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Minimum Randić Index of Trees with Fixed Total Domination Number

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Abstract: The Randić index is among the most famous degree-based topological indices in chemical graph theory. It was introduced due to its application in modeling the properties of certain molecular structures and has been extensively studied. In this paper, we study the lower bound of the Randić index of trees in terms of the order and the total domination number. Finally, trees with the minimal Randić index are characterized.

Keywords: Randić index; total domination number; tree

MSC: 05C05; 05C35; 05C69

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1. Introduction

Let G be a simple and connected graph with vertex set $V(G)$ and edge set $E(G)$. An edge connecting two vertices u and v in the graph G are denoted by uv. For any vertex $v \in V$, the open neighborhood of v is the set $N(v) = \{u \in V | uv \in E\}$ and the closed neighborhood is the set $N[v] = N(v) \cup v$. The degree of a vertex u is denoted by $deg(u)$ and it is the number of edges that are incident with u in the graph G. A vertex u in G is a leaf if $deg(u) = 1$. The diameter of a tree is the longest path between two leaves. If $v_1, v_2, \ldots, v_d$ is a path where the diameter is attained, we say that $v_1, v_2, \ldots, v_d$ is a diameter path in T. We use $T - \{u_1, \ldots, u_k\}$ to denote the tree obtained from T by deleting the vertices $u_1, \ldots, u_k$ of T. As usual, by P_n and S_n, we denote the path and the star with n vertices, respectively. For other notations and terminologies not defined here, please refer to the book by West [1].

Graph theory has provided chemists with a variety of useful tools, such as topological indices. A topological index is a numeric quantity from the structural graph of a chemical compound [2]. Among many topological indices, the Randić index is the most widely used in applications to chemistry, especially in QSPR/QSAR investigations [3].

The Randić index was introduced by Randić [4] and is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg(u)deg(v)}},$$

where $deg(u)$ and $deg(v)$ denote the degrees of the vertices $u, v \in V(G)$, and uv denotes the edge connecting these two vertices.

A subset $D \subseteq V(G)$ is a dominating set of G if every vertex in $V(G) \setminus D$ has a neighbor in D. The minimum cardinality of a dominating set of G is called the domination number, denoted by $\gamma(G)$. A subset $D \subseteq V(G)$ is a total dominating set of G with no isolated vertices if every vertex G has a neighbor in D. The total domination number of G, denoted by $\gamma_t(G)$, is the minimal cardinality of a total dominating set [5]. Please refer to [6] for a survey of the selected findings on total domination number in graphs before 2009. Domination in graphs has been an active research area in graph theory [7,8].

The relationship between topological indices and the parameters of domination has attracted the attention of many researchers. Borovićanin and Furtula [9] showed the sharp upper bounds on the Zagreb indices of n-vertex trees with the domination number and characterized the extremal trees. In [10], the authors obtained the extremal harmonic index of trees in terms of the order and domination number. Furthermore, Pei and Pan [11] considered the upper bounds for the Zagreb indices of n-vertex trees with a given distance k-domination number and the extremal trees are characterized. Wang et al. [12] determined sharp upper and lower bounds of multiplicative Zagreb indices in terms of the arbitrary domination number. Moreover, the corresponding extremal graphs are characterized. In the paper, [13], upper and lower bounds on the zeroth-order general Randić index for trees with a given order and domination number are presented. In addition, the authors showed that the bounds are the best possible. Şahin [14] obtained the extremal values of the Hosoya index and the Merrifield–Simmons index of trees with a given domination number. Recently, Sun et al. [15] provided the maximum and minimum Sombor index of trees with fixed domination numbers and identified the corresponding extremal trees.

In [16], the upper bounds on the Zagreb indices of the tree, unicyclic, and bicyclic graphs with a given domination number and total domination number were obtained. Bermudo et al. [17] obtained the upper and lower bounds of the Randić index of trees with a given domination number. Recently, Ahmad Jamri et al. [18] discovered an upper bound for the Randić index of trees with a given total domination number. This paper investigates the lower bound of the Randić index of trees with a given total domination number. Finally, trees with a given order and total domination number with minimal Randić index are characterized.

2. Main Results

Here, the sharp lower bound of the Randić index of trees in terms of the total domination number and the characterization of those that attain this lower bound are presented. In order to do that, we used a similar approach as in [17].

The following lemmas are useful for our main results.

Lemma 1 ([12])**.** *If G is a connected graph of order $n \geq 3$, then $\gamma_t \leq \frac{2n}{3}$.*

Lemma 2. *Assume that for any number $n > 4$*

$$f(n,k) = \left(n - \frac{1}{2}(3k-1) + \frac{k-1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-1}} - \frac{1}{\sqrt{n-k}}\right) - \frac{1}{\sqrt{n-k-1}},$$

then $f(n,k+1) < f(n,k)$ and $f(n,k) < f(n+1,k)$, for any $2 \leq k < n-2$.

Proof. Firstly, we show that $f(n,k+1) < f(n,k)$ for any $k < n-2$.

$$\begin{aligned} f(n,k+1) &= \left(n - \frac{1}{2}(3k+2) + \frac{k}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-2}} - \frac{1}{\sqrt{n-k-1}}\right) - \frac{1}{\sqrt{n-k-2}} \\ &= \left(n - \frac{1}{2}(3k-1) + \frac{k-1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-2}} - \frac{1}{\sqrt{n-k-1}}\right) - \frac{1}{\sqrt{n-k-2}} \\ &\quad -\left(\frac{3}{2} - \frac{1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-2}} - \frac{1}{\sqrt{n-k-1}}\right), \end{aligned}$$

then $f(n,k+1) < f(n,k)$ if and only if

$$\begin{aligned}&\left(n-\frac{1}{2}(3k-1)+\frac{k-1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-2}}-\frac{1}{\sqrt{n-k-1}}\right)-\frac{1}{\sqrt{n-k-2}}\\&-\left(\frac{3}{2}-\frac{1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-2}}-\frac{1}{\sqrt{n-k-1}}\right)\\&<\left(n-\frac{1}{2}(3k-1)+\frac{k-1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-1}}-\frac{1}{\sqrt{n-k}}\right)-\frac{1}{\sqrt{n-k-1}}.\end{aligned}$$

