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## Maximal independent sets in graphs with at most one cycle<sup>☆</sup>

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### Abstract

In this paper, we determine the largest number of maximal independent sets among all connected graphs of order  $n$ , which contain at most one cycle. We also characterize those extremal graphs achieving this maximum value. As a consequence, the corresponding results for graphs with at most one cycle but not necessarily connected are also given.

*Keywords:* (Maximal) independent set; Cycle; Connected graph; Isolated vertex; Leaf; Baton

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### 1. Introduction

In a graph  $G = (V, E)$ , an *independent set* is a subset  $S$  of  $V$  such that no two vertices in  $S$  are adjacent. A *maximal independent set* is an independent set that is not a proper subset of any other independent set. The number of maximal independent sets of  $G$  is denoted by  $\text{mi}(G)$ .

The problem of determining the maximum value of  $\text{mi}(G)$  in a general graph of order  $n$  and those graphs achieving the maximum value was proposed by Erdős and Moser, and solved by Moon and Moser [7]. The problem was independently solved by Füredi [1] and Griggs et al. [3] for connected graphs; for triangle-free graphs by Hujter and Tuza [4]; for bipartite graphs by Liu [6]; for trees independently by Wilf [9], Sagan [8], Griggs and Grinstead [2], and Jou [5]. Sagan's solution for trees uses an induction from a vertex whose neighbors are all leaves except possibly one. Jou's method is to get the solution for forests and then use this to prove the results for trees.

The main purpose of this paper is to study the problem for connected graphs with at most one cycle. We first give alternative proofs for the solutions to the problem in trees and forests by a method combining the ideas in Sagan's and Jou's papers. The idea then is used to solve the problem for connected graphs with at most one

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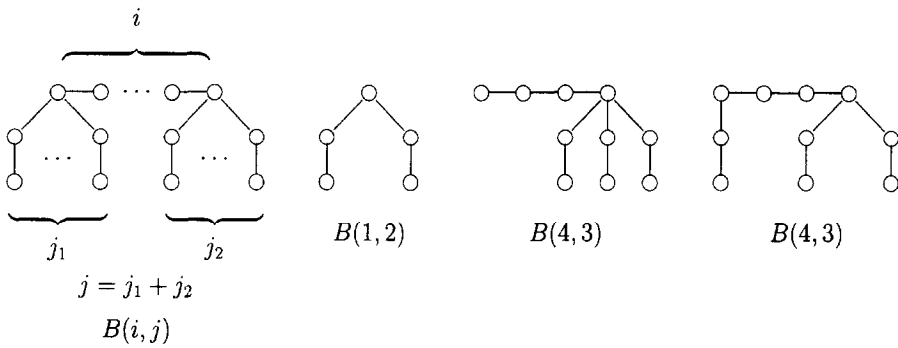


Fig. 1. Batons.

cycle. The corresponding results for graphs with at most one cycle, but not necessarily connected, are also obtained.

## 2. Trees and forests

This section gives an alternative proof for the solution to the problem of determining the maximum value  $t(n)$  (respectively,  $f(n)$ ) of  $mi(G)$  for a tree (respectively, forest) of order  $n$  and those trees (respectively, forests) achieving this maximum value.

The *neighborhood*  $N(x)$  of a vertex  $x$  is the set of vertices adjacent to  $x$  and the *closed neighborhood*  $N[x]$  is  $\{x\} \cup N(x)$ . A vertex  $x$  is an *isolated vertex* if  $N(x) = \emptyset$  and a *leaf* if  $|N(x)| = 1$ . For a graph  $G = (V, E)$  and  $S \subseteq V$ , the *deletion* of  $S$  from  $G$  is the graph  $G - S$  obtained from  $G$  by removing all vertices in  $S$  and all edges incident to these vertices. We use  $C_n$  to denote the cycle with  $n$  vertices.

