Maximal Independent Sets in Graphs with at Most *r* Cycles

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Abstract: We find the maximum number of maximal independent sets in two families of graphs. The first family consists of all graphs with *n* vertices

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and at most r cycles. The second family is all graphs of the first family which are connected and satisfy $n \ge 3r$. © 2006 Wiley Periodicals, Inc. J Graph Theory 53: 270–282, 2006

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INTRODUCTION

Let G = (V, E) be a simple graph. A subset $I \subseteq V$ is *independent* if there is no edge of G between any two vertices of I. Also, I is maximal if it is not properly contained in any other independent set. We let m(G) be the number of maximal independent sets of G.

Around 1960, Erdős and Moser asked for the maximum value of m(G) as G runs over all graphs with n vertices as well as for a characterization of the graphs achieving this maximum. (Actually, they asked the dual question about cliques in such graphs.) Shortly thereafter Erdős, and slightly later Moon and Moser [5], answered both questions. The extremal graphs turn out to have most of their components isomorphic to the complete graph K_3 . Wilf [10] raised the same questions for the family of connected graphs. Independently, Fűredi [2] determined the maximum number for n > 50, while Griggs, Grinstead, and Guichard [3] found the maximum for all n as well as the extremal graphs. Many of the blocks (maximal subgraphs containing no cutvertex) of these graphs are also K_3 's.

Since these initial articles, there has been a string of articles about the maximum value of m(G) as G runs over various families of graphs. In particular, graphs with a bounded number of cycles have received attention. Wilf [10] determined the maximum number of maximal independent sets possible in a tree, while Sagan [6] characterized the extremal trees. These involve attaching copies of K_2 to the endpoints of a given path. Later Jou and Chang [4] settled the problem for graphs and connected graphs with at most one cycle. Here we consider the family of graphs with n vertices and at most r cycles, and the family of connected graphs with nvertices and at most r cycles where $n \geq 3r$. The extremal graphs are obtained by taking copies of K_2 and K_3 either as components (for all such graphs) or as blocks (for all such connected graphs). We define the extremal graphs and prove some lemmas about them in the next section. Then Section 3 gives the proof of our main result, Theorem 3.1.

2. EXTREMAL GRAPHS AND LEMMAS

For any two graphs G and H, let $G \uplus H$ denote the disjoint union of G and H, and for any nonnegative integer t, let tG stand for the disjoint union of t copies of G. We will need the original result of Moon and Moser. To state it, suppose $n \geq 2$ and

let

$$G(n) := \begin{cases} \frac{n}{3}K_3 & \text{if } n \equiv 0 \text{ (mod 3),} \\ 2K_2 \uplus \frac{n-4}{3}K_3 & \text{if } n \equiv 1 \text{ (mod 3),} \\ K_2 \uplus \frac{n-2}{3}K_3 & \text{if } n \equiv 2 \text{ (mod 3).} \end{cases}$$

Also let

$$G'(n) := K_4 \uplus \frac{n-4}{3} K_3$$
 if $n \equiv 1 \pmod{3}$.

Using the fact that $m(G \uplus H) = m(G)m(H)$ we see that

$$g(n) := m(G(n)) = \begin{cases} 3^{\frac{n}{3}} & \text{if } n \equiv 0 \pmod{3}, \\ 4 \cdot 3^{\frac{n-4}{3}} & \text{if } n \equiv 1 \pmod{3}, \\ 2 \cdot 3^{\frac{n-2}{3}} & \text{if } n \equiv 2 \pmod{3}. \end{cases}$$

Note also that if $n \equiv 1 \pmod{3}$ then m(G'(n)) = m(G(n)).

Theorem 2.1 (Moon and Moser [5]). Let G be a graph with $n \ge 2$ vertices. Then

$$m(G) \le g(n)$$

with equality if and only if $G \cong G(n)$ or, for $n \equiv 1 \pmod{3}$, $G \cong G'(n)$.

Note that G(n) has at most $\lfloor n/3 \rfloor$ cycles. Therefore, the Moon–Moser Theorem gives the maximum number of maximal independent sets for the family of all graphs with n vertices and at most r cycles when $r \geq \lfloor n/3 \rfloor$. To complete the characterization, we need only handle the cases where $r < \lfloor n/3 \rfloor$. To make our proof cleaner, we will assume the stronger condition that $n \geq 3r - 1$.