This inequality is equivalent to

$$\begin{aligned}&\left(n-\frac{1}{2}(3k-1)+\frac{k-1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-2}}-\frac{1}{\sqrt{n-k-1}}\right)\\&-\left(n-\frac{1}{2}(3k-1)+\frac{k-1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-1}}-\frac{1}{\sqrt{n-k}}\right)\\&<\left(\frac{3}{2}-\frac{1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-2}}-\frac{1}{\sqrt{n-k-1}}\right)-\frac{1}{\sqrt{n-k-1}}+\frac{1}{\sqrt{n-k-2}}.\end{aligned}$$

After rearranging, we have

$$\begin{aligned}&\left(n-\frac{1}{2}(3k-1)+\frac{k-1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-2}}-\frac{2}{\sqrt{n-k-1}}+\frac{1}{\sqrt{n-k}}\right)\\&<\left(\frac{3}{2}-\frac{1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-2}}-\frac{1}{\sqrt{n-k-1}}\right)-\frac{1}{\sqrt{n-k-1}}+\frac{1}{\sqrt{n-k-2}}.\end{aligned}$$

Since we have

$$\begin{aligned}n-\frac{1}{2}(3k-1)+\frac{k-1}{2\sqrt{2}}&=n-k-\frac{1}{2}(k-1)+\frac{k-1}{2\sqrt{2}}\\&=n-k-\frac{1}{2}(k-1)\left(1-\frac{1}{\sqrt{2}}\right)\\&\leq n-k,\end{aligned}$$

it is enough to check that

$$\begin{aligned}&(n-k)\left(\frac{1}{\sqrt{n-k-2}}-\frac{2}{\sqrt{n-k-1}}+\frac{1}{\sqrt{n-k}}\right)\\&<\left(\frac{3}{2}-\frac{1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-2}}-\frac{1}{\sqrt{n-k-1}}\right)-\frac{1}{\sqrt{n-k-1}}+\frac{1}{\sqrt{n-k-2}},\end{aligned}$$

which is obtained by using the fact that the function

$$r(x) = \left(\frac{3}{2}-\frac{1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{x-2}}-\frac{1}{\sqrt{x-1}}\right)-\frac{1}{\sqrt{x-1}}+\frac{1}{\sqrt{x-2}}-x\left(\frac{1}{\sqrt{x-2}}-\frac{2}{\sqrt{x-1}}+\frac{1}{\sqrt{x}}\right),$$

is a positive function for any $x > 2$.

Finally, we show that $f(n,k) < f(n+1,k)$ implies

$$\begin{aligned}&\left(n-\frac{1}{2}(3k-1)+\frac{k-1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-1}}-\frac{1}{\sqrt{n-k}}\right)-\frac{1}{\sqrt{n-k-1}}\\&<\left(n+1-\frac{1}{2}(3k-1)+\frac{k-1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k}}-\frac{1}{\sqrt{n-k+1}}\right)-\frac{1}{\sqrt{n-k}},\end{aligned}$$

for any $n > k + 2$. Hence, this inequality is equivalent to

$$\left(n - \frac{1}{2}(3k-1) + \frac{k-1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-k-1}} + \frac{1}{\sqrt{n-k+1}} - \frac{2}{\sqrt{n-k}}\right)$$
$$< \frac{1}{\sqrt{n-k-1}} - \frac{1}{\sqrt{n-k+1}}.$$

Since

$$n - \frac{1}{2}(3k-1) + \frac{k-1}{2\sqrt{2}} = n - k - \frac{1}{2}(k-1)\left(1 - \frac{1}{\sqrt{2}}\right) \leq n - k,$$

for any $k \geq 2$ and the function

$$\frac{1}{\sqrt{x-1}} - \frac{1}{\sqrt{x+1}} - x\left(\frac{1}{\sqrt{x-1}} + \frac{1}{\sqrt{x+1}} - \frac{2}{\sqrt{x}}\right),$$

is a positive function for any $x \geq 2$, we have the required inequality. □

Now, we present our main results.

Theorem 1. *If T is a tree of order n and total domination number γ_t, then*

$$R(T) \geq \left(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-\gamma_t}}\right) + \frac{(\gamma_t-1)(\sqrt{2}+1)}{4} - \frac{(-1)^{\gamma_t}+1}{2\gamma_t - 1}. \quad (1)$$

Proof. The result is proved by induction on the number of vertices. If $n = 3$, $R(P_3) = \sqrt{2} > g(3,2) \approx 0.7904$. If $n = 4$, then $R(P_4) = \sqrt{2} + \frac{1}{2} > g(4,2) \approx 1.2475$ and $R(S_4) = \sqrt{3} > g(4,2)$. Therefore, we suppose that $n \geq 5$ and the result holds for any trees of order $n-1$. We will check if it is true for the tree with n vertices.