**Lemma 1** (Hujter and Tuza [4] and Jou [5]). *If  $G$  is a graph in which  $x$  is adjacent to exactly one vertex  $y$ , then  $mi(G) = mi(G - N[x]) + mi(G - N[y])$ .*

**Lemma 2** (Füredi [1]). *If  $n \geq 6$ , then  $mi(C_n) = mi(C_{n-2}) + mi(C_{n-3})$ .*

**Lemma 3** (Hujter and Tuza [4] and Jou [5]). *If  $G$  is the disjoint union of two graphs  $G_1$  and  $G_2$ , then  $mi(G) = mi(G_1)mi(G_2)$ .*

For simplicity, let  $r = \sqrt{2}$ . For  $i, j \geq 0$ , 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 endpoints of  $P$ ; see Fig. 1. Note that  $B(i, j)$  is a tree with  $i + 2j$  vertices.

**Lemma 4.** *For any  $j \geq 0$ ,  $mi(B(1, j)) = 2^j$ ,  $mi(B(2, j)) = 2^j + 1$  and  $mi(B(4, j)) = 2^{j+1} + 1$ .*

**Proof.** The lemma follows from repeatedly applying Lemma 1 to the leaves of the batons.  $\square$

We now give an alternative proof for the solution to the problem in trees.

**Theorem 5** (Wilf [9], Griggs and Grinstead [2], Sagan [8] and Jou [5]). *If  $T$  is a tree with  $n \geq 1$  vertices, then  $mi(T) \leq t(n)$ , where*

$$t(n) = \begin{cases} r^{n-2} + 1 & \text{if } n \text{ is even,} \\ r^{n-1} & \text{if } n \text{ is odd.} \end{cases}$$

Furthermore,  $mi(T) = t(n)$  if and only if  $T \cong T(n)$ , where

$$T(n) = \begin{cases} B(2, \frac{n-2}{2}) \text{ or } B(4, \frac{n-4}{2}) & \text{if } n \text{ is even,} \\ B(1, \frac{n-1}{2}) & \text{if } n \text{ is odd.} \end{cases}$$

**Proof.** First, note that  $mi(T(n)) = t(n)$  by Lemma 4. We shall prove the theorem by induction on  $n$ . The theorem is obviously true for  $n \leq 3$ . Assume that it is true for all  $n' < n$ . Suppose  $T$  is a tree of order  $n \geq 4$ . Choose an end vertex  $x$  of a longest path in  $T$ . Then  $x$  is a vertex adjacent to exactly one vertex  $y$  such that  $T - N[x] \cong T' \cup iK_1$  for some  $i \geq 0$  and a tree  $T'$  with  $n - 2 - i$  vertices; and  $T - N[y] \cong T'' \cup jK_1 \cup kK_2$  for some  $j, k \geq 0$  and a tree  $T''$  with  $n - 3 - i - j - 2k$  vertices. (We may assume that  $T'' = \emptyset$  or  $T''$  contains at least 3 vertices.) Note that  $t(m) \leq r^{m-1}$  for  $m \neq 2$ . By Lemmas 1 and 3 and the induction hypothesis,

$$\begin{aligned} mi(T) &= mi(T - N[x]) + mi(T - N[y]) \\ &\leq t(n - 2 - i) + t(n - 3 - i - j - 2k)2^k \\ &\leq \begin{cases} t(n - 2 - i) + r^{2k} & \text{if } T'' = \emptyset, \text{ i.e., } 2k = n - 3 - i - j, \\ t(n - 2 - i) + r^{n-3-i-j-2k-1}r^{2k} & \text{otherwise} \end{cases} \\ &\leq \begin{cases} t(n - 2) + r^{n-3} & \text{if } n = 2k + 3, \\ t(n - 2) + r^{n-4} & \text{otherwise} \end{cases} \\ &\leq t(n). \end{aligned}$$

