{1}{3d(z_1)} + \frac{1}{3d(z_2)} - \frac{1}{d(z_1)d(z_2)} \\ &\leq \frac{15(n-2)+C}{56} + \frac{1}{3} + \frac{1}{3}\left(\frac{1}{d(z_1)} + \frac{1}{d(z_2)}\right) - \frac{1}{d(z_1)d(z_2)} \\ &\leq \frac{15n+C}{56}, \end{aligned}$$

provided

$$\frac{1}{3}\left(\frac{1}{d(z_1)} + \frac{1}{d(z_2)}\right) - \frac{1}{d(z_1)d(z_2)} - \frac{17}{84} \leq 0. \tag{2.2}$$

By considering the cases that both $d(z_1)$ and $d(z_2) \geq 4$; one of $d(z_i) = 3$ and the other ≥ 2; one of $d(z_i) = 2$ and the other ≥ 2, we can see that (2.2) holds.

Hence, $m = l = 1$. For convenience, from now on we use the symbol d instead of $d(z)$. If $d(z) = d = 2$, then

$$(2.1) = \frac{15(n-1)+C}{56} + \frac{1}{2} - \frac{1}{4} < \frac{15n+C}{56}.$$

We use the notion of suspended path in [9]. From above, since $m + l$ is as large as possible, we only leave the case that each leaf x in T is on a path x, y, z with $d(y) = 2$ and $d(z) \geq 3$. We call x, y, z a suspended path from x to z. Let $x_1 y_1 z, \cdots, x_s y_s z$ be the distinct suspended paths adjacent to z, and $w_1, \cdots, w_{d-s}$ be the vertices of T, other than $y_1, \cdots, y_s$, adjacent to z (which is called a (s,d)-system centered at z). Since

$T \not\cong S^*_{2m+1}$, we have $1 \leq s \leq d-1$. Then

$$\begin{aligned} R_{-1}(T) &= R_{-1}(T - \{x_1, y_1\}) + \frac{1}{2} + \frac{1}{2d} + (s-1)(\frac{1}{2d} - \frac{1}{2(d-1)}) \\ &\quad +(\frac{1}{d} - \frac{1}{d-1}) \sum_{i=1}^{d-s} \frac{1}{d(w_i)} \\ &\leq \frac{15(n-2)+C}{56} + \frac{1}{2} + \frac{1}{2d} - \frac{s-1}{2d(d-1)} - \frac{1}{d(d-1)} \sum_{i=1}^{d-s} \frac{1}{d(w_i)} \\ &= \frac{15n+C}{56} - \frac{1}{28} + \frac{d-s}{2d(d-1)} - \frac{1}{d(d-1)} \sum_{i=1}^{d-s} \frac{1}{d(w_i)} \\ &\leq \frac{15n+C}{56}, \end{aligned}$$

provided

$$\frac{d-s}{2d(d-1)} \leq \frac{1}{28} + \frac{1}{d(d-1)} \sum_{i=1}^{d-s} \frac{1}{d(w_i)}. \tag{2.3}$$

We examine (2.3) for all pairs (s, d) with $1 \leq s \leq d-1$, $d \geq 3$. Since

$$\frac{d-s}{2d(d-1)} \leq \frac{1}{28}$$

holds for $s = 1$, $d \geq 14$; $s = 2$, $d \geq 13$; $s = 3$, $d \geq 12$ and $s \geq 4$, d could be any integers larger than 3. One can see that (2.3) also holds for these (s, d) pairs. So we only need to consider the following (s, d)-systems: $s = 1$, $3 \leq d \leq 13$; $s = 2$, $3 \leq d \leq 12$; $s = 3$, $4 \leq d \leq 11$.

If T has a vertex w of degree 2 not in any suspended path, namely, let u, v be the neighbors of w, then $d(u), d(v) \geq 2$.

$$\begin{aligned} R_{-1}(T) &= R_{-1}(T - \{w\} + uv) + \frac{1}{2d(u)} + \frac{1}{2d(v)} - \frac{1}{d(u)d(v)} \\ &\leq \frac{15(n-1)+C}{56} + \frac{1}{2d(u)} + \frac{1}{2d(v)} - \frac{1}{d(u)d(v)} \\ &\leq \frac{15n+C}{56}, \end{aligned}$$

provided

$$\frac{1}{2d(u)} + \frac{1}{2d(v)} - \frac{1}{d(u)d(v)} \leq \frac{15}{56}. \tag{2.4}$$

By considering the cases that both $d(u)$ and $d(v) \geq 4$; one of $d(z_i) = 3$ and the other ≥ 2; one of $d(z_i) = 2$ and the other ≥ 2, we can see that (2.4) holds. Hence we can suppose that if the vertex w of T is not in a suspended path, then $d(w) \geq 3$.

