# Trees with the second and third largest number of maximum independent sets

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#### **Abstract**

An independent set in a graph G is a subset I of the vertices such that no two vertices in I are adjacent. We say that I is a maximum independent set in G if no other independent set is larger than I. In this paper, we study the problem of determining the second and third largest number of maximum independent sets among all trees and forests. Extremal graphs achieving these values are also given.

### 1 Introduction

For a simple undirected graph G = (V, E), a subset I of V(G) is said to be an *independent set* of G if there is no edge of G between any two vertices of I. 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. The set of all maximum independent sets (respectively, maximal independent sets) of a graph G is denoted by XI(G) (respectively, MI(G)) and its cardinality by xi(G) (respectively, mi(G)).

The problem of determining the largest value of mi(G) in a general graph G of order n and those graphs achieving the largest number was proposed by Erdős and Moser, and solved by Moon and Moser [6]. It was then extensively studied for various classes of graphs in the literature, including trees, forests, (connected) graphs with at most one cycle, bipartite graphs, connected graphs, k-connected graphs, (connected) triangle-free graphs; for a survey see [3]. Later, Jin and Li [1] determined the second largest number of maximal independent sets among all graphs of order n. As for trees and forests, it was solved by Jou and Lin [5].

Compared to mi(G), there are fewer results about counting xi(G). The problem of determining the largest number of maximum independent sets among all trees of order n was first solved by Zito [8]. Later, Jou and Chang [4] gave an alternative proof for the solution to the same problem and further explored the problem for various classes of graphs, including general graphs, trees, forests, (connected) graphs with at most one cycle, connected graphs and triangle-free graphs. Recently, Sagan and Vatter [7] settled the problem for the family of graphs with at most r cycles.

The purpose of this paper is to determine the second and third largest number of maximum independent sets among all trees and forests. Extremal graphs achieving these values are also given.

## 2 Preliminary

For our discussions, some terminology and notation are needed. For a graph G = (V, E), the cardinality of V(G) is called the *order*, and it is denoted by |G|. The neighborhood  $N_G(x)$  of a vertex  $x \in V(G)$ is the set of vertices adjacent to x in G and the closed neighborhood  $N_G[x]$  is  $\{x\} \cup N_G(x)$ . Two distinct vertices u and v are called duplicated vertices if  $N_G(u) = N_G(v)$ . The degree of x is the number of edges that are incident with x in G, denoted by  $\deg_G(x)$ . A vertex x is a leaf if  $\deg_{G}(x) = 1$ . A vertex is called a support vertex if it is adjacent to a leaf. For a set  $A \subseteq V(G)$ , the deletion of A from G is the graph G-A obtained from G by removing all vertices in A and their incident edges. Two graphs  $G_1$  and  $G_2$  are disjoint if  $V(G_1) \cap V(G_2) = \emptyset$ . The union of two disjoint graphs  $G_1$  and  $G_2$ is the graph  $G_1 \cup G_2$  with vertex set  $V(G_1 \cup G_2) = V(G_1) \cup V(G_2)$ and edge set  $E(G_1 \cup G_2) = E(G_1) \cup E(G_2)$ . Let nG be the short notation for the union of n copies of disjoint graphs isomorphic to G. A component of odd (respectively, even) order is called an odd (respectively, even) component. Denote by  $P_n$  a path with n vertices.

Throughout this paper, for simplicity, let  $r = \sqrt{2}$ .

**Lemma 2.1.** ([2], [5]) If x is a leaf adjacent to y in a graph G, then (1)  $xi(G) \leq xi(G - N_G[x]) + xi(G - N_G[y])$ .

$$(2) xi(G) \leq 2xi(G - N_G[x]).$$

**Lemma 2.2.** ([2], [5]) If  $x_1, x_2, \ldots, x_k$  are  $k \geq 2$  leaves adjacent to the same vertex y in a graph G, then  $xi(G) = xi(G - \{x_1, x_2, \ldots, x_k, y\})$ .

**Lemma 2.3.** ([2], [5]) If G is the union of two disjoint graphs  $G_1$  and  $G_2$ , then  $xi(G) = xi(G_1) \cdot xi(G_2)$ .

