Trees with the second and third largest number of maximal independent sets

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Abstract

Let G be a simple undirected graph. Denote by $\mathrm{mi}(G)$ the number of maximal independent sets in G. In this paper we determine the second and third largest number of maximal independent sets in trees. Extremal trees achieving these values are also determined.

Key Words: combinatorial problems, maximal independent sets, trees.

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1 Introduction

An *independent set* is a subset S of $V(G)$ such that no two vertices in S are adjacent in G. A *maximal independent set* is an independent set that is not a proper subset of any other independent set. A *maximum independent set* is an independent set of maximum size. Note that a maximum independent set is maximal but the converse is not always true. Denote by $\mathrm{mi}(G)$ (respectively, $\mathrm{xi}(G)$) the number of maximal (respectively, maximum) independent sets in G.

One reason why upper bounds on $\mathrm{mi}(G)$ are of interest is that better estimates on the size of $\mathrm{mi}(G)$ lead to improvements on the time analysis of algorithms determining several hard graph invariants. Erdős and Moser raised the problem of determining the maximum value of $\mathrm{mi}(G)$ for a general graph of order n and the extremal graphs achieving the maximum

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value. This problem was solved by Moon and Moser [20]. Since then, researchers have studied the problem for graphs with some basic properties, see [1, 4, 6, 9, 14, 19, 21, 22, 23, 24]. For other related, including algorithmic, results on mi(G), see [3, 7, 10, 11, 12, 15, 16]. Compared to mi(G), there are fewer results for the parameter xi(G), see [2, 8, 17]. A survey on counting maximal independent sets in graphs can be found in [13].

In this paper, we determine the second and third largest number of maximal independent sets in trees. Extremal trees achieving these values are also determined.

2 Preliminaries

Lemma 2.1 [9] *For any vertex x in a graph G, the followings hold.*
(1) $\mathrm{mi}(G) \le \mathrm{mi}(G-x) + \mathrm{mi}(G-N[x])$.
(2) *If x is a leaf adjacent to y, then* $\mathrm{mi}(G) = \mathrm{mi}(G-N[x]) + \mathrm{mi}(G-N[y])$.

Lemma 2.2 [9] *For any two vertex disjoint graphs G and H,* $\mathrm{mi}(G \cup H) = \mathrm{mi}(G)\mathrm{mi}(H)$.

The following lemma is obvious.

Lemma 2.3 *Let G be a graph of order n. If G contains two vertices x and y, with $d(x) = d(y) = 1$ and $N(x) = N(y)$, then* $\mathrm{mi}(G) = \mathrm{mi}(G-x)$.

Define a *baton* $B(i, j)$ as follows: Start with a basic path P with i vertices and attach j paths of length two to the endpoints of P. Throughout the paper, we use r to denote $\sqrt{2}$.

For any $n \ge 1$, let

$$T_1(n) = \begin{cases} B(2, \frac{n-2}{2}) \text{ or } B(4, \frac{n-4}{2}), & \text{if } n \equiv 0 \pmod 2; \\ B(1, \frac{n-1}{2}), & \text{if } n \equiv 1 \pmod 2. \end{cases}$$

It follows from Lemma 2.1 that

$$\mathrm{mi}(T_1(n)) = t_1(n) = \begin{cases} r^{n-2} + 1, & \text{if } n \equiv 0 \pmod 2; \\ r^{n-1}, & \text{if } n \equiv 1 \pmod 2. \end{cases}$$

Theorem 2.4 [5, 11, 14, 21, 23] *If T is a tree of order n, then* $\mathrm{mi}(T) \le t_1(n)$. *Furthermore, the equality holds if and only if $T \cong T_1(n)$.*

For forests, Jou [11] obtained the following result.

Theorem 2.5 [11] *If F is a forest of order n, then*

$$\mathrm{mi}(F) \le f(n) = \begin{cases} r^n, & \text{if } n \equiv 0 \pmod 2; \\ r^{n-1}, & \text{if } n \equiv 1 \pmod 2. \end{cases}$$

Furthermore, the equality holds if and only if $F \cong F(n)$, *where*

$$F(n) = \begin{cases} \frac{n}{2}K_2, & \textit{if } n \equiv 0 \pmod 2; \\ B(1, \frac{n-1-2s}{2}) \cup sK_2, & \textit{if } n \equiv 1 \pmod 2. \end{cases}$$