For any positive integers n, r with $n \ge 3r - 1$ we define

$$G(n,r) := \begin{cases} rK_3 \uplus \frac{n-3r}{2}K_2 & \text{if } n \equiv r \pmod{2}, \\ (r-1)K_3 \uplus \frac{n-3r+3}{2}K_2 & \text{if } n \not\equiv r \pmod{2}. \end{cases}$$

Note that if n and r have different parity then $G(n, r) \cong G(n, r-1)$. This duplication is to facilitate the statement and proof of our main result where G(n, r) will be extremal among all graphs with |V| = n and at most r cycles. Further, define

$$g(n,r) := m(G(n,r)) = \begin{cases} 3^r \cdot 2^{\frac{n-3r}{2}} & \text{if } n \equiv r \pmod{2}, \\ 3^{r-1} \cdot 2^{\frac{n-3r+3}{2}} & \text{if } n \not\equiv r \pmod{2}. \end{cases}$$

For the connected case, we will use the result of Griggs, Grinstead, and Guichard. We obtain the extremal graphs as follows. Let G be a graph all of whose components

are complete and let K_m be a complete graph disjoint from G. Construct the graph $K_m * G$ by picking a vertex v_0 in K_m and connecting it to a single vertex in each component of G. If $n \ge 6$ then let

$$C(n) := \begin{cases} K_3 * \frac{n-3}{3} K_3 & \text{if } n \equiv 0 \pmod{3}, \\ K_4 * \frac{n-4}{3} K_3 & \text{if } n \equiv 1 \pmod{3}, \\ K_4 * \left(K_4 \uplus \frac{n-8}{3} K_3\right) & \text{if } n \equiv 2 \pmod{3}. \end{cases}$$

The graph C(14) is displayed in Figure 1. Counting maximal independent sets by whether they do or do not contain v_0 gives

$$c(n) := m(C(n)) = \begin{cases} 2 \cdot 3^{\frac{n-3}{3}} + 2^{\frac{n-3}{3}} & \text{if } n \equiv 0 \pmod{3}, \\ 3^{\frac{n-1}{3}} + 2^{\frac{n-4}{3}} & \text{if } n \equiv 1 \pmod{3}, \\ 4 \cdot 3^{\frac{n-5}{3}} + 3 \cdot 2^{\frac{n-8}{3}} & \text{if } n \equiv 2 \pmod{3}. \end{cases}$$

Theorem 2.2 (Griggs, Grinstead, and Guichard [3]). Let G be a connected graph with $n \ge 6$ vertices. Then

$$m(G) \le c(n)$$

with equality if and only if $G \cong C(n)$.

To limit the number of cases in the proof of our main theorem we will only find the maximum of m(G) for the family of all connected graphs when $n \geq 3r$. Unlike the arbitrary graphs case, this result, together with the Griggs-Grinstead-Guichard Theorem, does not completely determine the maximum of m(G) for all n and r. For example, when n = 10 the extremal connected graph given by the Griggs-Grinstead-Guichard Theorem has 9 cycles, while our proof will only characterize extremal connected graphs with at most 3 cycles. Although this gap between our main theorem and the Griggs-Grinstead-Guichard Theorem is relatively small

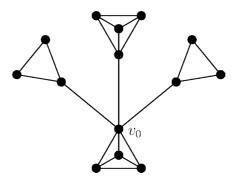


FIGURE 1. The graph C(14).

(C(n) contains $\lfloor n/3 \rfloor$, $\lfloor n/3 \rfloor + 6$, $\lfloor n/3 \rfloor + 12$ cycles when $n \equiv 0, 1, 2 \pmod{3}$, respectively), it takes considerable care to handle it. This work is undertaken in [7]. When $n \geq 3r$ we define

$$C(n,r) := \begin{cases} K_3 * \left((r-1)K_3 \uplus \frac{n-3r}{2}K_2 \right) & \text{if } n \equiv r \pmod{2}, \\ K_1 * \left(rK_3 \uplus \frac{n-3r-1}{2}K_2 \right) & \text{if } n \not\equiv r \pmod{2}. \end{cases}$$

The graphs C(13, 2) and C(15, 3) are shown in Figure 2. As usual, we let

$$c(n,r) := m(C(n,r)) = \begin{cases} 3^{r-1} \cdot 2^{\frac{n-3r+2}{2}} + 2^{r-1} & \text{if } n \equiv r \pmod{2}, \\ 3^r \cdot 2^{\frac{n-3r-1}{2}} & \text{if } n \not\equiv r \pmod{2}. \end{cases}$$

We also need the bounds for maximal independent sets in trees and forests, although we will not need the extremal graphs. Define

$$f(n) := 2^{\lfloor \frac{n}{2} \rfloor}$$

and

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

Using our upcoming Proposition 2.8, it is easy to establish the following result.