**Lemma 2.4.** ([2]) For any graph G,  $XI(G) \subseteq MI(G)$  and  $xi(G) \le mi(G)$ . Moreover, xi(G) = mi(G) if and only if XI(G) = MI(G).

The results of the largest numbers of maximum independent sets among all trees and forests are described in Theorems 2.5 and 2.6, respectively.

**Theorem 2.5.** ([2], [5]) If T is a tree with  $n \geq 2$  vertices, then

$$xi(T) \le t'(n) = \left\{ egin{array}{ll} r^{n-2} + 1, & \mbox{if $n$ is even}; \\ r^{n-3}, & \mbox{if $n$ is odd.} \end{array} 
ight.$$

Furthermore, xi(T) = t'(n) if and only if T = T'(n), where T'(n) is shown in Figure 1.

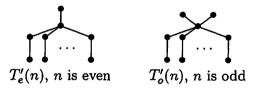


Figure 1: The graph T'(n)

**Theorem 2.6.** ([2], [5]) If F is a forest with  $n \ge 1$  vertices, then

$$xi(F) \le f'(n) = \begin{cases} r^n, & \text{if } n \text{ is even}; \\ r^{n-1}, & \text{if } n \text{ is odd}. \end{cases}$$

Furthermore, xi(F) = f'(n) if and only if F = F'(n), where

$$F'(n) = \left\{ \begin{array}{ll} \frac{n}{2}P_2, & \text{if } n \text{ is even}; \\ P_1 \cup \frac{n-1}{2}P_2, & \text{if } n \text{ is odd}. \end{array} \right.$$

The result of the second largest number of maximal independent sets among all forests of even order is described in Theorems 2.7.

**Theorem 2.7.** ([4]) If F is a forest of even order  $n \geq 4$  having  $F \neq \frac{n}{2}P_2$ , then  $mi(F) \leq 3r^{n-4}$ . Furthermore, the equality holds if and only if  $F = P_4 \cup \frac{n-4}{2}P_2$ .

## 3 Main results

In this section, we will prove the following two results.

**Theorem 3.1.** If F is a forest with  $n \ge 4$  vertices having  $F \ne F'(n)$ , then  $xi(F) \le f''(n)$ , where

$$f''(n) = \begin{cases} 3r^{n-4}, & \text{if } n \ge 4 \text{ is even}; \\ 3r^{n-5}, & \text{if } n \ge 5 \text{ is odd.} \end{cases}$$

Furthermore, xi(F) = f''(n) if and only if F = F''(n), where

$$F''(n)=\left\{\begin{array}{ll} P_4\cup\frac{n-4}{2}P_2, & \text{if } n\geq 4 \text{ is even};\\ P_1\cup P_4\cup\frac{n-5}{2}P_2, & \text{if } n\geq 5 \text{ is odd}. \end{array}\right.$$

**Theorem 3.2.** If T is a tree with  $n \ge 7$  vertices having  $T \ne T'(n)$ , then  $xi(T) \le t''(n)$ , where

$$t''(n) = \left\{ \begin{array}{ll} 3r^{n-7}, & \mbox{if } n \geq 7 \mbox{ is odd}; \\ 3r^{n-6} + 2, & \mbox{if } n \geq 8 \mbox{ is even}. \end{array} \right.$$

Furthermore, xi(T) = t''(n) if and only if T = T''(n), where T''(n) is shown in Figure 2.

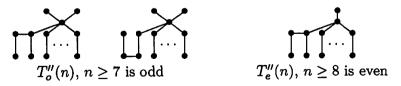


Figure 2: The graph T''(n)

We prove Theorems 3.1 and 3.2 by establishing the following four lemmas.

**Lemma 3.3.** If F is a forest of even order  $n \geq 4$  vertices having  $F \neq F'(n)$ , then  $xi(F) \leq 3r^{n-4}$  with the equality holding if and only if  $F = P_4 \cup \frac{n-4}{2}P_2$ .

*Proof.* Note that an independent set of  $P_4 \cup \frac{n-4}{2}P_2$  is maximal if and only if it is maximum, that is,  $XI(P_4 \cup \frac{n-4}{2}P_2) = MI(P_4 \cup \frac{n-4}{2}P_2)$ . By Lemma 2.4 and Theorem 2.7, we have the desired conclusion.  $\square$ 

**Lemma 3.4.** If F is a forest of odd order  $n \geq 5$  vertices having  $F \neq F'(n)$ , then  $xi(F) \leq 3r^{n-5}$  with the equality holding if and only if  $F = P_1 \cup P_4 \cup \frac{n-5}{2}P_2$ .