Let $T_2(n)$ denote the tree of order n defined as follows (see Figure 1): (1) For $n \equiv 0$ $(mod\ 2)$ and $n \geq 4$, start with a star $K_{1,3}$ and attach $\frac{n-4}{2}$ paths of length two to at most two leaves of the star $K_{1,3}$. (2) For $n \equiv 1$ $(mod\ 2)$ and $n \geq 7$, start with a path P_5 and attach $\frac{n-5}{2}$ paths of length two to an endpoint of the path P_5. From Lemma 2.1, we have

$$\mathrm{mi}(T_2(n)) = t_2(n) = \begin{cases} r^{n-2}, & \text{if } n \equiv 0 \pmod 2; \\ \frac{3}{4}r^{n-1} + 1, & \text{if } n \equiv 1 \pmod 2. \end{cases}$$

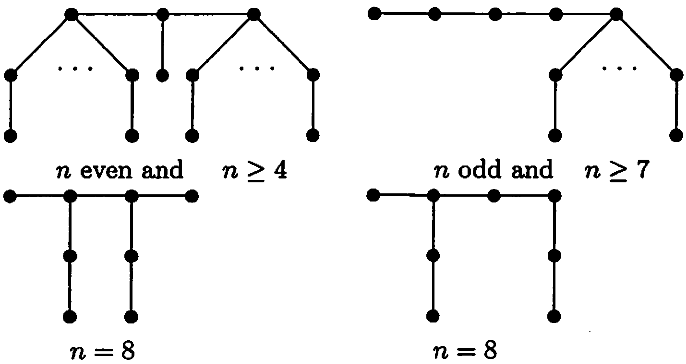

Figure 1: The tree $T_2(n)$.

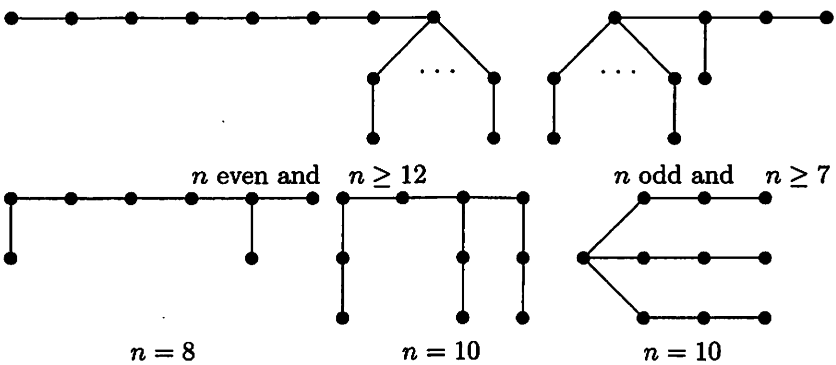

Figure 2: The tree $T_3(n)$.

Let $T_3(n)$ denote the tree of order n defined as follows (see Figure 2): (1) For $n \equiv 0$ $(mod\ 2)$ and $n \geq 12$, start with a path P_8 and attach $\frac{n-8}{2}$

paths of length two to an endpoint of the path P_8. (2) For $n \equiv 1 \pmod 2$ and $n \geq 5$, start with a path P_4 and the tree $T_1(n-4)$, and add an edge between the center of $T_1(n-4)$ and an internal vertex of the path P_4. It follows from Lemma 2.1 that

$$\mathrm{mi}(T_3(n)) = t_3(n) = \begin{cases} 7, & \text{if } n = 8; \\ \frac{7}{16}r^n + 1, & \text{if } n = 10; \\ \frac{7}{16}r^n + 2, & \text{if } n \equiv 0 \pmod 2 \text{ and } n \neq 8, 10; \\ \frac{3}{4}r^{n-1}, & \text{if } n \equiv 1 \pmod 2. \end{cases}$$

3 Main Results

Theorem 3.1 *let T be a tree of order n. If $T \not\cong P_{10}, T_i(n)$, $i = 1, 2$, then $mi(T) \leq t_3(n)$. Furthermore, the equality holds if and only if $T \cong T_3(n)$ or $T \cong P_9$.*

Proof. We prove the theorem by induction on n. It is a straightforward exercise to verify that the result holds for trees with at most eight vertices. Let $n \geq 9$ and assume that the result holds for all trees of order less than n. Let T be a tree of order n.

