Trees with Large Maximal Independent Sets

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Abstract

In this paper, we determine the fourth and fifth largest number of maximal independent sets in trees. Also, the extremal trees achieving these value are determined.

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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. Denote by $m_i(G)$ the number of maximal independent sets in $G$.

Due to the important roles in designing algorithms of graph colorings, the enumeration of the maximal independent sets in graphs have been studied widely. Erdős and Moser raised the problem of determining the maximum value of $m_i(G)$ among all graphs of order $n$ and the extremal graphs achieving the maximum value. This problem was solved by Moon and Moser [14]. Later researchers focused on the problem for special classes of graphs, see [1,3-6,8-17]. For other related, including algorithmic, results on $m_i(G)$, see [2, 11]. In current days, a main direction is to consider the number of maximal independent sets in graphs with some constrained conditions. Usually, the extremal graphs with large number of maximal independent sets are useful in it, see [7, 8, 18].
In this paper, we determine the fourth and fifth largest number of maximal independent sets in trees. Also, the extremal trees achieving these values are determined.

2 Preliminary

Lemma 2.1 [6] For any vertex \( x \) in a graph \( G \),
(1) \( \text{mi}(G) \leq \text{mi}((G - x) + \text{mi}((G - N[x])) \);
(2) If \( x \) is a leaf adjacent to \( y \), then \( \text{mi}(G) = \text{mi}((G - N[x]) + \text{mi}((G - N[y])) \).

Lemma 2.2 [6] For any two vertex disjoint graphs \( G \) and \( H \), \( \text{mi}((G \cup H)) = \text{mi}((G)\text{mi}((H)). \)

Lemma 2.3 Let \( G \) be a graph of order \( n \). If \( G \) contains two leaves \( x \) and \( y \) such that \( N(x) = N(y) \), then \( \text{mi}(G) = \text{mi}(G - x) \).

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

Clearly,
\[
\text{mi}(T(n)) = t_1(n) = \begin{cases} 
r^{n-2} + 1, & n \equiv 0 \pmod{2}; \\
r^{n-1}, & n \equiv 1 \pmod{2}.
\end{cases}
\]

Theorem 2.4 [10, 17] If \( T \) is a tree of order \( n \), then \( \text{mi}(T) \leq t_1(n) \). Furthermore, the equality holds if and only if \( T \cong T_1(n) \).

Theorem 2.5 [9] If \( F \) is a forest of order \( n \), then
\[
\text{mi}(F) \leq f(n) = \begin{cases} 
r^n, & n \equiv 0 \pmod{2}; \\
r^{n-1}, & n \equiv 1 \pmod{2}.
\end{cases}
\]

Furthermore, the equality holds if and only if \( F \cong F(n) \), where
\[
F(n) = \begin{cases} 
\frac{n}{2}K_2, & n \equiv 0 \pmod{2}; \\
B(1, \frac{n-1-2s}{2}) \cup sK_2, & n \equiv 1 \pmod{2}.
\end{cases}
\]
Let \( T_2(n) \) denote the tree of order \( n \) defined as follows (see Figure 1): (1) For \( n \equiv 0 \pmod{2} \) 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 \( n \equiv 1 \pmod{2} \) 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

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

![Figure 1: The tree \( T_2(n) \).](image1)

Let \( T_3(n) \) denote the tree of order \( n \) defined as follows (see Figure 2): (1) For \( n \equiv 0 \pmod{2} \) 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

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

**Theorem 2.6** [8] let \( T \) be a tree of order \( n \). If \( T \nlessneq P_10, T_i(n), i = 1, 2, \) then \( \text{mi}(T) \leq t_3(n) \). Furthermore, the equality holds if and only if \( T \cong T_3(n) \) or \( T \cong P_9 \).

### 3 Main results

**Theorem 3.1** Let \( T \) be a tree of order \( n \). If \( T \nlessneq P_9, P_{10}, T_i(n), i = 1, 2, 3, \) then \( \text{mi}(T) \leq t_4(n) \), where

\[
t_4(n) = \begin{cases} 
\frac{7}{16}r^n + 1, & n \equiv 0 \pmod{2}; \\
\frac{3}{8}r^{n-1} + 3, & n \equiv 1 \pmod{2}.
\end{cases}
\]

Furthermore, the equality holds if and only if \( T \cong T_4(n) \), where \( T_4(n) \) is illustrated in Figure 3.