Proof. It is straightforward to check that  $xi(P_1 \cup P_4 \cup \frac{n-5}{2}P_2) = 3r^{n-5}$ . Let F be a forest of odd order  $n \geq 5$  having  $F \neq F'(n)$  such that xi(F) is as large as possible. Then  $xi(F) \geq 3r^{n-5}$ . Since F is a forest of odd order, there exists an odd component, say H. Suppose that  $|H| = m \geq 3$ , by Lemma 2.3, Theorems 2.5 and 2.6,  $3r^{n-5} \leq xi(F) = xi(H) \cdot xi(F - V(H)) \leq r^{m-3} \cdot r^{n-m} = r^{n-3}$ , which is a contradiction. It follows that  $H = P_1$ . Since  $F \neq F(n)$ , by Lemma 3.3, we can see that  $F - V(H) = P_4 \cup \frac{n-5}{2}P_2$ . In conclusion,  $F = P_1 \cup P_4 \cup \frac{n-5}{2}P_2$ .

**Lemma 3.5.** If T is a tree of odd order  $n \geq 7$  having  $T \neq T'(n)$ , then  $xi(T) \leq 3r^{n-7}$  with the equality holding if and only if  $T = T''_o(n)$ .

Proof. It is straightforward to check that  $xi(T_0''(n)) = 3r^{n-7}$ . Let T be a tree of odd order  $n \geq 7$  having  $T \neq T'(n)$  such that xi(T) is as large as possible. Then  $xi(T) \geq 3r^{n-7}$ . Suppose that T has duplicated leaves  $x_1, x_2, x_3, \ldots, x_k$   $(k \geq 3)$  which are adjacent to the same vertex y, by Lemma 2.2 and Theorem 2.6,  $3r^{n-7} \leq xi(T) = xi(T - \{x_1, x_2, \ldots, x_k, y\}) \leq \max\{f'(n-4), f'(n-5)\} = r^{n-5}$ , which is a contradiction. On the other hand, suppose that there exist duplicated leaves  $x_1$  and  $x_2$  which are adjacent to the same vertex  $y_1$ , and duplicated leaves  $x_3$  and  $x_4$  which are adjacent to the same vertex  $y_2$ , by Lemma 2.2 and Theorem 2.6 again, we have that  $3r^{n-7} \leq xi(T) = xi(T - \{x_1, x_2, y_1\}) = xi(T - \{x_1, x_2, y_1\} - \{x_3, x_4, y_2\}) \leq f'(n-6) = r^{n-7}$ , which is a contradiction. Thus T contains at most one pair duplicated leaves.

We claim that the result is true for n=7. Since T contains at most one pair duplicated leaves, there are six possibilities for T. See Figure 3. Note that  $T_7^{(1)} = T''(7)$ ,  $T_7^{(4)} = T''(7)$  and  $T_7^{(2)} = T'(7)$ . On the other hand, by simple calculation, we have  $xi(T_7^{(i)}) < 3$  for i=3,5,6, a contradiction to  $xi(T) \ge 3r^{n-7} = 3$ .

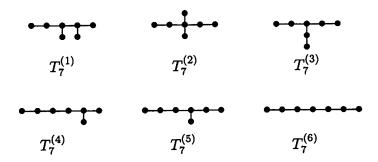


Figure 3: The graphs  $T_7^{(i)}$  (i = 1, 2, 3, 4, 5, 6)

Let n=2k+1. We prove the result by induction on  $k \geq 3$ . The result is true for k=3. Assume that it is true for all k' < k. Let x be a leaf lying on a longest path P of T, say  $P=x,y,z,\ldots$ . Since T contains at most one pair duplicated leaves, we assume that  $T-N_T[x]$  is a tree of odd order n-2. Suppose that T has no duplicated leaf, there are three cases depending on the structure of  $T-N_T[x]$ .

Case 1.  $T - N_T[x] = T'(n-2)$ .