Moreover, the equalities holding imply that either  $n = 2k + 3$  or  $n$  is even with  $i = j = 0$ ,  $T - N[x] \cong T(n - 2)$ , and  $T - N[y] \cong B(1, \frac{n-4-2k}{2}) \cup kK_2$  by the induction hypothesis. For the case of  $n = 2k + 3$ ,  $T \cong B(1, \frac{n-1}{2}) = T(n)$ . For the later case,  $N_G(y) = \{x, z\}$  and  $z$  is an endpoint of the basic path of the baton  $T - N[x] \cong T(n - 2) = B(2, \frac{n-4}{2})$  or  $B(4, \frac{n-6}{2})$ , except possibly when  $T - N[x] \cong B(2, 1) = B(4, 0) = P_4$ . For the exceptional case, we can view  $P_4$  as a suitable  $B(2, 1)$  or  $B(4, 0)$ ; and still assume that  $z$  is an endpoint of the basic path of the baton. Thus,  $T \cong B(2, \frac{n-2}{2})$  or  $B(4, \frac{n-4}{2})$ , i.e.,  $T = T(n)$ .  $\square$

**Theorem 6** (Jou [5]). *If  $F$  is a forest of  $n \geq 1$  vertices, then  $mi(F) \leq f(n)$ , where*

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

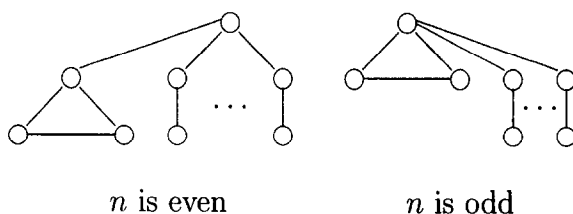


Fig. 2.  $H(n)$ .

Furthermore,  $mi(F) = f(n)$  if and only if  $F = F(n)$ , where

$$F(n) = \begin{cases} \frac{n}{2}K_2 & \text{if } n \text{ is even,} \\ B(1, \frac{n-1-2s}{2}) \cup sK_2 \text{ for some } s \text{ with } 0 \leq s \leq \frac{n-1}{2} & \text{if } n \text{ is odd.} \end{cases}$$

**Proof.** First of all,  $mi(F(n)) = f(n)$  by Lemmas 3 and 4. Suppose  $F = sK_2 \cup (\bigcup_{i=1}^m T_i)$ , where  $s \geq 0$ ,  $m \geq 0$ , and each  $T_i$  is a tree with  $n_i \neq 2$  vertices. Note that  $t(n) \leq r^{n-1}$  when  $n \neq 2$ . By Lemma 3 and Theorem 5,

$$mi(F) \leq 2^s \prod_{i=1}^m t(n_i) \leq r^{2s} \prod_{i=1}^m r^{n_i-1} = r^{n-m} \leq f(n).$$

Furthermore, if the equalities hold, then either  $m = 0$  or  $m = 1$  with  $n_1$  odd and  $t(n_1) = r^{n_1-1}$ . For the former case,  $F \cong \frac{n}{2}K_2 = F(n)$ . For the later case, by Theorem 5,  $T_1 \cong B(1, \frac{n_1-1}{2})$  and so  $F \cong F(n)$ .  $\square$

### 3. Graphs with at most one cycle

This section gives solutions to the problem of determining the maximum value  $h(n)$  (respectively,  $g(n)$ ) of  $mi(G)$  in a connected graph (respectively, general graph) of order  $n$  that contains at most one cycle.

Define the graph  $H(n)$  of order  $n$  as follows, see Fig. 2. For even  $n$ ,  $H(n)$  is the graph obtained from  $B(1, \frac{n-4}{2})$  by adding a  $K_3$  and a new edge joining a vertex of  $K_3$  and the only vertex in the basic path of  $B(1, \frac{n-4}{2})$ . For odd  $n$ ,  $H(n)$  is the graph obtained from  $B(1, \frac{n-3}{2})$  by adding a  $K_3$  with one vertex identified with the only vertex in the basic path of  $B(1, \frac{n-3}{2})$ .