Let r and x denote two vertices of T at maximum distance from each other. Both r and x are necessarily leaves, and we may assume that the distance between r and x is a least three. We root T at r and let y and z denote the father and grandfather of the leaf x. We distinguish the following cases.

Case 1. $n \equiv 1 \pmod 2$ and $n \geq 9$.

If $d(y) \geq 3$, then y has at least two leaf sons, so it follows from Lemma 2.3 that

$$\mathrm{mi}(T) = \mathrm{mi}(T - x) \leq t_1(n-1) < t_3(n).$$

We now consider the case $d(y) = 2$. Suppose that $T - N[x] \cong T_1(n-2)$. Since $T \not\cong T_i(n)$, $i = 1, 2$, it follows from the structure of $T_1(n-2)$ that $T \cong T_3(n)$. We now assume that $T - N[x] \not\cong T_1(n-2)$. If z has a leaf son, it follows from the induction hypothesis and Theorem 2.5 that

$$\begin{aligned} \mathrm{mi}(T) &= \mathrm{mi}(T - N[x]) + \mathrm{mi}(T - N[y]) \\ &\leq t_2(n-2) + f(n-4) \\ &= \tfrac{5}{8}r^{n-1} + 1 < \tfrac{3}{4}r^{n-1}. \end{aligned}$$

Thus we may assume that all the descendants of z induce a matching.

Suppose that $T - N[x] \cong T_2(n-2)$. Since $T \not\cong T_i(n)$, $i = 1, 2$, and the descendants of z induce a matching, it is not difficult to see that $z \in \{a, b, c\}$, where a, b, and c are as indicated in Figure 3.

If $z = a$, it follows from Lemma 2.1 that

$$\begin{aligned} \text{mi}(T) &= \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\ &= t_2(n-2) + t_1(n-3) \\ &= \tfrac{5}{8}r^{n-1} + 2 \le \tfrac{3}{4}r^{n-1}. \end{aligned}$$

Equality holds if and only if $n = 9$ and $T \cong P_9$.

Suppose that $z = b$. Since $T \not\cong T_2(n)$, we have $n \ge 11$. It follows from Lemma 2.1 that

$$\begin{aligned} \text{mi}(T) &= \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\ &= t_2(n-2) + 2t_1(n-5) \\ &= \tfrac{5}{8}r^{n-1} + 3 < \tfrac{3}{4}r^{n-1}. \end{aligned}$$

If $z = c$, it follows from Lemma 2.1 that

$$\begin{aligned} \text{mi}(T) &= \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\ &= t_2(n-2) + \text{mi}(T - N[y] - N[e]) + \text{mi}(T - N[y] - N[d]) \\ &= \tfrac{3}{4}r^{n-3} + 1 + 3r^{n-9} + 2 \\ &= \tfrac{9}{16}r^{n-1} + 3 \le \tfrac{3}{4}r^{n-1}. \end{aligned}$$

Equality holds if and only if $n = 9$ and $T \cong P_9$.

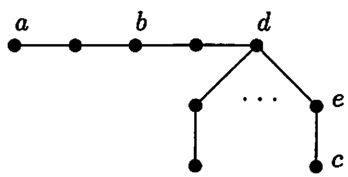

Figure 3: The tree $T - N[x] \cong T_2(n-2)$.

We now consider the case that $T - N[x] \not\cong T_i(n-2)$, $i = 1, 2$. Suppose that $d(z) = \frac{n-3}{2}$. Since all the descendants of z induce a matching, it follows from the definitions of z and r that $T \cong T_2(n)$ or $T_3(n)$. Thus we may assume that $d(z) \le \frac{n-5}{2}$. Since $T - N[y]$ consists of a matching of $d(z) - 2$ edges and a tree of order $n - 2d(z) + 1$, it now follows from the induction hypothesis that

$$\begin{aligned} \text{mi}(T) &= \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\ &\le t_3(n-2) + r^{2(d(z)-2)}t_1(n - 2d(z) + 1) \\ &= \tfrac{3}{4}r^{n-3} + r^{n-5} + r^{2d(z)-4} \\ &= \tfrac{5}{8}r^{n-1} + r^{2d(z)-4} \\ &\le \tfrac{5}{8}r^{n-1} + r^{n-9} < \tfrac{3}{4}r^{n-1}. \end{aligned}$$

Case 2. $n \equiv 0$ $(mod\ 2)$ and $n \ge 10$.

The case $n = 10$ can be proved in the similar way as follows, so here we only present the details of the case $n \geq 12$.