If the Max Tree T have two (s, d)-systems sharing one edge denoted by $(s_1, d_1) \sim (s_2, d_2)$. We distinguish six cases to show that our result holds.

Case 1. $(1, d_1) \sim (1, d_2)$, where $3 \leq d_1 \leq 13$ and $3 \leq d_2 \leq 13$.

Let $x_1, y_1, z_1, w_1, \cdots, w_{d_1-2}$ be the $(1, d_1)$-system centered at z_1 where $d(z_1) = d_1$, and $x_2, y_2, z_2, \bar{w}_1, \cdots, \bar{w}_{d_2-2}$ be the $(1, d_2)$-system centered at z_2 where $d(z_2) = d_2$. Then $d(w_i) \geq 3$ and $d(\bar{w}_j) \geq 3$, $(1 \leq i \leq d_1 - 2$, and $1 \leq j \leq d_2 - 2)$. By deleting the vertices x_k, y_k, z_k, $(k = 1, 2)$, adding a path xyz of length 2, and then connecting $w_i z$ and $\bar{w}_j z$, we get a new tree T'. Then $|V(T')| = n - 3$, and $d_{T'}(z) = d_1 + d_2 - 3$. Now $n - 3 \geq 3(d_1 + d_2) - 12$ and

$$\begin{aligned}
R_{-1}(T) &= R_{-1}(T') + \frac{1}{2} + \frac{1}{2d_1} + \frac{1}{2} + \frac{1}{2d_2} + \frac{1}{d_1 d_2} - \frac{1}{2} - \frac{1}{2(d_1 + d_2 - 3)} \\
&\quad + \left(\frac{1}{d_1} - \frac{1}{d_1 + d_2 - 3}\right) \sum_{i=1}^{d_1-2} \frac{1}{d(w_i)} + \left(\frac{1}{d_2} - \frac{1}{d_1 + d_2 - 3}\right) \sum_{i=1}^{d_2-2} \frac{1}{d(\bar{w}_i)} \\
&\leq \frac{15(n-3) + C}{56} + \frac{1}{2} + \frac{1}{2d_1} + \frac{1}{2d_2} + \frac{1}{d_1 d_2} - \frac{1}{2(d_1 + d_2 - 3)} \\
&\quad + \frac{d_1 - 2}{3} \cdot \frac{d_2 - 3}{d_1(d_1 + d_2 - 3)} + \frac{d_2 - 2}{3} \cdot \frac{d_1 - 3}{d_2(d_1 + d_2 - 3)} \\
&\leq \frac{15n + C}{56}.
\end{aligned}$$

The last inequality holds for all (d_1, d_2) such that $3 \leq d_1 \leq 13$ and $3 \leq d_2 \leq 13$, unless $(d_1, d_2) = (11, 13)$, $(12, 12)$, $(12, 13)$, $(13, 13)$.

Case 2. $(1, d_1) \sim (2, d_2)$ where $3 \leq d_1 \leq 13$ and $3 \leq d_2 \leq 12$.

Let $x_1, y_1, z_1, w_1, \cdots, w_{d_1-2}$ be the $(1, d_1)$-system centered at z_1 where $d(z_1) = d_1$, and $x_2, y_2, x_3, y_3, z_2, \bar{w}_1, \cdots, \bar{w}_{d_2-3}$ be the $(2, d_2)$-system centered at z_2 where $d(z_2) = d_2$. Then $d(w_i) \geq 3$ and $d(\bar{w}_j) \geq 3$, $(1 \leq i \leq d_1 - 2$, and $1 \leq j \leq d_2 - 3)$. By deleting the vertices x_k, y_k and z_h, $(k = 1, 2, 3,\ h = 1, 2)$, adding a path xyz of length 2, and then connecting $w_i z$ and $\bar{w}_j z$, we get a new tree T'. Then $|V(T')| = n - 5$, and