![Figure 3: The tree \( T_4(n) \)](image)

**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 11 vertices. Let \( n \geq 12 \) 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 at least three. We root \( T \) at \( r \) and let \( y \) and \( z \) denote the father and grandfather of the leaf \( x \). Suppose that \( T \) contains two leaves \( u \) and \( v \) which has the same neighbor. If \( T - u \cong T_1(n - 1) \), then from the construction of \( T_1(n - 1) \), we have \( T \cong T_2(n) \). So \( T - u \nlessneq T_1(n - 1) \), and then \( \text{mi}(T) = \text{mi}(T - u) \leq t_2(n - 1) = \frac{3}{4}r^{n-2} + 1 < \frac{7}{16}r^n + 1 \). So assume that \( T \) contains no any two leaves with the same neighbor, and clearly, \( d(y) = 2 \).
**Case 1.** \( n \equiv 0(\text{mod } 2) \).

If \( T - N[x] \cong T_1(n-2) \), see Figure 4, then \( z \in \{a, b, c, d, e\} \).

If \( z = a \), then since \( T(n) \not\cong T_1(n) \), we have \( d(u) \geq 3 \), i.e., \( d(v) \leq \frac{n-6}{2} \). Then

\[
\text{mi}(T) = \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\
= t_1(n-2) + \text{mi}(T - N[y] - N[b]) + \text{mi}(T - N[y] - N[u]) \\
\leq t_1(n-2) + f(n-5) + r^{2d(v)-2} \\
\leq r^{n-4} + (r^{n-6} + 1) + r^{n-8} \\
= \frac{7}{16}r^n + 1.
\]

It is to see that the equality holds if and only if \( d(u) = 3 \), i.e., \( T(n) \cong T_1(n) \).

If \( z = b, e \), then since \( T(n) \not\cong T_3(n) \), we have \( d(u) \geq 3 \). Then

\[
\text{mi}(T) = \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\
= t_1(n-2) + t_1(n-4) \\
= \frac{3}{8}r^n + 2 \\
< \frac{7}{16}r^n + 1.
\]

If \( z = c \), then since \( T(n) \not\cong T_1(n) \), we have \( d(w) \geq 2 \), i.e., \( d(g) \leq \frac{n-6}{2} \). Then,

\[
\text{mi}(T) = \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\
= t_1(n-2) + (r^{2(d(u)-2)} + 1)r^{2d(g)-2} \\
= r^{n-4} + 1 + r^{2d(u)+2d(g)-4} + r^{2d(g)-2} \\
\leq r^{n-4} + r^{n-6} + r^{n-8} + 1 \\
= \frac{7}{16}r^n + 1.
\]

The equality holds if and only if \( d(w) = 2 \) and \( d(g) = \frac{n-6}{2} \), i.e., \( T(n) \cong T_4(n) \).

If \( z = d \), then since \( T(n) \not\cong T_3(n) \), we have \( d(w) \geq 3 \), i.e., \( d(g) \leq \frac{n-8}{2} \). Then,

\[
\text{mi}(T) = \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\
\leq t_1(n-2) + \text{mi}(T - N[y] - N[c]) + \text{mi}(T - N[y] - N[w]) \\
= t_1(n-2) + r^{2d(u)-2}r^{2d(g)} + r^{2d(g)-2} + 1 \\
\leq r^{n-4} + 1 + r^{n-6} + r^{n-10} + 1 \\
= (\frac{1}{4} + \frac{1}{8} + \frac{1}{32})r^n + 2 \\
\leq \frac{7}{16}r^n + 1.
\]
The equality holds if and only if $d(w) = 3$, i.e., $d(g) = \frac{n - 8}{2}$, i.e., $T(n) \cong T_4(n)$.

Suppose that $T - N[x] \not\cong T_1(n - 2)$. If $z$ have a leaf son $w$, then $T - N[w]$ consists of a tree of order $n - 2d(z) + 2$ and a matching of $d(z) - 2$ edges and $T - N[z]$ consists of $d(z) - 2$ isolated vertices and a forest of order $n - 2d(z) + 1$.

So we have

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

So assume that $z$ has no leaf sons, i.e., all the descendants of $z$ induce a matching. If $T - N[x] \cong T_2(n - 2)$, since $T \not\cong T_i(n), i = 1, 2$, we have $z \in a, b, c$, see Figure 5.

Figure 5: The tree $T_2(n - 2)$

If $z = a$, then $mi(T) = t_2(n - 2) + r^{2d(c) - 4}r^{2d(d)} + r^{2d(d)} < r^{n - 4} + r^{n - 8} + r^{n - 6} < \frac{7}{16}r^n + 1$.