If $d(y) \geq 3$, then y has at least two leaf sons. Suppose that $T - x \cong T_1(n-1)$; then it follows from the structure of $T_1(n-1)$ that $T \cong T_2(n)$. Thus we may assume that $T - x \ncong T_1(n-1)$. It follows from the induction hypothesis and Lemma 2.3 that

$$\mathrm{mi}(T) = \mathrm{mi}(T - x) \leq t_2(n-1) = \frac{3}{4}r^{n-2} + 1 < \frac{7}{16}r^n + 2.$$

We now consider the case $d(y) = 2$. Suppose that $T - N[x] \cong T_1(n-2)$. Since $T \ncong T_i(n)$, $i = 1, 2$, it is not difficult to see that $z \in \{a, b, c, d, e\}$, where a, b, c, d, and e are as indicated in Figure 4.

Suppose that $z = a$; then it follows from $T \ncong T_1(n)$ that $d(u) \geq 3$, i.e., $d(v) \leq \frac{n}{2} - 3$. It follows from Lemma 2.1 that

$$\begin{aligned}
\mathrm{mi}(T) &= \mathrm{mi}(T - N[x]) + \mathrm{mi}(T - N[y]) \\
&= t_1(n-2) + \mathrm{mi}(T - N[y] - N[b]) + \mathrm{mi}(T - N[y] - N[u]) \\
&= t_1(n-2) + f(n-5) + r^{2(d(v)-1)} \\
&\leq \tfrac{7}{16}r^n + 1 < \tfrac{7}{16}r^n + 2.
\end{aligned}$$

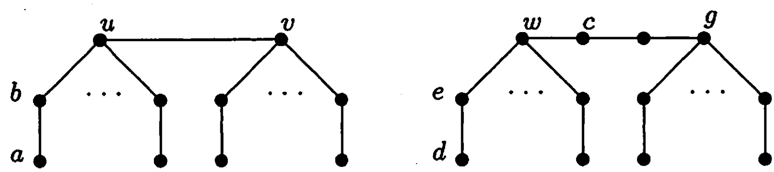

Figure 4: The tree $T - N[x] \cong T_1(n-2)$.

If $z = b$, it follows from Lemma 2.1 that

$$\begin{aligned}
\mathrm{mi}(T) &= \mathrm{mi}(T - N[a]) + \mathrm{mi}(T - N[b]) \\
&= 2t_1(n-4) + f(n-5) \\
&= \tfrac{3}{8}r^n + 2 < \tfrac{7}{16}r^n + 2.
\end{aligned}$$

Suppose that $z = c$; then it follows from $T \ncong T_1(n)$ that $d(g) \geq 2$. It follows from Lemma 2.1 that

$$\begin{aligned}
\mathrm{mi}(T) &= \mathrm{mi}(T - N[x]) + \mathrm{mi}(T - N[y]) \\
&= t_1(n-2) + r^{n-2d(g)-4}(r^{2(d(g)-1)} + 1) \\
&= r^{n-4} + 1 + r^{n-6} + r^{n-2d(g)-4} \\
&\leq \tfrac{7}{16}r^n + 1 < \tfrac{7}{16}r^n + 2.
\end{aligned}$$

If $z = d$ and $d(w) = 2$, then $T \cong T_3(n)$. Suppose that $z = d$ and

$d(w) \geq 3$; then it follows from Lemma 2.1 that

$$\begin{aligned} \mathrm{mi}(T) &= \mathrm{mi}(T - N[x]) + \mathrm{mi}(T - N[y]) \\ &= t_1(n-2) + \mathrm{mi}(T - N[y] - N[e]) + \mathrm{mi}(T - N[y] - N[w]) \\ &= t_1(n-2) + r^{2(d(w)-2)} r^{n-2d(w)-2} + r^{n-2d(w)-4} + 1 \\ &= r^{n-4} + 1 + r^{n-6} + r^{n-2d(g)-4} + 1 \\ &\leq \tfrac{13}{32} r^n + 2 < \tfrac{7}{16} r^n + 2. \end{aligned}$$

If $z = e$, then it follows from Lemma 2.1 that

$$\begin{aligned} \mathrm{mi}(T) &= \mathrm{mi}(T - N[d]) + \mathrm{mi}(T - N[e]) \\ &= \tfrac{3}{8} r^n + 2 < \tfrac{7}{16} r^n + 2. \end{aligned}$$