Theorem 2.3. If G is a forest with $n \ge 1$ vertices then $m(G) \le f(n)$.

Somewhat surprisingly, the tree analog is significantly more difficult.

Theorem 2.4 (Wilf [10]). *If* G *is a tree with* n *vertices then* $m(G) \le t(n)$.

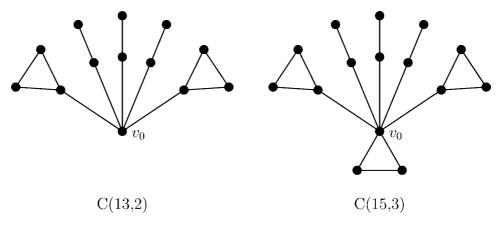


FIGURE 2. Examples of C(n, r) for $n \ge 3r$.

For the extremal trees the reader is referred to Sagan [6].

Next, we have a list of inequalities that will be useful in the proof of our main theorem. It will be convenient to let g(n, 0) = f(n) and c(n, 0) = t(n).

Lemma 2.5. We have the following monotonicity results.

(1) If $r \ge 1$ and $n > m \ge 3r - 1$ then

$$g(n, r) > g(m, r)$$
.

(2) If $r \ge 1$ and $n > m \ge 3r$ then

$$c(n, r) > c(m, r)$$
.

(3) If $r > q \ge 0$ and $n \ge 3r - 1$ then

with equality if and only if n and r have different parity and q = r - 1.

(4) If $r > q \ge 0$ and $n \ge 3r$ then

$$c(n,r) \ge c(n,q)$$

with equality if and only if (n, r, q) = (4, 1, 0) or (7, 2, 1).

Proof. The proofs of all of these results are similar, so we will content ourselves with a demonstration of (4). It suffices to consider the case when q = r - 1. Suppose that $r \ge 2$ since the r = 1 case is similar. If n and r have the same parity, then we wish to show

$$3^{r-1} \cdot 2^{\frac{n-3r+2}{2}} + 2^{r-1} > 3^{r-1} \cdot 2^{\frac{n-3r+2}{2}}$$

which is clear. If n and r have different parity, then $n \ge 3r$ forces $n \ge 3r + 1$. We want

$$3^r \cdot 2^{\frac{n-3r-1}{2}} \ge 3^{r-2} \cdot 2^{\frac{n-3r+5}{2}} + 2^{r-2}.$$

Combining the terms with powers of 3, we have the equivalent inequality

$$3^{r-2} \cdot 2^{\frac{n-3r-1}{2}} \ge 2^{r-2}.$$

The bounds on n and r show that this is true, with equality exactly when both sides equal1.

We also need two results about m(G) for general graphs G. In what follows, if $v \in V$ then the *open* and *closed neighborhoods of* v are

$$N(v) = \{ u \in V \mid uv \in E \}$$

and

$$N[v] = \{v\} \cup N(v),$$

respectively. We also call a block an *endblock of G* if it has at most one cutvertex in the graph as a whole. We first verify that certain types of endblocks exist.

Proposition 2.6. Every graph has an endblock that intersects at most one non-endblock.

Proof. The block-cutvertex graph of G, G', is the graph with a vertex v_B for each block B of G, a vertex v_x for each cutvertex x of G, and edges of the form v_Bv_x whenever $x \in V(B)$. It is well known that G' is a forest. Now consider a longest path P in G'. The final vertex of P corresponds to a block B of G with the desired property.

Any block with at least 3 vertices is 2-connected, that is, one must remove at least 2 vertices to disconnect or trivialize the graph. Such graphs are exactly those which can be obtained from a cycle by adding a sequence of *ears*. This fact is originally due to Whitney [9], and can also be found in Diestel [1, Proposition 3.1.2] and West [8, Theorem 4.2.8].