If γ_t is even, then we can have the inequality (1) as follows

$$R(T) \geq \left(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-\gamma_t}}\right) + \frac{(\gamma_t-1)(\sqrt{2}+1)}{4} - \frac{2}{2\gamma_t - 1}. \quad (2)$$

Meanwhile, if γ_t is odd, the inequality (1) is obtained as follows

$$R(T) \geq \left(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-\gamma_t}}\right) + \frac{(\gamma_t-1)(\sqrt{2}+1)}{4}. \quad (3)$$

Without loss of generality, suppose that γ_t is odd. Therefore, we prove inequality (3). To simplify the computations, we denote

$$g(n,\gamma_t) = \left(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n-\gamma_t}}\right) + \frac{(\gamma_t-1)(\sqrt{2}+1)}{4}.$$

Let $v_1, v_2, \ldots, v_d$ is a diameter path in the tree T. Let $deg(v_2) = i$, $N(v_2) = \{v_1, v_3, u_1, \ldots, u_{i-2}\}$, $deg(v_3) = j$ and $N(v_3) = \{v_2, v_4, w_1, w_2, \ldots, w_{j-2}\}$ and $deg(w_l) = s_l$ for $l \in \{1, \ldots, j-2\}$. Suppose $\widehat{T} = T - v_1$. Since $\gamma_t(T) - 1 \leq \gamma_t(\widehat{T}) \leq \gamma_t(T)$, we study the following cases.

Case 1. Suppose that $\gamma_t(\widehat{T}) = \gamma_t(T)$. Then, we have

$$
\begin{aligned}
R(T) &= R(\widehat{T}) - \Big(\frac{1}{\sqrt{i-1}} - \frac{1}{\sqrt{i}}\Big)\Big(i-2+\frac{1}{\sqrt{j}}\Big) + \frac{1}{\sqrt{i}} \\
&\geq \Big((n-1) - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-1-\gamma_t}}\Big) + \frac{(\gamma_t - 1)(\sqrt{2}+1)}{4} \\
&- \Big(\frac{1}{\sqrt{i-1}} - \frac{1}{\sqrt{i}}\Big)\Big(i-2+\frac{1}{\sqrt{j}}\Big) + \frac{1}{\sqrt{i}} \\
&= g(n,\gamma_t) + \Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}} - \frac{1}{\sqrt{n-\gamma_t}}\Big) - \frac{1}{\sqrt{n-\gamma_t-1}} \\
&- \Big(\frac{1}{\sqrt{i-1}} - \frac{1}{\sqrt{i}}\Big)\Big(i-2+\frac{1}{\sqrt{j}}\Big) + \frac{1}{\sqrt{i}}.
\end{aligned}
$$

If $n = i+2$, we have the graph shown in Figure 1 with $r = 1$ (see below). In this case, $\gamma_t(T^2_{s,1}) = 2$ and $R(T^2_{s,1}) = \frac{\sqrt{2}(i-1)+(\sqrt{i}+1)}{\sqrt{2i}}$. It is easy to check that $R(T^2_{s,1}) > g(i+2,2)$.

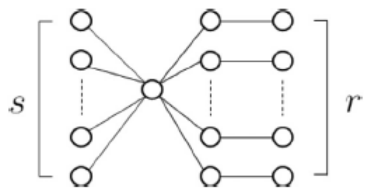

Figure 1. The graph $T^2_{s,r}$.

Thus, we consider $n \geq i+3$. Since $\gamma_t \leq n-(i-2)-2 = n-i$ and $n \geq i+3$, by Lemma 2, we have

$$
\begin{aligned}
&\Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}} - \frac{1}{\sqrt{n-\gamma_t}}\Big) - \frac{1}{\sqrt{n-\gamma_t-1}} \\
&\geq \Big(n - \frac{1}{2}(3(n-i)-1) + \frac{n-i-1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{i-1}} - \frac{1}{\sqrt{i}}\Big) - \frac{1}{\sqrt{i-1}} \\
&\geq (i-1+\frac{1}{\sqrt{2}})\Big(\frac{1}{\sqrt{i-1}} - \frac{1}{\sqrt{i}}\Big) - \frac{1}{\sqrt{i-1}}.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
R(T) &\geq g(n,\gamma_t) + \Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}} - \frac{1}{\sqrt{n-\gamma_t}}\Big) \\
&- \frac{1}{\sqrt{n-\gamma_t-1}} - \Big(\frac{1}{\sqrt{i-1}} - \frac{1}{\sqrt{i}}\Big)\Big(i-1+\frac{1}{\sqrt{j}}\Big) + \frac{1}{\sqrt{i-1}} \\
&= g(n,\gamma_t) + (i-1+\frac{1}{\sqrt{2}})\Big(\frac{1}{\sqrt{i-1}} - \frac{1}{\sqrt{i}}\Big) - \frac{1}{\sqrt{i-1}} \\
&- \Big(i-1+\frac{1}{\sqrt{j}}\Big)\Big(\frac{1}{\sqrt{i-1}} - \frac{1}{\sqrt{i}}\Big) + \frac{1}{\sqrt{i-1}} \\
&\geq g(n,\gamma_t) + \Big(\frac{1}{\sqrt{i-1}} - \frac{1}{\sqrt{i}}\Big)\Big(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}}\Big) \\
&= g(n,\gamma_t),
\end{aligned}
$$

for any $i \geq 2$. Thus, $R(T) \geq g(n,\gamma_t)$. The equalities hold if and only if $j = 2$ and in this case, the graph is one of the graphs shown in Figure 1.

Case 2. Suppose that $\gamma_t(\widehat{T}) = \gamma_t(T) - 1$. In this case, we have $i = 2$. Then, there exists a minimum total dominating set D of T such that $v_3 \in D$. Therefore, we obtain

$$\begin{aligned} R(T) &= R(\widehat{T}) - \Big(1 - \frac{1}{\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{j}}\Big) + \frac{1}{\sqrt{2}} \\ &\geq \Big((n-1) - \frac{1}{2}(3(\gamma_t - 1) - 1) + \frac{\gamma_t - 2}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t}}\Big) + \frac{(\gamma_t - 2)(\sqrt{2}+1)}{4} \\ &- \frac{2}{(2\gamma_t - 3)} - \Big(1 - \frac{1}{\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{j}}\Big) + \frac{1}{\sqrt{2}} \\ &= g(n,\gamma_t) + \Big(1 - \frac{1}{\sqrt{2}}\Big)\Big(\frac{1}{2\sqrt{n-\gamma_t}} - \frac{1}{\sqrt{j}}\Big) + \frac{\sqrt{2}-1}{4} - \frac{2}{(2\gamma_t - 3)}. \end{aligned}$$