We now assume that $T - N[x] \not\cong T_1(n-2)$. If z has a leaf son w, then $d(z) \geq 3$ and x is isolated in $T - N[z]$. If z has the unique leaf son w, then all the descendants of z, other than w, induce a matching, and $T - N[z]$ is a forest of order $n - d(z) - 1$ which contains at least $d(z) - 2$ isolated vertices. Hence, it follows from Lemma 2.1 that

$$\begin{aligned} \mathrm{mi}(T) &= \mathrm{mi}(T - N[w]) + \mathrm{mi}(T - N[z]) \\ &\leq r^{2(d(z)-2)} t_1(n - 2d(z) + 2) + f(n - 2d(z) + 1) \\ &= r^{n-4} + r^{2d(z)-4} + r^{n-2d(z)} \\ &\leq r^{n-4} + r^2 + r^{n-6} < \tfrac{7}{16} r^n + 2. \end{aligned}$$

If z has at least two leaf sons, then it follows from the structure of $T_i(n-1)$ that $T - w \not\cong T_i(n-1)$, $i = 1, 2$. Hence, it follows from the induction hypothesis and Lemma 2.3 that

$$\mathrm{mi}(T) = \mathrm{mi}(T - w) \leq t_3(n-1) = \frac{3}{4} r^{n-2} < \frac{7}{16} r^n + 2.$$

We now assume that z has no leaf sons, i.e., all the descendants of z induce a matching. Suppose that $T - N[x] \cong T_2(n-2)$. Since $T \not\cong T_i(n)$, $i = 1, 2$, and all the descendants of z induce a matching, we may assume that $z \in \{a, d\}$, where a and d are as indicated in Figure 5.

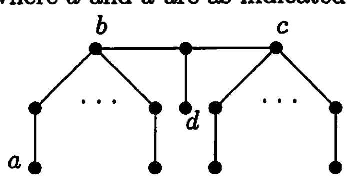

Figure 5: The tree $T - N[x] \cong T_2(n-2)$.

If $z = a$, then $T - N[y]$ is a tree of order $n - 3$ and $T - N[y] \not\cong T_i(n-3)$, $i = 1, 2$. It follows from the induction hypothesis that

$$\begin{aligned} \mathrm{mi}(T) &= \mathrm{mi}(T - N[x]) + \mathrm{mi}(T - N[y]) \\ &\leq t_2(n-2) + t_3(n-3) \\ &= \tfrac{7}{16} r^n < \tfrac{7}{16} r^n + 2. \end{aligned}$$

Suppose that $z = d$. Since $T \not\cong T_2(n)$, we have $d(b) \geq 2$ and $d(c) \geq 2$. Therefore $T - N[y]$ is a tree of order $n-3$ and $T - N[y] \not\cong T_1(n-3)$. It follows from the induction hypothesis that

$$\begin{aligned} \text{mi}(T) &= \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\ &\leq t_2(n-2) + t_2(n-3) \\ &= \tfrac{7}{16}r^n + 1 < \tfrac{7}{16}r^n + 2. \end{aligned}$$

We now consider the case $T - N[x] \not\cong T_i(n-2)$, $i = 1, 2$. Denote by T' the tree obtained from T by deleting z and all its descendants. Clearly, T' is a tree of order $n - 2d(z) + 1$. If $T' \not\cong T_i(n - 2d(z) + 1)$, $i = 1, 2$, it follows from the induction hypothesis that

$$\begin{aligned} \text{mi}(T) &= \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\ &\leq t_3(n-2) + r^{2(d(z)-2)} t_3(n - 2d(z) + 1) \\ &= \tfrac{13}{32}r^n + 2 < \tfrac{7}{16}r^n + 2. \end{aligned}$$

If $T' \cong T_1(n-2d(z)+1)$, it follows from the structure of $T_1(n-2d(z)+1)$ that $T \cong T_1(n)$ or $T \cong T_2(n)$.

If $T' \cong T_2(n-2d(z)+1)$, then the father of z must be one of the vertices a, b, c, d, e, f, or g indicated in Figure 6. We note for later use that it follows from the definition of $T_2(n - 2d(z) + 1)$ that $d(z) \leq \frac{n-6}{2}$.

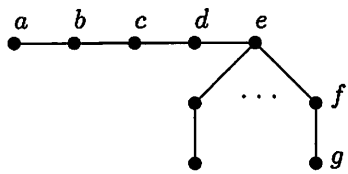

Figure 6: The tree $T' \cong T_2(n - 2d + 1)$.