If $z = b$, since $T \not\cong T_i(n), i = 1, 2$, we have $d(c) \geq 2$ and $d(d) \geq 2$. Note that $T - N[y] \not\cong T_1(n - 3)$. Then

$$
mi(T) = mi(T - N[x]) + mi(T - N[y]) \\
\leq t_2(n - 2) + t_2(n - 3) \\
\leq \frac{7}{16}r^n + 1.
$$

The equality holds if and only if $d(c) \geq 2$ or $d(d) \geq 2$, i.e., $T(n) \cong T_4(n)$.

If $z = e$, we have $mi(T) = t_2(n - 2) + t_2(n - 4) = r^{n - 4} + r^{n - 6} = \frac{7}{16}r^n < \frac{7}{16}r^n + 1$.

So assume that $T - N[x] \not\cong T_i(n - 2), i = 1, 2$, and $z$ has no any leaf sons. Denote by $T'$ the tree obtained from $T$ by deleting $z$ and its descendants. Clearly, $T'$ is a tree of order $n - 2d(z) + 1$. If $T' \cong T_1(n - 2d(z) + 1)$, from the structure of $T_1(n - 2d(z) + 1)$, we have $T \cong T_1(n)$ or $T \cong T_2(n)$. So
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Let \( T \not\cong T_1(n - 2d(z) + 1) \). Let \( d(z) \leq \frac{n-8}{2} \). If \( n \geq 14 \), then,

\[
\text{mi}(T) = \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\
\leq t_3(n - 2) + r^{2d(z)-4}t_2(n - 2d(z) + 1) \\
= \frac{7}{32}r^n + 2 + r^{2d(z)-4}(\frac{3}{4}r^{n-2d(z)} + 1) \\
= \frac{7}{32}r^n + 2 + \frac{3}{16}r^n + r^{2d(z)-4} \\
\leq \frac{7}{32}r^n + 2 + \frac{3}{16}r^n + r^{n-12} \\
< \frac{7}{16}r^n + 1.
\]

If \( n = 12 \), then,

\[
\text{mi}(T) = \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\
\leq t_3(n - 2) + r^{2d(z)-4}t_2(n - 2d(z) + 1) \\
= \frac{7}{32}r^n + 1 + r^{2d(z)-4}(\frac{3}{4}r^{n-2d(z)} + 1) \\
= \frac{7}{32}r^n + 1 + \frac{3}{16}r^n + r^{2d(z)-4} \\
\leq \frac{7}{32}r^n + 1 + \frac{3}{16}r^n + r^{n-12} \\
< \frac{7}{16}r^n + 1.
\]

So let \( d(z) \geq \frac{n-6}{2} \). By the symmetry of \( r \) and \( x \), when we root the tree in \( x \), we may assume that the grandfather of \( r \), denoted by \( z' \), has degree at least \( \frac{n-6}{2} \) and \( z' \) has no any leaf sons. Clearly, \( z \neq z' \). Let \( D_r(z) \) denote the set of all the descendants of \( z \) when \( T \) is rooted in \( r \) and \( D_x(z') \) denote the set of all the descendants of \( z' \) when \( T \) is rooted in \( x \). It is easy to see that \( D_r(z) \cap D_x(z') = \emptyset \). So \( n > |D_x(z)| + |D_x(z')| + 2 \geq 2n - 14 \), i.e., \( n = 12 \). Since \( d(z), d(z') \geq 3 \) and both \( D_r(z) \) and \( D_x(z') \) induce a matching, it must hold that \( T \cong T_i(n) \) for \( i = 1 \) or \( 2 \).

**Case 2.** \( n \equiv 1(\text{mod } 2) \)

Suppose that \( T - N[x] \cong T_1(n - 2) \). Since \( T \not\cong T_1(n) \), we have \( z \in \{a, b\} \), where \( a \) and \( c \) are illustrated in Figure 6. If \( z = a \), we have \( T \cong T_2(n) \), a contradiction. If \( z = b \), we have \( T \cong T_3(n) \), a contradiction. So \( T - N[x] \not\cong T_1(n - 2) \). If \( z \) have a leaf \( w \), then we have

\[
T - N[x] \cong T_1(n - 2) \quad T - N[x] \cong T_2(n - 2)
\]