The only possible graph with this property is the graph  $T^*(n)$  shown in Figure 4. By simple calculation, we have  $xi(T^*(n)) = r^{n-5}$ , a contradiction to  $xi(T) \geq 3r^{n-7}$ .

Case 2.  $T - N_T[x] = T''(n-2)$ .

The possible graphs with this property are the graphs  $T^{**}(n)$  shown in Figure 4. By simple calculation, we have  $xi(T^{**}(n)) = 3r^{n-9}$ , a contradiction to  $xi(T) \geq 3r^{n-7}$ .

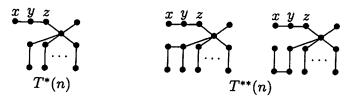


Figure 4: The graphs  $T^*(n)$  and  $T^{**}(n)$ 

Case 3.  $T - N_T[x] \neq T'(n-2)$  and  $T - N_T[x] \neq T''(n-2)$ .

By induction hypothesis and Lemma 2.1 (2),  $3r^{n-7} \le xi(T) \le 2xi(T - N_T[x]) < 2t''(n-2) = 3r^{n-7}$ , which is a contradiction.

From the above arguments, we have that there exists exactly one pair duplicated leaves in T, say  $v_1$  and  $v_2$ , which are adjacent to the same vertex u. Since  $T \neq T'(n)$ , then  $T - \{v_1, v_2, u\} \neq F'(n-3)$ . By Lemmas 2.2 and 3.3, we have that  $3r^{n-7} \leq xi(T) = xi(T - \{v_1, v_2, u\}) \leq f''(n-3) = 3r^{n-7}$ , the equalities holding imply that  $T - \{v_1, v_2, u\} = F''(n-3)$ . Hence we obtain that  $T = T''_o(n)$ .  $\square$ 

**Lemma 3.6.** If T is a tree of even order  $n \ge 8$  having  $T \ne T'(n)$ , then  $xi(T) \le 3r^{n-6} + 2$  with the equality holding if and only if  $T = T''_e(n)$ .

*Proof.* It is straightforward to check that  $xi(T_e''(n)) = 3r^{n-6} + 2$ . Let T be a tree of even order  $n \geq 8$  having  $T \neq T'(n)$  such that xi(T) is as large as possible. Then  $xi(T) \geq 3r^{n-6} + 2$ . Suppose that T has duplicated leaves  $x_1, x_2, x_3, \ldots, x_k$   $(k \geq 2)$  which are adjacent to the same vertex y, by Lemma 2.2 and Theorem 2.6,  $3r^{n-6} + 2 \leq xi(T) = xi(T - \{x_1, x_2, \ldots, x_k, y\}) \leq \max\{f'(n-3), f'(n-4)\} = r^{n-4}$ . This is a contradiction, thus T has no duplicated leaf.

We claim that the result is true for n=8. Since T has no duplicated leaf, there are six possibilities for T. See Figure 5. Note that  $T_8^{(1)} = T'(8)$  and  $T_8^{(2)} = T''(8)$ . On the other hand, by simple calculation, we have  $xi(T_8^{(i)}) < 8$  for i=3,4,5,6, a contradiction to  $xi(T) \ge 3r^{n-6} + 2 = 8$ .

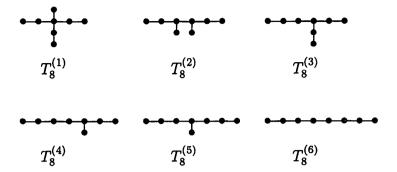


Figure 5: The graphs  $T_8^{(i)}$  (i = 1, 2, 3, 4, 5, 6)

Let n=2k. We prove the result by induction on  $k \geq 4$ . The result is true for k=4. Assume that it is true for all k' < k. Let x be a leaf lying on a longest path P of T, say  $P=x,y,z,\ldots$  Then  $T-N_T[x]$  is a tree of even order n-2. By Theorem 2.5, we have that  $xi(T-N_T[x]) \leq t'(n-2) = r^{n-4} + 1$ . Let H be the component of  $T-N_T[y]$  containing  $P-N_T[y]$ . Since P is a longest path of T, it follows that  $|H| \geq 2$  and every component of  $T-(N_T[y] \cup V(H))$  is  $P_1$  or  $P_2$ , see Figure 6.