Suppose that $az \in E(T)$. If $d(z) = 2$, then $T \cong T_3(n)$. Thus we may assume that $3 \leq d(z) \leq \frac{n-6}{2}$. Hence $T - N[x] \not\cong T_i(n-2)$, $i = 1, 2$, and $T - N[y]$ is a forest consisting of a matching of $d(z) - 2$ edges and a tree of order $n - 2d(z) + 1$ which is not isomorphic to $T_1(n - 2d(z) + 1)$. It follows from the induction hypothesis that

$$\begin{aligned} \text{mi}(T) &= \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\ &\leq t_3(n-2) + r^{2(d(z)-2)} t_2(n - 2d(z) + 1) \\ &= \tfrac{13}{32}r^{n-2} + 2 + r^{2d(z)-4} \leq \tfrac{7}{16}r^n + 2. \end{aligned}$$

Equality holds if and only if $T - N[x] \cong T_3(n-2)$ and $d(z) = \frac{n-6}{2}$, i.e., $T \cong T_3(n)$.

If $bz \in E(T)$, it follows from Lemma 2.1 that

$$\begin{aligned} \mathrm{mi}(T) &= \mathrm{mi}(T-N[a])+\mathrm{mi}(T-N[b]) \\ &= r^{2d(z)-2}r^{n-2d(z)-2}+r^{2d(z)-2}(r^{n-2d(z)-4}+1) \\ &= \tfrac{3}{8}r^n + r^{2d(z)-2} \\ &\le \tfrac{7}{16}r^n < \tfrac{7}{16}r^n+2. \end{aligned}$$

If $cz \in E(T)$, it follows from Lemma 2.1 that

$$\begin{aligned} \mathrm{mi}(T) &= \mathrm{mi}(T-N[a])+\mathrm{mi}(T-N[b]) \\ &= t_1(n-2)+r^{2d(z)-2}t_1(n-2d(z)-2) \\ &= \tfrac{3}{8}r^n + r^{2d(z)-2}+1 \\ &\le \tfrac{7}{16}r^n+1 < \tfrac{7}{16}r^n+2. \end{aligned}$$

Suppose that $dz \in E(T)$. Clearly, $T-N[a] \not\cong T_1(n-2)$ and $T-N[b] \not\cong T_1(n-3)$. It follows from the induction hypothesis that

$$\begin{aligned} \mathrm{mi}(T) &= \mathrm{mi}(T-N[a])+\mathrm{mi}(T-N[b]) \\ &\le t_2(n-2)+t_2(n-3) \\ &= \tfrac{7}{16}r^n+1 < \tfrac{7}{16}r^n+2. \end{aligned}$$

Suppose that $ez \in E(T)$. Clearly, $T-N[b] \not\cong T_i(n-3)$, $i=1,2$. It follows from the induction hypothesis that

$$\begin{aligned} \mathrm{mi}(T) &= \mathrm{mi}(T-N[a])+\mathrm{mi}(T-N[b]) \\ &\le t_1(n-2)+t_3(n-3) \\ &= \tfrac{7}{16}r^n+1 < \tfrac{7}{16}r^n+2. \end{aligned}$$

If $fz \in E(T)$, then $T-N[a] \cong T_2(n-2)$ and $T-N[b] \not\cong T_i(n-3)$, $i=1,2$. It follows from the induction hypothesis that

$$\begin{aligned} \mathrm{mi}(T) &= \mathrm{mi}(T-N[a])+\mathrm{mi}(T-N[b]) \\ &\le t_2(n-2)+t_3(n-3) \\ &= \tfrac{7}{16}r^n < \tfrac{7}{16}r^n+2. \end{aligned}$$

Suppose that $gz \in E(T)$. If $d(e)=2$, then $T \cong T_3(n)$. If $d(e)\ge 3$, then $T-N[b] \not\cong T_i(n-3)$, $i=1,2$. It follows from the induction hypothesis that

$$\begin{aligned} \mathrm{mi}(T) &= \mathrm{mi}(T-N[a])+\mathrm{mi}(T-N[b]) \\ &\le t_1(n-2)+t_3(n-3) \\ &= \tfrac{7}{16}r^n+1 < \tfrac{7}{16}r^n+2. \end{aligned}$$

This completes the proof. ∎

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