If $j \geq 4(n - \gamma_t)$, then $\gamma_t \leq n - j + 1$, thus, $4n - 4\gamma_t \leq n - \gamma_t + 1$. Therefore, $n \leq \gamma_t + \frac{1}{3}$ and, consequently, we have $n - \frac{1}{3} \leq \gamma_t \leq \frac{2n}{3}$. However, it is $n \leq 1$. Therefore, we consider $j < 4(n - \gamma_t) - 1$. We denote $N(v_3) = \{v_2, v_4, w_1, \ldots, w_{j-2}\}$ and $deg(w_l) = s_l$ for any $l \in \{1, 2, \ldots, j-2\}$. By considering this case, $s_l = 1$ or $s_l = 2$ for $l \in \{1, 2, \ldots, j-2\}$. If v_4 is a leaf or support vertex with $deg(v_4) = 2$, then the graph is the one shown in Figure 1, which the result holds. In the other cases, we consider $s_1 = \cdots = s_{r_1} = 1$, $s_{r_1+1} = \cdots = s_{r_1+r_2} = 2$, where $r_1 + r_2 = j - 2$ and $deg(v_4) \geq 2$. We have the following cases.

Case 2.1. Let $r_1 \geq 1$. If $w_1 \in N(v_3)$ is one vertex, such that $deg(v_1) = 1$ and we take $T_1 = T - w_1$, then $\gamma_t(T) = \gamma_t(\widehat{T})$. Since $\gamma_t - 2 - r_2 \leq \frac{2\left(n-(j+1+r_2)\right)}{3}$; thus, $\gamma_t \leq \frac{2n-2j+r_2+4}{3}$. Hence, we have

$$\begin{aligned} R(T) &= R(T_1) - \Big(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\Big)\Big(\frac{1}{\sqrt{deg(v_4)}} + r_1 - 1 + \frac{r_2+1}{\sqrt{2}}\Big) + \frac{1}{\sqrt{j}} \\ &\geq \Big(n - 1 - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}}\Big) + \frac{(\gamma_t - 1)(\sqrt{2}+1)}{4} \\ &- \Big(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\Big)\Big(r_1 + \frac{r_2+2}{\sqrt{2}}\Big) + \frac{1}{\sqrt{j-1}} \\ &= g(n,\gamma_t) + \Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}} - \frac{1}{\sqrt{n-\gamma_t}}\Big) - \frac{1}{\sqrt{n-\gamma_t-1}} \\ &- \Big(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\Big)\Big(r_1 + \frac{r_2+2}{\sqrt{2}}\Big) + \frac{1}{\sqrt{j-1}}. \end{aligned}$$

If $d \leq 5$, then T is one of the graphs P_3, S_3, P_4 or the graph shown in Figure 1, thus we can consider $d \geq 6$. In this case, $n \geq r_1 + 2r_2 + 6$ and there exists $r \geq 0$, such that $n = r_1 + 2r_2 + 6 + r$. Therefore,

$$\gamma_t \leq \frac{2(r_1 + 2r_2 + 6 + r) - 2j + r_2 + 4}{3} = r_2 + 4 + \frac{2}{3}r.$$

By applying Lemma 1 and since $\gamma_t \leq r_2 + 4 + \frac{2}{3}r$ and $n = r_1 + 2r_2 + 6 + r$, we have

$$
\begin{aligned}
&\Big(n-\frac{1}{2}(3\gamma_t-1)+\frac{\gamma_t-1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}}-\frac{1}{\sqrt{n-\gamma_t}}\Big)-\frac{1}{\sqrt{n-\gamma_t-1}}\\
&\geq\Big(r_1+\frac{r_2+1}{2}+\frac{r_2+\frac{2}{3}r+3}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{(r_1+r_2)+\frac{r}{3}+1}}-\frac{1}{\sqrt{(r_1+r_2)+\frac{r}{3}+2}}\Big)\\
&-\frac{1}{\sqrt{(r_1+r_2)+\frac{r}{3}+1}}\\
&\geq\frac{2(j+\frac{r}{3})+(\sqrt{2}-1)(2r_1+r_2+1)}{2\sqrt{2}}\Big(\frac{1}{\sqrt{(j+\frac{r}{3})-1}}-\frac{1}{\sqrt{(j+\frac{r}{3})}}\Big)-\frac{1}{\sqrt{(j+\frac{r}{3})-1}}.
\end{aligned}
$$

By putting $x=j+\frac{r}{3}$, we have the function

$$h(x)=\Big(\frac{2x+(\sqrt{2}-1)(2r_1+r_2+1)}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{x-1}}-\frac{1}{\sqrt{x}}\Big)-\frac{1}{\sqrt{x-1}},$$

whose

$$h'(x)=\frac{1}{\sqrt{2}}\Big(\frac{1}{\sqrt{x-1}}-\frac{1}{\sqrt{x}}\Big)+\frac{1}{2(x-1)^{\frac{3}{2}}}-\frac{1}{2}\Big(\frac{2x+(\sqrt{2}-1)(2r_1+r_2+1)}{2\sqrt{2}}\Big)\Big(\frac{1}{(x-1)^{\frac{3}{2}}}-\frac{1}{(x)^{\frac{3}{2}}}\Big).$$

If $2x\geq(2r_1+r_2+1)$, we have that

$$h'(x)\geq\frac{1}{\sqrt{2}}\Big(\frac{1}{\sqrt{x-1}}-\frac{1}{\sqrt{x}}\Big)+\frac{1}{2(x-1)^{\frac{3}{2}}}-\Big(\frac{x(\sqrt{2}-1)}{\sqrt{2}}\Big)\Big(\frac{1}{(x-1)^{\frac{3}{2}}}-\frac{1}{(x)^{\frac{3}{2}}}\Big).$$