**Theorem 7.** If  $G$  is a connected graph with  $n \geq 3$  vertices such that  $G$  contains at most one cycle, then  $mi(G) \leq h(n)$ , where

$$h(n) = \begin{cases} 3r^{n-4} & \text{if } n \text{ is even,} \\ r^{n-1} + 1 & \text{if } n \text{ is odd.} \end{cases}$$

Furthermore, for  $n \geq 6$ ,  $mi(G) = h(n)$  if and only if  $G \cong H(n)$ .

**Proof.** By repeatedly applying Lemma 1, we have  $mi(H(n)) = h(n)$ . We shall prove the theorem by induction on  $n$ . The theorem is clearly true for  $3 \leq n \leq 5$ . Assume that it is true for all  $n' < n$ . Suppose  $G$  is a connected graph with  $n \geq 6$  vertices such that  $G$  contains at most one cycle. If  $G$  is the cycle  $C_n$ , then, by Lemma 2 and the induction hypothesis,

$$\begin{aligned}
 mi(G) &= mi(C_n) = mi(C_{n-2}) + mi(C_{n-3}) \\
 &\leq \begin{cases} 5 & \text{if } n=6, \\ h(n-2) + h(n-3) & \text{if } n \geq 7 \end{cases} \\
 &\leq \begin{cases} 5 & \text{if } n=6, \\ 3r^{n-6} + (r^{n-4} + 1) & \text{if } n \geq 8 \text{ is even,} \\ (r^{n-3} + 1) + 3r^{n-7} & \text{if } n \geq 7 \text{ is odd} \end{cases} \\
 &= \begin{cases} 5 & \text{if } n=6, \\ 5r^{n-6} + 1 & \text{if } n \geq 8 \text{ is even,} \\ 7r^{n-7} + 1 & \text{if } n \geq 7 \text{ is odd} \end{cases} \\
 &< h(n).
 \end{aligned}$$

Now, assume that  $G \not\cong C_n$ . Either  $G$  contains a unique cycle  $C$ , or else  $G$  is a tree in which a leaf  $C$  is chosen. Choose a vertex  $x$  which is farthest to  $C$ . Then  $x$  is a leaf adjacent to  $y$  such that  $G - N[x]$  is the union of  $i \geq 0$  isolated vertices and a connected graph  $G'$  with  $n - 2 - i$  vertices. Note that the connected subgraph  $G'$  contains at most one cycle. By the induction hypothesis,  $mi(G') \leq h(n - 2 - i)$ . Thus, by Lemma 3,

$$mi(G - N[x]) = mi(iK_1) mi(G') \leq h(n - 2 - i) \leq h(n - 2).$$

Also,  $mi(G - N[x]) = h(n - 2)$  implies that  $i = 0$  and  $G - N[x] \cong H(n - 2)$  by the induction hypothesis. On the other hand,  $G - N[y]$  has at most  $n - 3 - i$  vertices, which is either a forest or the union of a forest  $F$  and a connected subgraph  $G''$  with  $t$  vertices,  $3 \leq t \leq n - 3 - i$ , that contains exactly one cycle. So  $mi(F) \leq f(n - 3 - i - t)$  by Theorem 6 and  $mi(G'') \leq h(t)$  by the induction hypothesis. Thus,

$$\begin{aligned}
 mi(G - N[y]) &\leq \begin{cases} f(n - 3 - i) & \text{if } G - N[y] \text{ is a forest,} \\ f(n - 3 - i - t)h(t) & \text{if } G - N[y] \text{ is not a forest} \end{cases} \\
 &\leq \begin{cases} \max\{r^{n-4}, r^{n-4-t}(3r^{t-4}), r^{n-3-t}(r^{t-1} + 1)\} & \text{if } n \text{ is even,} \\ \max\{r^{n-3}, r^{n-3-t}(3r^{t-4}), r^{n-4-t}(r^{t-1} + 1)\} & \text{if } n \text{ is odd} \end{cases} \\
 &\leq \begin{cases} 3r^{n-6} & \text{if } n \text{ is even,} \\ r^{n-3} & \text{if } n \text{ is odd.} \end{cases}
 \end{aligned}$$