$d_{T'}(z) = d_1 + d_2 - 4$. Now $n - 5 \geq 3(d_1 + d_2) - 15$ and

$$\begin{aligned}
R_{-1}(T) &= R_{-1}(T') + \frac{1}{2} + \frac{1}{2d_1} + (\frac{1}{2} + \frac{1}{2d_2}) \cdot 2 + \frac{1}{d_1 d_2} - \frac{1}{2} - \frac{1}{2(d_1 + d_2 - 4)} \\
&\quad + (\frac{1}{d_1} - \frac{1}{d_1 + d_2 - 4}) \sum_{i=1}^{d_1 - 2} \frac{1}{d(w_i)} + (\frac{1}{d_2} - \frac{1}{d_1 + d_2 - 4}) \sum_{i=1}^{d_2 - 3} \frac{1}{d(\bar{w}_i)} \\
&\leq \frac{15(n-5) + C}{56} + 1 + \frac{1}{2d_1} + \frac{1}{d_2} + \frac{1}{d_1 d_2} - \frac{1}{2(d_1 + d_2 - 4)} \\
&\quad + \frac{d_1 - 2}{3} \cdot \frac{d_2 - 4}{d_1(d_1 + d_2 - 4)} + \frac{d_2 - 3}{3} \cdot \frac{d_1 - 4}{d_2(d_1 + d_2 - 4)} \\
&\leq \frac{15n + C}{56}.
\end{aligned}$$

The last inequality holds for all $3 \leq d_1 \leq 13$ and $3 \leq d_2 \leq 12$.

Case 3. $(1, d_1) \sim (3, d_2)$ where $3 \leq d_1 \leq 13$ and $4 \leq d_2 \leq 11$.

Let $x_1, y_1, z_1, w_1, \cdots, w_{d_1 - 2}$ be the $(1, d_1)$-system centered at z_1 where $d(z_1) = d_1$, and $x_2, y_2, x_3, y_3, x_4, y_4, z_2, \bar{w}_1, \cdots, \bar{w}_{d_2 - 4}$ be the $(3, d_2)$-system centered at z_2 where $d(z_2) = d_2$. Then $d(w_i) \geq 3$ and $d(\bar{w}_j) \geq 3$, $(1 \leq i \leq d_1 - 2$, and $1 \leq j \leq d_2 - 4)$. By deleting the vertices x_k, y_k and z_h, $(k = 1, 2, 3, 4,\ h = 1, 2)$, adding a path xyz of length 2, and then connecting $w_i z$ and $\bar{w}_j z$, we get a new tree T'. Then $|V(T')| = n - 7$, and $d_{T'}(z) = d_1 + d_2 - 5$. Now $n - 7 \geq 3(d_1 + d_2) - 18$ and

$$\begin{aligned}
R_{-1}(T) &= R_{-1}(T') + \frac{1}{2} + \frac{1}{2d_1} + (\frac{1}{2} + \frac{1}{2d_2}) \cdot 3 + \frac{1}{d_1 d_2} - \frac{1}{2} - \frac{1}{2(d_1 + d_2 - 5)} \\
&\quad + (\frac{1}{d_1} - \frac{1}{d_1 + d_2 - 5}) \sum_{i=1}^{d_1 - 2} \frac{1}{d(w_i)} + (\frac{1}{d_2} - \frac{1}{d_1 + d_2 - 5}) \sum_{i=1}^{d_2 - 4} \frac{1}{d(\bar{w}_i)} \\
&\leq \frac{15(n-7) + C}{56} + \frac{3}{2} + \frac{1}{2d_1} + \frac{3}{2d_2} + \frac{1}{d_1 d_2} - \frac{1}{2(d_1 + d_2 - 5)} \\
&\quad + \frac{d_1 - 2}{3} \cdot \frac{d_2 - 5}{d_1(d_1 + d_2 - 5)} + \frac{d_2 - 4}{3} \cdot \frac{d_1 - 5}{d_2(d_1 + d_2 - 5)} \\
&\leq \frac{15n + C}{56}.
\end{aligned}$$

The last inequality holds for all $3 \leq d_1 \leq 13$ and $4 \leq d_2 \leq 11$.

Case 4. $(2, d_1) \sim (2, d_2)$ where $3 \leq d_1 \leq 12$ and $3 \leq d_2 \leq 12$.