The above function for any $x\geq 2$ is a positive function. Thus, $h(x)$ is an increasing function for any $x\geq\frac{(2r_1+r_2+1)}{2}$. Since $j+\frac{r}{3}\geq j\geq\frac{(2r_1+r_2+1)}{2}$, if $r=0$, then the graph with $n=r_1+2r_2+6$ and $\gamma_t=4+r_2$ satisfies (1). In other cases, we have $h(j+\frac{r}{3})>h(j)$, which implies that

$$
\begin{aligned}
&\Big(n-\frac{1}{2}(3\gamma_t-1)+\frac{\gamma_t-1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}}-\frac{1}{\sqrt{n-\gamma_t}}\Big)-\frac{1}{\sqrt{n-\gamma_t-1}}\\
&\geq\frac{2(j+\frac{r}{3})+(\sqrt{2}-1)(2r_1+r_2+1)}{2\sqrt{2}}\Big(\frac{1}{\sqrt{(j+\frac{r}{3})-1}}-\frac{1}{\sqrt{(j+\frac{r}{3})}}\Big)-\frac{1}{\sqrt{(j+\frac{r}{3})-1}}\\
&\geq\frac{2j+(\sqrt{2}-1)(2r_1+r_2+1)}{2\sqrt{2}}\Big(\frac{1}{\sqrt{j-1}}-\frac{1}{\sqrt{j}}\Big)-\frac{1}{\sqrt{j-1}}.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
R(T) &\geq g(n,\gamma_t) + \Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}} - \frac{1}{\sqrt{n-\gamma_t}}\Big) - \frac{1}{\sqrt{n-\gamma_t-1}} \\
&- \Big(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\Big)\Big(r_1 + \frac{r_2+2}{\sqrt{2}}\Big) + \frac{1}{\sqrt{j-1}} \\
&> g(n,\gamma_t) + \frac{2j + (\sqrt{2}-1)(2r_1 + r_2 + 1)}{2\sqrt{2}}\Big(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\Big) - \frac{1}{\sqrt{j-1}} \\
&- \Big(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\Big)\Big(r_1 + \frac{r_2+2}{\sqrt{2}}\Big) + \frac{1}{\sqrt{j-1}} \\
&= g(n,\gamma_t) + \Big(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\Big)\Big(\frac{(\sqrt{2}-1)(r_2+1)}{2\sqrt{2}}\Big).
\end{aligned}
$$

Therefore, $R(T) > g(n,\gamma_t)$ for $j \geq 2$ and $r_2 \geq 0$.

Case 2.2. Assume that $r_1 = 0$. We study the following cases.

Case 2.2.1. Let $j \geq 3$. If $w_1 \in N(v_3)$ is one vertex such that $deg(w_1) = 2$ and z_1 is adjacent to w_1 with $deg(z_1) = 1$, we take $T_2 = T - \{v_1, v_2, z_1\}$. In this case, $\gamma_t(T_2) = \gamma_t(T) - 2$ and we have

$$
\begin{aligned}
R(T) &= R(T_2) - \Big(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\Big)\Big(\frac{j}{\sqrt{2}}\Big) + \frac{2-\sqrt{2}}{\sqrt{2(j-1)}} + \sqrt{2} \\
&\geq \Big(n - 3 - \frac{1}{2}(3(\gamma_t - 2) - 1) + \frac{\gamma_t - 3}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}}\Big) + \frac{(\gamma_t - 3)(\sqrt{2}+1)}{4} \\
&- \Big(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\Big)\Big(\frac{j}{\sqrt{2}}\Big) + \frac{2-\sqrt{2}}{\sqrt{2(j-1)}} + \sqrt{2} \\
&= g(n,\gamma_t) + \Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}} - \frac{1}{\sqrt{n-\gamma_t}}\Big) - \frac{\sqrt{2}}{2}\Big(\frac{1}{\sqrt{n-\gamma_t-1}}\Big) \\
&+ \Big(\frac{\sqrt{2}-1}{2}\Big) - \Big(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\Big)\Big(\frac{j}{\sqrt{2}}\Big) + \frac{2-\sqrt{2}}{\sqrt{2(j-1)}}.
\end{aligned}
$$

Since $\gamma_t \leq \frac{2n}{3}$, we have

$$
\begin{aligned}
&\Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}} - \frac{1}{\sqrt{n-\gamma_t}}\Big) - \frac{\sqrt{2}}{2}\Big(\frac{1}{\sqrt{n-\gamma_t-1}}\Big) \\
&\quad \geq \Big(n - \frac{1}{2}(2n-1) + \frac{2(\frac{n}{3}) - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{(\frac{n}{3}) - 1}} - \frac{1}{\sqrt{(\frac{n}{3})}}\Big) - \frac{\sqrt{2}}{2}\Big(\frac{1}{\sqrt{(\frac{n}{3}) - 1}}\Big).
\end{aligned}
$$

We consider the function

$$
h(x) = \frac{1}{2}\Big(1 + \frac{2x-1}{\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{x-1}} - \frac{1}{\sqrt{x}}\Big) - \frac{\sqrt{2}}{2}\Big(\frac{1}{\sqrt{x-1}}\Big),
$$

which is an increasing function for $x > 1$.