Theorem 2.7 (Ear Decomposition Theorem). A graph B is 2-connected if and only if there is a sequence

$$B_0, B_1, \ldots, B_l = B$$

such that B_0 is a cycle and B_{i+1} is obtained by taking a nontrivial path and identifying its two endpoints with two distinct vertices of B_i .

Proposition 2.8. The invariant m(G) satisfies the following.

(1) If $v \in V$ then

$$m(G) < m(G - v) + m(G - N[v]).$$

(2) If G has an endblock B that is isomorphic to a complete graph then

$$m(G) = \sum_{v \in V(B)} m(G - N[v]).$$

In fact, the same equality holds for any complete subgraph B having at least one vertex that is adjacent in G only to other vertices of B.

Proof. For any $v \in V$ there is a bijection between the maximal independent sets I of G that contain v and the maximal independent sets of G - N[v], given by $I \mapsto I - v$. Also, the identity map gives an injection from those I that do not contain v into the maximal independent sets of G - v. This proves (1). For (2), merely use the previous bijection and the fact that, under either hypothesis, any maximal independent set of G must contain exactly one of the vertices of B.

We will refer to the formulas in parts (1) and (2) of this proposition as the *m-bound* and *m-recursion*, respectively.

PROOF OF THE MAIN THEOREM

We are now in a position to state and prove our main result. The path and cycle on n vertices will be denoted by P_n and C_n , respectively. Also, let E denote the graph pictured in Figure 3.

Theorem 3.1. Let G be a graph with n vertices and at most r cycles where $r \ge 1$.

(I) If $n \ge 3r - 1$ then for all such graphs we have

$$m(G) \leq g(n,r)$$

with equality if and only if $G \cong G(n, r)$.

(II) If $n \ge 3r$ then for all such graphs that are connected we have

$$m(G) \le c(n, r)$$

with equality if and only if $G \cong C(n,r)$ or if G is one of the exceptional cases listed in the following table.

$n r $ Possible $G \ncong C(n,r)$	
4 1	P_4
5 1	C_5
7 2	C(7, 1), E

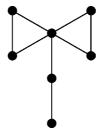


FIGURE 3. The exceptional graph *E*.

Proof. The proof will be by double induction on n and r. The base case r = 1 has been done by Jou and Chang [4], so we assume from now on that $r \ge 2$. We will also assume that $n \ge 8$, as the smaller cases have been checked by computer.

We first show that graphs with a certain cycle structure can not be extremal by proving the following pair of claims. Here we assume that G has n vertices and at most r cycles.

Claim 1. If G is a graph with two or more intersecting cycles and $n \ge 3r - 1$ then m(G) < g(n, r).

Claim 2. If G is a connected graph with an endblock B containing two or more cycles and $n \ge 3r$ then m(G) < c(n, r).

To prove Claim 1 suppose to the contrary that v is a vertex where two cycles intersect, so G-v has n-1 vertices and at most r-2 cycles. Furthermore, among all such vertices we can choose v with deg $v \ge 3$. It follows that G-N[v] has at most n-4 vertices and at most r-2 cycles. If r=2 then using Theorem 2.3 and the m-bound gives

$$m(G) \le f(n-1) + f(n-4)$$

$$= \begin{cases} 2^{\frac{n-2}{2}} + 2^{\frac{n-4}{2}} & \text{if } n \text{ is even,} \\ 2^{\frac{n-1}{2}} + 2^{\frac{n-5}{2}} & \text{if } n \text{ is odd} \end{cases}$$

$$= \begin{cases} 3 \cdot 2^{\frac{n-4}{2}} & \text{if } n \text{ is even,} \\ 5 \cdot 2^{\frac{n-5}{2}} & \text{if } n \text{ is odd} \end{cases}$$

$$\le g(n, 2).$$

If $r \ge 3$ then we use the induction hypothesis of the theorem, Lemma 2.5 (1) and (3), and the *m*-bound to get

$$m(G) \le g(n-1, r-2) + g(n-4, r-2)$$

$$= \begin{cases} 3^{r-3} \cdot 2^{\frac{n-3r+8}{2}} + 3^{r-2} \cdot 2^{\frac{n-3r+2}{2}} & \text{if } n \equiv r \pmod{2}, \\ 3^{r-2} \cdot 2^{\frac{n-3r+5}{2}} + 3^{r-3} \cdot 2^{\frac{n-3r+5}{2}} & \text{if } n \not\equiv r \pmod{2}, \end{cases}$$