Let $x_1, y_1, x_2, y_2, z_1, w_1, \cdots, w_{d_1 - 3}$ be the $(2, d_1)$-system centered at z_1 where $d(z_1) = d_1$, and $x_3, y_3, x_4, y_4, z_2, \bar{w}_1, \cdots, \bar{w}_{d_2 - 3}$ be the $(2, d_2)$-system centered at z_2 where $d(z_2) =$

d_2. Then $d(w_i) \geq 3$ and $d(\bar{w}_j) \geq 3$, $(1 \leq i \leq d_1 - 3$, and $1 \leq j \leq d_2 - 3)$. By deleting the vertices x_k, y_k and z_h, $(k = 1, 2, 3, 4,\ h = 1, 2)$, adding a path xyz of length 2, and then connecting $w_i z$ and $\bar{w}_j z$, we get a new tree T'. Then $|V(T')| = n - 7$, and $d_{T'}(z) = d_1 + d_2 - 5$. Now $n - 7 \geq 3(d_1 + d_2) - 18$ and

$$\begin{aligned}
R_{-1}(T) &= R_{-1}(T') + (\frac{1}{2} + \frac{1}{2d_1}) \cdot 2 + (\frac{1}{2} + \frac{1}{2d_2}) \cdot 2 + \frac{1}{d_1 d_2} - \frac{1}{2} - \frac{1}{2(d_1 + d_2 - 5)} \\
&\quad + (\frac{1}{d_1} - \frac{1}{d_1 + d_2 - 5}) \sum_{i=1}^{d_1 - 3} \frac{1}{d(w_i)} + (\frac{1}{d_2} - \frac{1}{d_1 + d_2 - 5}) \sum_{i=1}^{d_2 - 3} \frac{1}{d(\bar{w}_i)} \\
&\leq \frac{15(n-7) + C}{56} + \frac{3}{2} + \frac{1}{d_1} + \frac{1}{d_2} + \frac{1}{d_1 d_2} - \frac{1}{2(d_1 + d_2 - 5)} \\
&\quad + \frac{d_1 - 3}{3} \cdot \frac{d_2 - 5}{d_1(d_1 + d_2 - 5)} + \frac{d_2 - 3}{3} \cdot \frac{d_1 - 5}{d_2(d_1 + d_2 - 5)} \\
&\leq \frac{15n + C}{56}.
\end{aligned}$$

The last inequality holds for all $3 \leq d_1 \leq 12$ and $3 \leq d_2 \leq 12$.

Case 5. $(2, d_1) \sim (3, d_2)$ where $3 \leq d_1 \leq 12$ and $4 \leq d_2 \leq 11$.

Let $x_1, y_1, x_2, y_2, z_1, w_1, \cdots, w_{d_1 - 3}$ be the $(2, d_1)$-system centered at z_1 where $d(z_1) = d_1$, and $x_3, y_3, x_4, y_4, x_5, y_5, z_2, \bar{w}_1, \cdots, \bar{w}_{d_2 - 4}$ be the $(2, d_2)$-system centered at z_2 where $d(z_2) = d_2$. Then $d(w_i) \geq 3$ and $d(\bar{w}_j) \geq 3$, $(1 \leq i \leq d_1 - 3$, and $1 \leq j \leq d_2 - 4)$. By deleting the vertices x_k, y_k and z_h, $(k = 1, 2, \cdots, 5,\ h = 1, 2)$, adding a path xyz of length 2, and then connecting $w_i z$ and $\bar{w}_j z$, we get a new tree T'. Then $|V(T')| = n - 9$, and $d_{T'}(z) = d_1 + d_2 - 6$. Now $n - 9 \geq 3(d_1 + d_2) - 21$ and

$$\begin{aligned}
R_{-1}(T) &= R_{-1}(T') + (\frac{1}{2} + \frac{1}{2d_1}) \cdot 2 + (\frac{1}{2} + \frac{1}{2d_2}) \cdot 3 + \frac{1}{d_1 d_2} - \frac{1}{2} - \frac{1}{2(d_1 + d_2 - 6)} \\
&\quad + (\frac{1}{d_1} - \frac{1}{d_1 + d_2 - 6}) \sum_{i=1}^{d_1 - 3} \frac{1}{d(w_i)} + (\frac{1}{d_2} - \frac{1}{d_1 + d_2 - 6}) \sum_{i=1}^{d_2 - 4} \frac{1}{d(\bar{w}_i)} \\
&\leq \frac{15(n-9) + C}{56} + 2 + \frac{1}{d_1} + \frac{3}{2d_2} + \frac{1}{d_1 d_2} - \frac{1}{2(d_1 + d_2 - 6)} \\
&\quad + \frac{d_1 - 3}{3} \cdot \frac{d_2 - 6}{d_1(d_1 + d_2 - 6)} + \frac{d_2 - 4}{3} \cdot \frac{d_1 - 6}{d_2(d_1 + d_2 - 6)} \\
&\leq \frac{15n + C}{56}.
\end{aligned}$$