If $n \geq 3j$, then $h(\frac{n}{3}) \geq h(j)$, which yields

$$\begin{aligned}
&\Big(n-\frac{1}{2}(3\gamma_t-1)+\frac{\gamma_t-1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}}-\frac{1}{\sqrt{n-\gamma_t}}\Big)-\frac{\sqrt{2}}{2}\Big(\frac{1}{\sqrt{n-\gamma_t-1}}\Big)\\
&+\Big(\frac{\sqrt{2}-1}{2}\Big)-\Big(\frac{1}{\sqrt{j-1}}-\frac{1}{\sqrt{j}}\Big)\Big(\frac{j}{\sqrt{2}}\Big)+\frac{2-\sqrt{2}}{\sqrt{2(j-1)}}\\
&\geq \frac{1}{2}\Big(1+\frac{2j-1}{\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{j-1}}-\frac{1}{\sqrt{j}}\Big)-\frac{\sqrt{2}}{2}\Big(\frac{1}{\sqrt{j-1}}\Big)+\Big(\frac{\sqrt{2}-1}{2}\Big)\\
&-\Big(\frac{1}{\sqrt{j-1}}-\frac{1}{\sqrt{j}}\Big)\Big(\frac{j}{\sqrt{2}}\Big)+\frac{2-\sqrt{2}}{\sqrt{2(j-1)}}.
\end{aligned}$$

This is a positive function for any $j \geq 3$. Therefore, $R(T) \geq g(n, \gamma_t)$. If $n < 3j$ and $j \geq 3$, in this case, the only graph with these conditions is the graph obtained from path P_6, such that P_2 is added to the vertex v_3. It is easy to check for this graph that $R(T) > g(8, 5)$.

Case 2.2.2. We suppose that $j = 2$. By the above cases, we can suppose that $n \geq 8$. We consider the following cases.

Case 2.2.2.1. If $v_4, v_5 \notin D$, then we take $T_2 = T - \{v_1, v_2\}$. In this case, $\gamma_t(T_2) = \gamma_t(T)$. Thus, we have

$$\begin{aligned}
R(T) &= R(T_2)+1\\
&\geq \Big(n-2-\frac{1}{2}(3\gamma_t-1)+\frac{\gamma_t-1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-3}}\Big)+\frac{(\gamma_t-1)(\sqrt{2}+1)}{4}+1\\
&= g(n,\gamma_t)+\Big(n-\frac{1}{2}(3\gamma_t-1)+\frac{\gamma_t-1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-3}}-\frac{1}{\sqrt{n-\gamma_t}}\Big)-\frac{2}{\sqrt{n-\gamma_t-3}}+1.
\end{aligned}$$

Since $\gamma_t \leq \frac{2n}{3}$, using Lemma 2, we have

$$\begin{aligned}
&\Big(n-\frac{1}{2}(3\gamma_t-1)+\frac{\gamma_t-1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-3}}-\frac{1}{\sqrt{n-\gamma_t}}\Big)-\frac{2}{\sqrt{n-\gamma_t-3}}\\
&\geq \Big(n-\frac{1}{2}(3(2n-1)+\frac{2(\frac{2n}{3})-1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{(\frac{n}{3})-3}}-\frac{1}{\sqrt{(\frac{n}{3})}}\Big)-\frac{2}{\sqrt{(\frac{n}{3})-3}}\\
&= \Big(\frac{1}{2}+\frac{2n-3}{6\sqrt{2}}\Big)\Big(\frac{\sqrt{3}}{\sqrt{n-9}}-\frac{\sqrt{3}}{\sqrt{n}}\Big)-\frac{2\sqrt{3}}{\sqrt{n-9}}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
R(T) &\geq g(n,\gamma_t)+\Big(n-\frac{1}{2}(3\gamma_t-1)+\frac{\gamma_t-1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-3}}-\frac{1}{\sqrt{n-\gamma_t}}\Big)-\frac{2}{\sqrt{n-\gamma_t-3}}+1,\\
&\geq g(n,\gamma_t)+\Big(\frac{1}{2}+\frac{2n-3}{6\sqrt{2}}\Big)\Big(\frac{\sqrt{3}}{\sqrt{n-9}}-\frac{\sqrt{3}}{\sqrt{n}}\Big)-\frac{2\sqrt{3}}{\sqrt{n-9}}+1,
\end{aligned}$$

which is a positive function for $n \geq 10$. Therefore, $R(T) > g(n, \gamma_t)$.

For $n = 8$ and $j = 2$, tree T is the path P_8, and for $n = 9$ and $j = 2$, the graph is one of graphs P_9 or the graph obtained from P_8, such that $deg(v_7) = 4$. Clearly, in these cases, $R(T) > g(n, \gamma_t)$.

Case 2.2.2.2. Let v_4 or v_5 not be in the minimum total dominating set D. We suppose that $v_4 \in D$ and $v_5 \notin D$. We take $T_2 = T - \{v_1, v_2, v_3\}$ and we consider the two following cases.

Case 2.2.2.2.1. We suppose that $\gamma_t(T_2) = \gamma_t(T) - 2$. Assume that $deg(v_4) = k \geq 2$. Then, we have

$$\begin{aligned}
R(T) &= R(T_2) + \Big(\frac{\sqrt{2}+1}{2}\Big) - \frac{1}{\sqrt{2}}\Big(\frac{1}{\sqrt{k-1}} - \frac{2}{\sqrt{k}}\Big) \\
&\geq \Big(n - 3 - \frac{1}{2}(3(\gamma_t - 2) - 1) + \frac{\gamma_t - 3}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}}\Big) + \frac{(\gamma_t - 3)(\sqrt{2}+1)}{4} \\
&+ \Big(\frac{\sqrt{2}+1}{2}\Big) - \frac{1}{\sqrt{2}}\Big(\frac{1}{\sqrt{k-1}} - \frac{2}{\sqrt{k}}\Big) \\
&= g(n,\gamma_t) + \Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}} - \frac{1}{\sqrt{n-\gamma_t}}\Big) \\
&- \frac{\sqrt{2}}{2}\Big(\frac{1}{\sqrt{n-\gamma_t-1}}\Big) - \frac{1}{\sqrt{2}}\Big(\frac{1}{\sqrt{k-1}} - \frac{2}{\sqrt{k}}\Big).
\end{aligned}$$