So we have that  $T - N_T[y] = aP_1 \cup bP_2 \cup H$ . Since T has no duplicated leaves, it follows that a = 0 or 1. Suppose that a = 0. Then H is a tree of odd order n - 3 - 2b > 3. By Theorem 2.5,

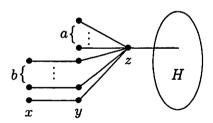


Figure 6: The tree T

 $xi(H) \le r^{n-6-2b}$ . By Lemma 2.3,  $xi(T - N_T[y]) \le r^{2b} \cdot r^{n-6-2b} = r^{n-6}$ . Hence, by Lemma 2.1 (1), we have

$$r^{n-4} + 1 = t'(n-2)$$

$$\geq xi(T - N_T[x])$$

$$\geq xi(T) - xi(T - N_T[y])$$

$$\geq (3r^{n-6} + 2) - r^{n-6}$$

$$= 2r^{n-6} + 2.$$

which is a contradiction. Hence we obtain that a = 1. There are two cases depending on the structure of  $T - N_T[x]$ .

Case 1. 
$$T - N_T[x] = T'(n-2)$$
.

Since a=1, it follows that z is a support vertex of  $T-N_T[x]$ . Note that  $T\neq T'(n)$ . Thus we obtain that  $T=T''_e(n)$ .

Case 2. 
$$T - N_T[x] \neq T'(n-2)$$
.

By induction hypothesis,  $xi(T - N_T[x]) \le 3r^{n-8} + 2$ . Since  $T \ne T'(n)$ , we can see that  $|H| = n - 4 - 2b \ge 4$  is even. It follows that  $b \le \frac{n-8}{2}$  and  $xi(H) \le r^{n-6-2b} + 1$ . By Lemmas 2.1 (1), 2.3 and Theorem 2.5, we have that

$$3r^{n-8} \ge r^{2b} \cdot (r^{n-6-2b} + 1)$$

$$\ge r^{2b} \cdot xi(H)$$

$$= xi(T - N_T[y])$$

$$\ge xi(T) - xi(T - N_T[x])$$

$$\ge (3r^{n-6} + 2) - (3r^{n-8} + 2)$$

$$= 3r^{n-8}$$

Hence the equalities holding imply that b = (n-8)/2,  $T - N_T[x] = T''(n-2)$  and  $H = P_4$ . This means that  $T = T''_e(n)$ .

Theorems 3.1 and 3.2 now follow from Lemmas 3.3, 3.4, 3.5 and 3.6.

In a similar manner as above, we will obtain the results of the third numbers of maximum independent sets among all forests and trees in Theorems 3.7 and 3.8, respectively. Here we omit the details of proof.

**Theorem 3.7.** If F is a forest with  $n \ge 6$  vertices having  $F \ne F'(n), F''(n)$ , then  $xi(F) \le f'''(n)$ , where

$$f'''(n) = \begin{cases} 5r^{n-6}, & \text{if } n \ge 6 \text{ is even}; \\ 5r^{n-7}, & \text{if } n \ge 7 \text{ is odd.} \end{cases}$$

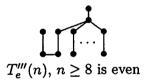
Furthermore, xi(T) = f'''(n) if and only if F = F'''(n), where

$$F'''(n) = \begin{cases} T'(6) \cup \frac{n-6}{2} P_2, & \text{if } n \ge 6 \text{ is even}; \\ P_1 \cup T'(6) \cup \frac{n-5}{2} P_2, & \text{if } n \ge 7 \text{ is odd.} \end{cases}$$

**Theorem 3.8.** If T is a tree with  $n \ge 8$  vertices having  $T \ne T'(n), T''(n)$ , then  $xi(T) \le t'''(n)$ , where

$$t'''(n) = \begin{cases} 3r^{n-6} + 1, & \text{if } n \ge 8 \text{ is even}; \\ 5r^{n-9}, & \text{if } n \ge 9 \text{ is odd}. \end{cases}$$

Furthermore, xi(T) = t'''(n) if and only if T = T'''(n), where T'''(n) is shown in Figure 7.



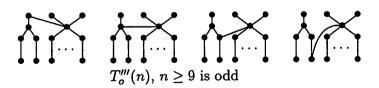


Figure 7: The graph T'''(n)

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