The last inequality holds for all $3 \leq d_1 \leq 12$ and $4 \leq d_2 \leq 11$.

Case 6. $(3, d_1) \sim (3, d_2)$ where $4 \leq d_1 \leq 11$ and $4 \leq d_2 \leq 11$.

Let $x_1, y_1, x_2, y_2, x_3, y_3, z_1, w_1, \cdots, w_{d_1-4}$ be the $(3, d_1)$-system centered at z_1 where $d(z_1) = d_1$, and $x_4, y_4, x_5, y_5, x_6, y_6, z_2, \bar{w}_1, \cdots, \bar{w}_{d_2-4}$ be the $(3, d_2)$-system centered at z_2 where $d(z_2) = d_2$. Then $d(w_i) \geq 3$ and $d(\bar{w}_j) \geq 3$, $(1 \leq i \leq d_1 - 4$, and $1 \leq j \leq d_2 - 4)$. By deleting the vertices x_k, y_k and z_h, $(k = 1, 2, \cdots, 6,\ h = 1, 2)$, adding a path xyz of length 2, and then connecting $w_i z$ and $\bar{w}_j z$, we get a new tree T'. Then $|V(T')| = n - 11$, and $d_{T'}(z) = d_1 + d_2 - 7$. Now $n - 11 \geq 3(d_1 + d_2) - 24$ and

$$\begin{aligned} R_{-1}(T) &= R_{-1}(T') + (\frac{1}{2} + \frac{1}{2d_1}) \cdot 3 + (\frac{1}{2} + \frac{1}{2d_2}) \cdot 3 + \frac{1}{d_1 d_2} - \frac{1}{2} - \frac{1}{2(d_1 + d_2 - 7)} \\ &\quad + (\frac{1}{d_1} - \frac{1}{d_1 + d_2 - 7}) \sum_{i=1}^{d_1-4} \frac{1}{d(w_i)} + (\frac{1}{d_2} - \frac{1}{d_1 + d_2 - 7}) \sum_{i=1}^{d_2-4} \frac{1}{d(\bar{w}_i)} \\ &\leq \frac{15(n-11) + C}{56} + \frac{5}{2} + \frac{3}{2d_1} + \frac{3}{2d_2} + \frac{1}{d_1 d_2} - \frac{1}{2(d_1 + d_2 - 7)} \\ &\quad + \frac{d_1 - 4}{3} \cdot \frac{d_2 - 7}{d_1(d_1 + d_2 - 7)} + \frac{d_2 - 4}{3} \cdot \frac{d_1 - 7}{d_2(d_1 + d_2 - 7)} \\ &\leq \frac{15n + C}{56}. \end{aligned}$$

The last inequality holds for all $4 \leq d_1 \leq 11$ and $4 \leq d_2 \leq 11$.

From above we can assume that for each (s, d)-system (unless $(1, d_1)$ where $d_1 = 11, 12, 13$). Let v_{ij} denote the neighbor of w_i, other than z, then $d(v_j) \geq 3$. Denote t_i the degree of w_i.

If the Max Tree T has the (s, d)-systems: $(1, 3)$, $(1, 4)$, $(1, 5)$, $(2, 3)$ $(2, 4)$, $(2, 5)$, $(3, 4)$, $(3, 5)$, then by deleting the suspended paths $x_i y_i z$ $(i = 1, \cdots, s)$ and identifying all w_j $(j = 1, \cdots d - s)$ to form a new vertex w, we get a new tree T'. So $|V(T')| = n - d - s$ and $d(w) = \sum_{i=1}^{d-s} (t_i - 1)$.