By applying $\gamma_t \leq \frac{2n}{3}$ and Lemma 2, we have

$$\begin{aligned}
&\Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}} - \frac{1}{\sqrt{n-\gamma_t}}\Big) - \frac{\sqrt{2}}{2}\Big(\frac{1}{\sqrt{n-\gamma_t-1}}\Big), \\
&\geq \frac{1}{2}\Big(1 + \frac{2(\frac{n}{3}) - 1}{\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{(\frac{n}{3}) - 1}} - \frac{1}{\sqrt{(\frac{n}{3})}}\Big) - \frac{\sqrt{2}}{2}\Big(\frac{1}{\sqrt{(\frac{n}{3}) - 1}}\Big).
\end{aligned}$$

Here, the function

$$\frac{1}{2}\Big(1 + \frac{2x - 1}{\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{x-1}} - \frac{1}{\sqrt{x}}\Big) - \frac{\sqrt{2}}{2}\Big(\frac{1}{\sqrt{x-1}}\Big),$$

is an increasing function for $x \geq 1$. Therefore, for $n \geq 3k$, we have $R(T) > g(n,\gamma_t)$.

Note that if $v_4 \notin D$ and $v_5 \in D$, by considering $T_2 = T - \{v_1, v_2, v_3\}$ and $\gamma_t(T_2) = \gamma_t - 2$, the result is obtained via the case given above.

Case 2.2.2.2.2. We suppose that $\gamma_t(T_2) = \gamma_t - 1$. We denote $N(v_4) = \{v_3, v_5, y_1, \ldots, y_{k-2}\}$. By the above cases and the definition of the total domination number, $deg(y_l) = 1$ for any $1 \leq l \leq k-2$. In such a case, we take $T_2 = T - \{v_1, v_2\}$ which yields

$$\begin{aligned}
R(T) &= R(T_2) + \Big(\frac{\sqrt{2}+1}{2}\Big) + \frac{1}{\sqrt{k}}\Big(\frac{1}{\sqrt{2}} - 1\Big) \\
&\geq \Big(n - 2 - \frac{1}{2}(3(\gamma_t - 1) - 1) + \frac{\gamma_t - 2}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}}\Big) + \frac{(\gamma_t - 2)(\sqrt{2}+1)}{4} \\
&+ \Big(\frac{\sqrt{2}+1}{2}\Big) + \frac{1}{\sqrt{k}}\Big(\frac{1}{\sqrt{2}} - 1\Big) \\
&= g(n,\gamma_t) + \Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}} - \frac{1}{\sqrt{n-\gamma_t}}\Big) \\
&- \frac{\sqrt{2}+1}{2\sqrt{2}}\Big(\frac{1}{\sqrt{n-\gamma_t-1}}\Big) + \Big(\frac{\sqrt{2}+1}{4}\Big) + \frac{1}{\sqrt{k}}\Big(\frac{1}{\sqrt{2}} - 1\Big).
\end{aligned}$$

Since $\gamma_t \leq \frac{2n}{3}$, using Lemma 2, we have

$$\begin{aligned}
&\Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n-\gamma_t-1}} - \frac{1}{\sqrt{n-\gamma_t}}\Big) - \frac{\sqrt{2}+1}{2\sqrt{2}}\Big(\frac{1}{\sqrt{n-\gamma_t-1}}\Big) \\
&\geq \frac{1}{2}\Big(1 + \frac{2(\frac{n}{3}) - 1}{\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{(\frac{n}{3}) - 1}} - \frac{1}{\sqrt{(\frac{n}{3})}}\Big) - \frac{\sqrt{2}+1}{2\sqrt{2}}\Big(\frac{1}{\sqrt{(\frac{n}{3}) - 1}}\Big).
\end{aligned}$$

Similar to the above case, for any $n > 4$ we have $R(T) > g(n, \gamma_t)$. $\square$

Remark 1. *In [17], the authors proposed a lower bound of the Randić index of trees in terms of the order n and the domination number γ as follows*

$$R(T) \geq \frac{n - 2\gamma + 1}{\sqrt{n - \gamma}} + \frac{\gamma - 1}{\sqrt{2}}\Big(1 + \frac{1}{\sqrt{n - \gamma}}\Big) = h(n, \gamma).$$

According to the discussion at the beginning of the proof of Theorem 1, let us consider

$$R(T) \geq \Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n - \gamma_t}}\Big) + \frac{(\gamma_t - 1)(\sqrt{2} + 1)}{4} = g(n, \gamma_t).$$

If $\gamma_t \leq \frac{4\gamma}{3}$, then

$$\begin{aligned} g(n, \gamma_t) &= \Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n - \gamma_t}}\Big) + \frac{(\gamma_t - 1)(\sqrt{2} + 1)}{4} \\ &= \Big(n - \frac{3}{2}\gamma_t + 1 - 1 + \frac{1}{2} + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n - \gamma_t}}\Big) + \frac{(\gamma_t - 1)(\sqrt{2} + 1)}{4} \\ &\geq \Big(n - 2\gamma + 1\Big)\Big(\frac{1}{\sqrt{n - \gamma_t}}\Big) + (-\frac{1}{2} + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n - \gamma_t}}\Big) + \frac{(\gamma_t - 1)(\sqrt{2} + 1)}{4}. \end{aligned}$$