Figure 6: The tree \( T_1(n - 2) \)  Figure 7: The tree \( T_2(n - 2) \)
\[
\text{mi}(T) = \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\
\leq t_2(n - 2) + f(n - 4) \\
= \frac{3}{4}r^{n-3} + 1 + r^{n-5} \\
= \frac{9}{8}r^{n-1} + 1 \\
< \frac{9}{8}r^{n-1} + 3.
\]

Suppose that \( z \) has no any leaf sons, i.e., all the descendants of \( z \) induce a matching. If \( T - N[x] \cong T_2(n - 2) \), see Figure 7, we may assume that \( z \in \{a, b, c, d, f, g\} \). Using Lemma 2.1, we have the followings results:

- If \( z = a \), then \( \text{mi}(T) = \frac{3}{8}r^{n-1} + 2 < \frac{5}{8}r^{n-1} + 3 \).
- If \( z = b \), then \( \text{mi}(T) = \frac{3}{8}r^{n-1} + 1 < \frac{5}{8}r^{n-1} + 3 \).
- If \( z = c \), then \( T \cong T_4(n) \) and \( \text{mi}(T) = \frac{5}{8}r^{n-1} + 3 \).
- If \( z = d \), then \( \text{mi}(T) = \frac{5}{8}r^{n-1} + 1 < \frac{5}{8}r^{n-1} + 3 \).
- If \( z = f \), then \( \text{mi}(T) = \frac{9}{16}r^{n-1} + 2 < \frac{5}{8}r^{n-1} + 3 \).
- If \( z = g \), then \( \text{mi}(T) = \frac{9}{16}r^{n-1} + 3 < \frac{5}{8}r^{n-1} + 3 \).

Suppose that \( T - N[x] \cong T_3(n - 2) \). Without loss of generality, we may assume that \( z \in \{a, b, d, e, f, g\} \), see Figure 8.

- If \( z = a \), then \( \text{mi}(T) = \frac{3}{8}r^{n-1} + \frac{3}{8}r^{n-1} + 2 = \frac{9}{16}r^{n-1} + 2 < \frac{5}{8}r^{n-1} + 3 \).
- If \( z = b \), then \( \text{mi}(T) = \frac{3}{8}r^{n-1} + \frac{1}{16}r^{n-1} = \frac{9}{16}r^{n-1} < \frac{5}{8}r^{n-1} + 3 \).
- If \( z = d, e, f \), then \( \text{mi}(T) = \frac{3}{8}r^{n-1} + \frac{1}{8}r^{n-1} = \frac{5}{8}r^{n-1} < \frac{5}{8}r^{n-1} + 3 \).
- If \( z = g \), then \( \text{mi}(T) = \frac{3}{8}r^{n-1} + \frac{3}{8}r^{n-1} = \frac{5}{8}r^{n-1} + 1 < \frac{5}{8}r^{n-1} + 3 \).

Suppose that \( T - N[x] \not\cong T_i(n - 2), i = 1, 2, 3 \). If \( d(z) \leq \frac{n-5}{2} \), then by induction we have

\[
\text{mi}(T) = \text{mi}(T - N[x]) + \text{mi}(T - N[y]) \\
\leq t_4(n - 2) + t_1(n - 2d(z) + 1)r^{2d(z)-4} \\
= \frac{5}{8}r^{n-3} + (r^{n-2d(z)-1} + 1)r^{2d(z)-4} \\
= \frac{5}{16}r^{n-1} + r^{n-5} + r^{2d(z)-4} \\
\leq \frac{5}{16}r^{n-1} + r^{n-5} + r^{n-9} \\
< \frac{5}{8}r^{n-1} + 3.
\]

So let \( d(z) \geq \frac{n-3}{2} \). Since \( z \) has no any leaf sons and \( T \not\cong T(n) \), it must hold that \( d(z) = \frac{n-3}{2} \). By the similar analysis of the last sentence of Case 1, we can prove the result. This completes the proof.

In the similar way, we can prove the following result. Here we omit the details of proof.

**Theorem 3.2** Let \( T \) be a tree of order \( n \geq 11 \). If \( T \not\cong T_i(n), i = 1, 2, 3, 4, \ldots \),
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Figure 8: The tree $T_3(n)$  
Figure 9: The tree $T_5(n)$

then $mi(T) \leq t_5(n)$, where

$$t_5(n) = \begin{cases} 
\frac{7}{16}r^n, & n \equiv 0 \pmod{2} \\
\frac{9}{8}r^{n-1} + 2, & n \equiv 1 \pmod{2} 
\end{cases}$$

Furthermore, the equality holds if and only if $T \cong T_5(n)$, where $T_5(n)$ is illustrated in Figure 9.

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