$$\begin{aligned} R_{-1}(T) &= R_{-1}(T') + (\frac{1}{2} + \frac{1}{2d}) \cdot s + \frac{1}{d} \sum_{i=1}^{d-s} \frac{1}{t_i} + \sum_{i=1}^{d-s} (\frac{1}{t_i} - \frac{1}{d(w)}) \sum_{j=1}^{t_i - 1} \frac{1}{d(v_{ij})} \\ &\leq \frac{15(n-d-s) + C}{56} + \frac{s}{2} + \frac{s}{2d} + \frac{1}{d} \sum_{i=1}^{d-s} \frac{1}{t_i} + \sum_{i=1}^{d-s} \frac{t_i - 1}{3} (\frac{1}{t_i} - \frac{1}{\sum_{i=1}^{d-s} (t_i - 1)}) \end{aligned}$$

$$
\begin{aligned}
&= \frac{15n+C}{56} - \frac{15(d+s)}{56} + \frac{s}{2} + \frac{s}{2d} + \frac{d-s}{3} - \frac{1}{3} + (\frac{1}{d} - \frac{1}{3}) \sum_{i=1}^{d-s} \frac{1}{t_i} \\
&< \frac{15n+C}{56} - \frac{15(d+s)}{56} + \frac{sd+s}{2d} + \frac{d-s-1}{3} \\
&\leq \frac{15n+C}{56}
\end{aligned}
$$

The last inequality holds for $(s,d) = (1,3)$, $(1,4)$, $(1,5)$, $(2,3)$ $(2,4)$, $(2,5)$, $(3,4)$, $(3,5)$.

Hence, we consider the (s,d)-systems where $s = 1$, $6 \leq d \leq 13$; $s = 2$, $6 \leq d \leq 12$; $s = 3$, $6 \leq d \leq 11$. We return to (2.3) and examine it for above all pairs. We can see that (2.3) holds (also the theorem holds) for $(s,d) = (1,6)$ unless some $d(w_i) \geq 4$; (1,7) unless some $d(w_i) \geq 5$; (1,8) unless some $d(w_i) \geq 5$; (1,9) unless some $d(w_i) \geq 6$; (1,10) unless some $d(w_i) \geq 8$; (1,11) unless some $d(w_i) \geq 10$; (1,12) unless some $d(w_i) \geq 15$; (1,13) unless some $d(w_i) \geq 29$; (2,6) unless some $d(w_i) \geq 5$; (2,7) unless some $d(w_i) \geq 6$; (2,8) unless some $d(w_i) \geq 7$; (2,9) unless some $d(w_i) \geq 8$; (2,10) unless some $d(w_i) \geq 11$; (2,11) unless some $d(w_i) \geq 16$; (2,12) unless some $d(w_i) \geq 36$; (3,6) unless some $d(w_i) \geq 8$; (3,7) unless some $d(w_i) \geq 9$; (3,8) unless some $d(w_i) \geq 11$; (3,9) unless some $d(w_i) \geq 15$; (3,10) unless some $d(w_i) \geq 25$; (3,11) unless some $d(w_i) \geq 113$.

For each such (s,d)-system centered at z, take the edges of the s suspended paths along with the distinguished edge $w_i z$ with $d(w_i)$ as specified above where, say, w_i is as small as possible (recall $V(T) = [n]$).

It is not hard to see that all such edge-sets is pairwise disjoint. Let $M_{s,d}$ denote the number of such (s,d)-systems in T. Then by calculating the weights of these specified edges belonging to these systems, we have

$$
\begin{aligned}
R_{-1}(T) \leq\ & (\frac{1}{2} + \frac{1}{12} + \frac{1}{24})M_{1,6} + (\frac{1}{2} + \frac{1}{14} + \frac{1}{35})M_{1,7} + (\frac{1}{2} + \frac{1}{16} + \frac{1}{40})M_{1,8} \\
& +(\frac{1}{2} + \frac{1}{18} + \frac{1}{54})M_{1,9} + (\frac{1}{2} + \frac{1}{20} + \frac{1}{80})M_{1,10} + (\frac{1}{2} + \frac{1}{22} + \frac{1}{110})M_{1,11} \\
& +(\frac{1}{2} + \frac{1}{24} + \frac{1}{180})M_{1,12} + (\frac{1}{2} + \frac{1}{26} + \frac{1}{377})M_{1,13} \\
& +(2 \cdot (\frac{1}{2} + \frac{1}{12})) + \frac{1}{30})M_{2,6} + (2 \cdot (\frac{1}{2} + \frac{1}{14})) + \frac{1}{42})M_{2,7}
\end{aligned}
$$