Using the fact that $\gamma \leq \gamma_t$ and $2 \leq n - \gamma_t$, we have

$$\begin{aligned} g(n, \gamma_t) &\geq \Big(n - 2\gamma + 1\Big)\Big(\frac{1}{\sqrt{n - \gamma_t}}\Big) + (-\frac{1}{2} + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n - \gamma_t}}\Big) + \frac{(\gamma_t - 1)(\sqrt{2} + 1)}{4} \\ &\geq \Big(n - 2\gamma + 1\Big)\Big(\frac{1}{\sqrt{n - \gamma}}\Big) - \frac{1}{2}\Big(\frac{1}{\sqrt{n - \gamma_t}}\Big) + \frac{\gamma - 1}{2\sqrt{2}}\Big(\frac{1}{\sqrt{n - \gamma}}\Big) + \frac{(\gamma - 1)(\sqrt{2} + 1)}{4} \\ &= h(n, \gamma) - \frac{1}{2}\Big(\frac{1}{\sqrt{n - \gamma_t}}\Big) - \frac{\gamma - 1}{2\sqrt{2}}\Big(\frac{1}{\sqrt{n - \gamma}}\Big) - \frac{\gamma - 1}{\sqrt{2}} + \frac{(\gamma - 1)(\sqrt{2} + 1)}{4} \\ &\geq h(n, \gamma) - \frac{1}{2}\Big(\frac{1}{\sqrt{2}}\Big) - \frac{\gamma - 1}{2\sqrt{2}}\Big(\frac{1}{\sqrt{n - \gamma}}\Big) - \frac{\gamma - 1}{\sqrt{2}} + \frac{(\gamma - 1)(\sqrt{2} + 1)}{4} \\ &> h(n, \gamma), \end{aligned}$$

for any $n \geq 4$ and $\gamma \geq 2$.

Therefore, for any $n \geq 4$ and $\gamma \leq \gamma_t \leq \frac{4\gamma}{3}$,

$$\begin{aligned} &\Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n - \gamma_t}}\Big) + \frac{(\gamma_t - 1)(\sqrt{2} + 1)}{4} \\ &> \frac{n - 2\gamma + 1}{\sqrt{n - \gamma}} + \frac{\gamma - 1}{\sqrt{2}}\Big(1 + \frac{1}{\sqrt{n - \gamma}}\Big). \end{aligned}$$

Consequently, the lower bound (1) is stronger than the lower bound obtained in [17] Theorem 2.4 for $n \geq 4$ and $\gamma \leq \gamma_t \leq \frac{4\gamma}{3}$.

Theorem 2. *Let T be a tree of order n and a total domination number γ_t. Then*

$$R(T) = \Big(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\Big)\Big(\frac{1}{\sqrt{n - \gamma_t}}\Big) + \frac{(\gamma_t - 1)(\sqrt{2} + 1)}{4} - \frac{(-1)^{\gamma_t} + 1}{2\gamma_t - 1},$$

if and only if $T = T_{s,r}$.

Proof. Suppose that there exists a tree $T_{s,r}$ ($s \geq 1$), shown in Figure 2 as below. In such a case, we have $n = s + 3r + 1$ and $\gamma_t = 2r + 1$. Therefore, we have

$$R(T_{s,r}) = \frac{s}{\sqrt{r+s}} + \frac{r}{\sqrt{2}} + \frac{r}{\sqrt{4}} + \frac{r}{\sqrt{2(r+s)}}.$$

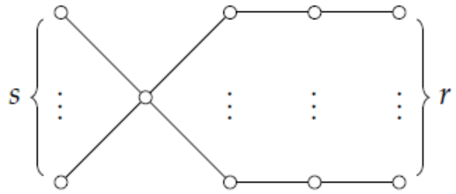

Figure 2. The graph$T_{s,r}$.

By substituting $r = \frac{\gamma_t - 1}{2}$ and $s = n - \frac{1}{2}(3\gamma_t - 1)$ on the right side of the above equation, we have

$$R(T_{s,r}) = \left(n - \frac{1}{2}(3\gamma_t - 1) + \frac{\gamma_t - 1}{2\sqrt{2}}\right)\left(\frac{1}{\sqrt{n - \gamma_t}}\right) + \frac{(\gamma_t - 1)(\sqrt{2} + 1)}{4} - \frac{(-1)^{\gamma_t} + 1}{2\gamma_t - 1}.$$

By following the proof of Theorem 1, we can see that in some cases of the proof, if $T \neq T_{s,r}$, then the inequality in that theorem is a strict inequality. Therefore, we suppose that there exists a tree $T \neq T_{s,r}$ in Cases 1 and 2.2, such that the equality holds. However, we show that there is no such tree.

In Case 1, if there exists a tree T such that the equality holds, then all of the inequalities become equalities. This happens when $n = i + 3$ and $\gamma_t = n - i = 3$. That is, the graph is one of the graphs shown in Figure 2 with $r = 1$. Therefore, $T = T_{s,1}$.

By considering Case 2.2 in the proof of Theorem 1, we investigate trees that satisfy the equality conditions $r_1 = 0$ and $j \geq 3$. If all inequalities become equal in Case 2.2, then we have

$$\frac{1}{2}\left(1 + \frac{2j-1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\right) - \frac{\sqrt{2}}{2}\left(\frac{1}{\sqrt{j-1}}\right) + \left(\frac{\sqrt{2}-1}{\sqrt{2}}\right)$$
$$- \left(\frac{1}{\sqrt{j-1}} - \frac{1}{\sqrt{j}}\right)\left(\frac{j}{\sqrt{2}}\right) + \frac{2-\sqrt{2}}{\sqrt{2(j-1)}} = 0.$$

By simplification of the above relation, we have

$$\frac{1}{4}\left(-2 + 2\sqrt{2} + \frac{\sqrt{2}-2}{\sqrt{j-1}} + \frac{\sqrt{2}-2}{\sqrt{j}}\right) = 0,$$

which we can easily check that $j < 3$. Therefore, the inequality, in this case, is also strict. □

3. Conclusions

This research looks at the link between the Randić index and the total domination number of trees. We provided a lower bound for the Randić index of trees in terms of the total domination number and characterized all trees that attained the equality case. Combined with the result in [18], the extremal results for the Randić index of trees (in terms of the order and the total domination number) were completely determined.

To conclude this paper, we suggest the following open problem.

Problem 1. Determine the upper and lower bounds for the Randić index of trees with respect to the order and the Roman domination number (or other domination parameters).

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