Also, the equalities holding imply that  $|G - N[y]| = n - 3$  and

$$G - N[y] \cong \begin{cases} K_3 \cup \frac{n-6}{2}K_2 & \text{if } n \text{ is even,} \\ \frac{n-3}{2}K_2 & \text{if } n \text{ is odd,} \end{cases}$$

by the induction hypothesis and Theorem 6. So, by Lemma 1,

$$\begin{aligned} \text{mi}(G) &= \text{mi}(G - N[x]) + \text{mi}(G - N[y]) \\ &\leq \begin{cases} h(n-2) + 3 \cdot r^{n-6} & \text{if } n \text{ is even,} \\ h(n-2) + r^{n-3} & \text{if } n \text{ is odd} \end{cases} \\ &= \begin{cases} 3 \cdot r^{n-6} + 3 \cdot r^{n-6} & \text{if } n \text{ is even,} \\ (r^{n-3} + 1) + r^{n-3} & \text{if } n \text{ is odd} \end{cases} \\ &= h(n). \end{aligned}$$

And the equalities holding imply that  $G \cong H(n)$ , since  $G - N[x] \cong H(n-2)$  and  $G - N[y]$  is as above.  $\square$

**Theorem 8.** *If  $G$  is a graph with  $n \geq 1$  vertices such that  $G$  contains at most one cycle, then  $\text{mi}(G) \leq g(n)$ , where*

$$g(n) = \begin{cases} r^n & \text{if } n \text{ is even,} \\ 3r^{n-3} & \text{if } n \text{ is odd.} \end{cases}$$

Furthermore,  $\text{mi}(G) = g(n)$  if and only if  $G \cong G(n)$ , where

$$G(n) = \begin{cases} \frac{n}{2}K_2 & \text{if } n \text{ is even,} \\ K_3 \cup \frac{n-3}{2}K_2 & \text{if } n \text{ is odd.} \end{cases}$$

**Proof.** By Lemma 3, it is clear that  $\text{mi}(G(n)) = g(n)$ . For the case when  $G$  is a forest, by Theorem 6,  $\text{mi}(G) \leq f(n) \leq g(n)$ ; and the equalities holding implies that  $n$  is even and  $G \cong F(n) = G(n)$ . For the case when  $G$  is connected with exactly one cycle, by Theorem 7,  $\text{mi}(G) \leq h(n) \leq g(n)$ ; and the equalities holding implies that  $n = 3$  and  $G \cong K_3 = G(3)$ . So we may suppose that  $G = F \cup H$ , where  $F$  is a forest of order  $n_1$  and  $H$  is a connected graph of order  $n_2$  with exactly one cycle. By Lemma 3 and the above two cases,

$$\text{mi}(G) = \text{mi}(F)\text{mi}(H) \leq f(n_1)h(n_2) \leq \begin{cases} r^{n_1}g(n_2) = g(n) & \text{if } n_1 \text{ is even,} \\ r^{n_1-1}g(n_2) < g(n) & \text{if } n_1 \text{ is odd.} \end{cases}$$

Furthermore, if the equalities hold, then  $n_1$  is even with  $\text{mi}(F) = f(n_1) = g(n_1)$  and  $\text{mi}(H) = h(n_2) = g(n_2)$ . By the first two cases,  $F \cong \frac{n_1}{2}K_2$  and  $H \cong K_3$ , i.e.,  $G \cong G(n)$ .  $\square$

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