$$= \begin{cases} 22 \cdot 3^{r-3} \cdot 2^{\frac{n-3r}{2}} & \text{if } n \equiv r \pmod{2}, \\ 8 \cdot 3^{r-3} \cdot 2^{\frac{n-3r+3}{2}} & \text{if } n \not\equiv r \pmod{2}, \end{cases}$$

$$< g(n, r).$$

To prove Claim 2 we first observe that by the Ear Decomposition Theorem, B contains two cycles C and C' such that $C \cap C'$ is a path with at least 2 vertices. Since B is an endblock, one of the endpoints of the path $C \cap C'$ is not a cutvertex in G. Label this endpoint v. Note that by construction deg $v \ge 3$ and v is on at least 3

cycles of G, namely C, C', and the cycle in $C \cup C'$ obtained by not taking any edge of the path $C \cap C'$. Proceeding as in the proof of Claim 1 and noting that G - v is connected by our choice of v, we have

$$m(G) \le \begin{cases} t(n-1) + f(n-4) & \text{if } r = 3, \\ c(n-1, r-3) + g(n-4, r-3) & \text{if } r > 3 \end{cases}$$

$$< c(n, r).$$

We now return to the proof of the theorem, first tackling the case where Gvaries over all graphs with n vertices and at most r cycles. For the base cases of n = 3r - 1 or 3r, we have g(n, r) = g(n) and G(n, r) = G(n) so we are done by the Moon-Moser Theorem.

Suppose that $n \ge 3r + 1$. From Claim 1 we can assume that the cycles of G are disjoint. It follows that the blocks of G must all be cycles or copies of K_2 . Let B be an endblock of G. We have three cases depending on whether $B \cong K_2$, K_3 , or C_p for $p \ge 4$.

If $B \cong K_2$ then let $V(B) = \{v, w\}$ where w is the cutvertex of B in G, if B has one. Then G - N[v] has n - 2 vertices and at most r cycles while G - N[w] has at most n-2 vertices and at most r cycles. By induction, Lemma 2.5 (1) and (3), and the m-recursion we have

$$m(G) \le 2g(n-2, r) = g(n, r)$$

with equality if and only if $G - N[v] = G - N[w] \cong G(n-2, r)$. It follows that B is actually a component of G isomorphic to K_2 and so $G \cong G(n, r)$.

The case $B \cong K_3$ is similar. Proceeding as before, one obtains

$$m(G) \le 3g(n-3, r-1) = g(n, r),$$

and equality is equivalent to $G \cong B \uplus G(n-3, r-1) \cong G(n, r)$.

To finish off the induction step, consider $B \cong C_p$, $p \ge 4$. Then there exist $v, w, x \in V(B)$ all of degree 2 such that $vw, vx \in E(B)$. So G - v has n - 1 vertices and at most r-1 cycles. Furthermore, $G-v \ncong G(n-1,r-1)$ since G-vcontains two vertices, w and x, both of degree 1 and in the same component but not adjacent. Also, G - N[v] has n - 3 vertices and at most r - 1 cycles. Using computations similar to those in Claim 1,

$$m(G) < g(n-1, r-1) + g(n-3, r-1) = g(n, r),$$

so these graphs cannot be extremal.

It remains to consider the connected case. It will be convenient to leave the base cases of n = 3r or 3r + 1 until last, so assume that $n \ge 3r + 2$. Among all the endblocks of the form guaranteed by Proposition 2.6, let B be one with the largest

number of vertices. Claim 2 shows that B is either K_2 or a cycle. Furthermore, the r=1 base case shows that cycles with more than 5 vertices are not extremal, so B must contain a cutvertex x. Again, there are three cases depending on the nature of B.

