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

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**Abstract**

We show that the main proof of the paper "*Solutions to Two Unsolved Questions on the Best Upper Bound for the Randić Index $R_{-1}$ of Trees*" by Yumei Hu, Xueliang Li and Yuan Yuan (*MATCH Commun. Math. Comput. Chem.* **54** (2005) 441–454) is not correct. Namely, in many cases they maximized incorrectly some sums and because of this their proof is not complete.

## INTRODUCTION

In 1975 Randić [ 9] 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 [9] that his indices are well correlated with a variety of physico–chemical properties. They have attracted considerable attention of chemists and mathematicians ([1–8]).

In [4] Clark and Moon gave a lower and upper bound for $R_{-1}(T)$ for trees,

$$1 \leq R_{-1}(T) \leq \frac{15n+8}{18}$$

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 that 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 $\mid V(T_{7n+1}) \mid = 7n+1$ and weight

$$R_{-1}(T_{7n+1}) = \frac{15n+2}{8} \qquad \text{and} \qquad \lim_{n\to\infty} \frac{R_{-1}(T_{7n+1})}{\mid V(T_{7n+1}) \mid} = \frac{15}{56} \, .$$

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 [10] gave an upper bound for $R_{-1}(T)$ of trees with maximum degree $3$. Li and Yang [8] 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 [6] investigated trees with maximum general Randić index $R_\alpha(T)$ among all trees of order $n$. They distinguished $\alpha$ 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 [7] have tried to give positive answers to the above two questions proposed by Clark and Moon and to find a 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. In this short comment we show that the main proof of the paper [7] is not correct. Namely, in many cases they maximized incorrectly some sums and because of this their proof is not complete.

## MAIN ERRORS

In this comment we want to point out the errors in the proof of **Theorem 2.1.** from [7]. All notations, terminology and presumed results can be found in [7].

In the paper [7] the authors prove the following theorem:

**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*

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

*which solves the first question in [4].*

We will show that their proof is not correct. They considered Max Tree which have two $(s, d)$-systems sharing one edge. In order to prove their result they distinguished six cases. In Cases 2, 3, 4, 5 and 6 they made the same error – incorrectly maximized some sums. We begin with Case 2 (page 447). We cite the Case 2.

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

*Let $x_1, y_1, z_1, \omega_1, \ldots, \omega_{d_1-2}$ be the $(1, d_1)$-system centered at $z_1$ where $d(z_1) = d_1$, and $x_2, y_2, x_3, y_3, z_2, \bar{\omega}_1, \ldots, \bar{\omega}_{d_2-3}$ be the $(2, d_2)$-system centered at $z_2$ where $d(z_2) = d_2$. Then $d(\omega_i) \geq 3$ and $d(\bar{\omega}_j) \geq 3$, ($1 \leq i \leq d_1 - 2$, 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 $\omega_i z$ and $\bar{\omega}_j z$, 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*

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

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

But, the first inequality is not correct. They put

$$\sum_{i=1}^{d_1-2} \frac{1}{d(\omega_i)} \leq \frac{d_1-2}{3} \qquad \text{and} \qquad \sum_{i=1}^{d_2-3} \frac{1}{d(\bar{\omega}_i)} \leq \frac{d_2-3}{3}$$

without taking into account the signs of

$$\left(\frac{1}{d_1} - \frac{1}{d_1+d_2-4}\right) \qquad \text{and} \qquad \left(\frac{1}{d_2} - \frac{1}{d_1+d_2-4}\right)$$

respectively. When $d_2 - 4 < 0$ or $d_1 - 4 < 0$ it is not possible to maximize $R_{-1}(T)$ by putting $d(\omega_i) = 3,\ 1 \leq i \leq d_1 - 2$ and $d(\bar{\omega}_j) = 3,\ 1 \leq j \leq d_2 - 3$. For example, if $d_2 = 3$ and $d_1 = 4$ we have:

$$\begin{aligned} R_{-1}(T) &= R_{-1}(T') + \frac{1}{2} + \frac{1}{8} + \frac{4}{3} + \frac{1}{12} - \frac{1}{2} - \frac{1}{6} - \frac{1}{12} \sum_{i=1}^{2} \frac{1}{d(\omega_i)} \\ &\leq \frac{15(n-5)+C}{56} + \frac{11}{8} - \frac{1}{12} \sum_{i=1}^{2} \frac{1}{d(\omega_i)} \\ &= \frac{15n+C}{56} + \frac{1}{28} - \frac{1}{12} \left( \frac{1}{d(\omega_1)} + \frac{1}{d(\omega_2)} \right) \end{aligned}$$