$$
\begin{aligned}
&+(2\cdot(\frac{1}{2}+\frac{1}{16}))+\frac{1}{56})M_{2,8}+(2\cdot(\frac{1}{2}+\frac{1}{18}))+\frac{1}{72})M_{2,9}\\
&+(2\cdot(\frac{1}{2}+\frac{1}{20}))+\frac{1}{110})M_{2,10}+(2\cdot(\frac{1}{2}+\frac{1}{22}))+\frac{1}{176})M_{2,11}\\
&+(2\cdot(\frac{1}{2}+\frac{1}{24}))+\frac{1}{432})M_{2,12}+(3\cdot(\frac{1}{2}+\frac{1}{12}))+\frac{1}{48})M_{3,6}\\
&+(3\cdot(\frac{1}{2}+\frac{1}{14}))+\frac{1}{63})M_{3,7}+(3\cdot(\frac{1}{2}+\frac{1}{16}))+\frac{1}{88})M_{3,8}\\
&+(3\cdot(\frac{1}{2}+\frac{1}{18}))+\frac{1}{135})M_{3,9}+(3\cdot(\frac{1}{2}+\frac{1}{20}))+\frac{1}{250})M_{3,10}\\
&+(3\cdot(\frac{1}{2}+\frac{1}{22}))+\frac{1}{1243})M_{3,11}\\
&+\frac{1}{4}[(n-1)-3\sum_{i=6}^{13}M_{1,i}-5\sum_{i=6}^{12}M_{2,i}-7\sum_{i=6}^{11}M_{3,i}]\\
=\ &\frac{n-1}{4}-\frac{1}{8}M_{1,6}-\frac{3}{20}M_{1,7}-\frac{13}{80}M_{1,8}-\frac{19}{108}M_{1,9}-\frac{3}{16}M_{1,10}\\
&-\frac{43}{220}M_{1,11}-\frac{73}{360}M_{1,12}-\frac{315}{1508}M_{1,13}-\frac{1}{20}M_{2,6}-\frac{1}{12}M_{2,7}-\frac{3}{28}M_{2,8}\\
&-\frac{1}{8}M_{2,9}-\frac{31}{220}M_{2,10}-\frac{27}{176}M_{2,11}-\frac{71}{432}M_{2,12}+\frac{1}{48}M_{3,6}-\frac{5}{252}M_{3,7}\\
&-\frac{9}{176}M_{3,8}-\frac{41}{540}M_{3,9}-\frac{12}{125}M_{3,10}-\frac{51}{452}M_{3,11}\\
<\ &\frac{n-1}{4}+\frac{1}{48}M_{3,6}.
\end{aligned}
$$

Since $M_{3,6}\le\frac{n-1}{7}$,

$$R_{-1}(T)\le\frac{n-1}{4}+\frac{1}{48}\cdot\frac{n-1}{7}=\frac{85}{336}(n-1)<\frac{15n+C}{56}.$$

The proof of the theorem is now complete. ∎

3 Solution to Question 2 - sharpness of our upper bound

Clark and Moon's first question is solved by our Theorem 2.1. In order to solve their second question, we note that if the constant C can be chosen as -1 for some n as our induction initial, then we can get the upper bound $\frac{15n-1}{56}$. This is because except for the induction initial n, our proof of Theorem 2.1 does not depend on the exact value of C. Since for the infinitely many trees T_r, defined in [6], the values of their R_{-1} can attain the upper bound, $\frac{15n-1}{56}$ is a sharp upper bound, and the second question is thus solved.

In fact, for $n \leq 71$ we first figure out various structural properties of a Max Tree to narrow the searching extent of possible trees, and then employ a good computer to calculate the values of R_{-1} for the rest trees of order 71. Finally, we get that T_{10} defined in [6] is the Max Tree. The value of R_{-1} for T_{10} is $19 = \frac{15\times 71-1}{56}$. So, $n = 71$ can be chosen as our induction initial, and the constant C in our theorem can really be chosen as -1. As r goes to infinity, there are infinitely many $n = 7r + 1$ for which the upper bound $\frac{15n-1}{56}$ is attained, and so in this sense $\frac{15n-1}{56}$ is a sharp upper bound for R_{-1} among all trees of order n. Here the exhausted searching by computers is omitted.

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