If $B \cong K_2$ then let $V(B) = \{x, v\}$ so that deg v = 1 and deg $x \ge 2$. By the choice of B, G - N[v] is the union of some number of K_1 's and a connected graph with at most n - 2 vertices and at most r cycles. Also, G - N[x] has at most n - 3 vertices and at most r cycles, so

$$m(G) \le c(n-2,r) + g(n-3,r) = c(n,r)$$

with equality if and only if both G - N[v] and G - N[x] are extremal. Except for the case where n = 9 and r = 2, this implies that $G - N[v] \cong C(n - 2, r)$ and $G - N[x] \cong G(n - 3, r)$, which is equivalent to $G \cong C(n, r)$. In the case where n = 9 and r = 2 we still must have $G - N[x] \cong G(6, 2) \cong 2K_3$, but now there are three possibilities for G - N[v]: C(7, 2), C(7, 1), or E. However, since G - N[x] is a subgraph of G - N[v] we must have $G - N[v] \cong C(7, 2)$, which shows that $G \cong C(9, 2)$, as desired.

Next consider $B \cong K_3$ and let $V(B) = \{x, v, w\}$ where x is the cutvertex. Let i be the number of K_3 endblocks other than B containing x. First we note that x is adjacent to some vertex y not in a K_3 endblock as otherwise n < 3r. It follows from our choice of B that G - N[v] = G - N[w] has some number of K_1 components, i components isomorphic to K_2 , and at most one other component, say H, with at most n - 2i - 3 vertices and at most r - i - 1 cycles. Furthermore, because x is adjacent to y, the graph G - N[x] has at most n - 2i - 4 vertices and at most r - i - 1 cycles. This gives us the upper bound

$$m(G) < 2^{i+1}c(n-2i-3,r-i-1) + g(n-2i-4,r-i-1).$$

As the right-hand side of this inequality is strictly decreasing for i of a given parity, it suffices to consider the cases where i is 0 or 1. When i = 1, we have

$$m(G) < 4c(n-5, r-2) + g(n-6, r-2) < c(n, r).$$

When i = 0 we have

$$m(G) \le 2c(n-3, r-1) + g(n-4, r-1) = c(n, r).$$

Using the same argument as in the case $B \cong K_2$ and (n, r) = (9, 2), one can show that this inequality is strict when c(n - 3, r - 1) could be achieved by one of the exceptional graphs. For other n, r we get equality if and only if $G \cong C(n, r)$.

The last case is where $B \cong C_p$ where $p \ge 4$. Label the vertices of B as x, u, v, w, \ldots so that they read one of the possible directions along the cycle, where x is the cutvertex. So $\deg u = \deg v = \deg w = 2$, $\deg x \ge 3$, and G - v

is connected with n-1 vertices and at most r-1 cycles. Furthermore, $G-v \ncong$ C(n-1,r-1) because it contains a vertex of degree 1 (namely u) adjacent to a vertex of degree at least 3 (namely x). Also, the graph G - N[v] is connected with n-3 vertices and at most r-1 cycles. These conditions give us

$$m(G) < c(n-1, r-1) + c(n-3, r-1) = c(n, r),$$

and since this inequality is strict, such G are not extremal.

We are left with the base cases. When n = 3r, c(n, r) = c(n) and $C(n, r) \cong C(n)$ so we are done by the Griggs-Grinstead-Guichard Theorem. If n = 3r + 1 then we can proceed as in the induction step except where $B \cong K_2$ since then c(n-2, r)and g(n-3,r) have arguments outside of the permissible range. However, since we have assumed $n \ge 8$, Theorems 2.1 and 2.2 apply to give

$$m(G) \le c(n-2) + g(n-3)$$

$$= c(3r-1) + g(3r-2)$$

$$= 4 \cdot 3^{r-2} + 3 \cdot 2^{r-3} + 4 \cdot 3^{r-2}$$

$$\le c(3r+1,r)$$

$$= c(n,r).$$

The latter inequality is strict for $r \neq 3$; when r = 3, the former inequality is strict because $C(8) = K_4 * K_4$ has more than 3 cycles. Therefore these graphs cannot be extremal, finishing the proof of the theorem.

As was mentioned in Section 1, Theorem 3.1 and the Moon-Moser Theorem combine to completely settle the maximal independent set question for the family of arbitrary graphs with n vertices and at most r cycles for all n and r, but this does not occur in the connected case. For these graphs, Theorem 3.1 handles the cases where n is large relative to r and the Griggs–Grinstead–Guichard Theorem handles the cases where n is small relative to r, but there is a gap between where these two results apply when $n \not\equiv 0 \pmod{3}$. This gap is handled in [7]. That article also answers related questions for maximum independent sets.

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