If $d(\omega_1) \geq 5$ and $d(\omega_2) \geq 5$, then

$$\frac{1}{28} - \frac{1}{12} \left( \frac{1}{d(\omega_1)} + \frac{1}{d(\omega_2)} \right) \geq \frac{1}{28} - \frac{1}{30} > 0$$

and we cannot conclude that

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

The same holds if $d_2 = 3$, $d_1 = 5$ and $d(\omega_i) \geq 5$, $i = 1, 2, 3$.

They made the same mistakes in Case 3 ($d_2 = 4,\ d_1 = 4,\ d(\omega_i) \geq 9, i = 1, 2$), Case 4 ($d_2 = 3,\ d_1 = 4,\ d(\omega_1) \geq 7$), Case 5 ($d_2 = 5,\ d_1 = 3,\ d(\bar{\omega}_1 \geq 8$), Case 6 ($d_2 = 4,\ d_1 = 5,\ d(\omega_1) \geq 11;\ d_2 = 4,\ d_1 = 6,\ d(\omega_i) \geq 7, i = 1, 2$). In parenthesis we gave some values of $d_1$ and $d_2$ when their claim is not correct, but we have not checked all possibilities for $d_1$ and $d_2$. The authors have to improve their proof for these cases.

The authors make the same mistakes when they consider Max Tree which has $(2, 3)$ or $(3, 4)$ system. They wrote:

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

They denoted by $v_{ij}$ the neighbor of $\omega_i$, other than $z$ $(d(v_{ij}) \geq 3)$ and by $t_i$ the degree of $\omega_i$.

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

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

They maximized $\sum_{j=1}^{t_i-1} 1/d(v_{ij})$ by $(t_i-1)/3$ using $(d(v_{ij}) \geq 3)$ without regard to the sign of $1/t_i - 1/d(\omega)$. When $1/t_i - 1/d(\omega) < 0$ they cannot do this. It will be if $d-s=1$,

$$\frac{1}{t_i} - \frac{1}{d(\omega)} = \frac{1}{t_i} - \frac{1}{t_i-1} = -\frac{1}{t_i(t_i-1)} < 0\,.$$

For example, if $(s,d) = (3,4)$, $d(v_{1j}) = 5, 1 \leq j \leq t_1 - 1$, then we have:

$$\begin{aligned}
R_{-1}(T) &= R_{-1}(T') + \frac{15}{8} + \frac{1}{4t_1} + \left(\frac{1}{t_1} - \frac{1}{t_1-1}\right)\sum_{j=1}^{t_1-1}\frac{1}{d(v_{1j})} \\
&\leq \frac{15(n-7)+C}{56} + \frac{15}{8} + \frac{1}{4t_1} - \frac{1}{t_1(t_1-1)}\sum_{j=1}^{t_1-1}\frac{1}{d(v_{1j})} \\
&= \frac{15n+C}{56} + \frac{1}{t_1}\left(\frac{1}{4} - \frac{1}{t_1-1}\right)\sum_{j=1}^{t_1-1}\frac{1}{d(v_{1j})} \\
&= \frac{15n+C}{56} + \frac{1}{t_1}\left(\frac{1}{4} - \frac{1}{t_1-1}\frac{t_1-1}{5}\right) = \frac{15n+C}{56} + \frac{1}{20t_1}
\end{aligned}$$

which is not less than $(15n+C)/56$.

Our advise to the authors of the respective paper is to reconsider their proof and to refine it. We hope that these errors will not much affect the rest of their proof.

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