

ON THE NUMBER OF INDEPENDENT SETS OF NODES IN A TREE

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1. INTRODUCTION

In [4] Wilf shows that the number of maximal independent sets of nodes (MIS) for a non-empty tree on n nodes is bounded above by

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

For each value of n , he gives a tree, depending upon the parity of n , that attains these bounds. The two general forms are shown below in Figure 1.



FIGURE 1

Throughout, we assume nonempty trees and, following the notation in [4], let $\mu(T)$ be the number of MIS's in a tree T . We will derive lower and upper bounds on $\mu(T)$ in terms of $\beta_1(T)$, the maximum number of independent edges in T .

First observe that, in any graph, two degree-one nodes having a common neighbor occur in the same MIS's. Thus, the number of MIS's is unaffected by the removal of one of these nodes. Such "pruning" can be repeated, and we formalize this fact as a lemma. Although the lemma is stated here for trees, it is actually valid for arbitrary graphs, and demonstrates, in some sense, the independence between the number of nodes and the number of maximal independent sets of nodes.

Lemma 1: Let T be a tree and T' the tree obtained by removing all but one degree-one neighbor from every node having two or more such neighbors. Then $\mu(T) = \mu(T')$ and $\beta_1(T) = \beta_1(T')$.

Any tree with diameter d , $2 \leq d \leq 4$, can be reduced by Lemma 1 to one of the forms in Figure 1. The n -even case arises from trees containing two degree-one nodes that are distance three from each other. Define T_e to be this set of trees and let T_o be the remaining trees with diameter between two and four. Notice that K_1 and K_2 are the only trees with diameter less than or equal to four that are not in $T_e \cup T_o$. Neither are they reducible to a tree of Figure 1. For these, though, we know that $\mu(K_1) = 1$ and $\mu(K_2) = 2$. We can determine exactly $\mu(T)$ for any tree T with diameter at most four.

Lemma 2: Let T be a tree with diameter at most four and $\beta_1 = \beta_1(T)$. Then

$$\mu(T) = \begin{cases} 2^{\beta_1-1} + 1 & \text{if } T \in T_e \cup \{K_2\}, \\ 2^{\beta_1} & \text{if } T \in T_o \cup \{K_1\}. \end{cases}$$

Proof: All trees in $T_e \cup T_o$ must, by the above discussion, reduce to either the n even (with $n = 2\beta_1$) or the n odd (with $n = 2\beta_1 + 1$) case in Figure 1. The result then follows from $f(n)$ given above. Finally, since $\beta_1(K_1) = 0$, $\mu(K_1) = 1$, $\beta_1(K_2) = 1$, and $\mu(K_2) = 2$, K_1 and K_2 also satisfy the lemma. \square

The trees in $T_e \cup T_o$ will be called **terminal trees** or **terminal subtrees** when part of a larger tree, and will have an assigned root node u . With one exception, the root node must be selected from those nodes that, after pruning, would be nodes of maximum degree. The star $K_{1,n}$, the exception, must be rooted at a leaf node. The root of a terminal subtree S has a single neighbor not in S . The neighborhoods of all other nodes in S are a subset of S . In a pruned tree, a subtree whose removal would disconnect the graph or leave an isolated K_1 or K_2 is not a terminal subtree. The trees in Figure 1 are terminal trees. The tree T' in Figure 2 below is formed by removing a terminal subtree from T . All trees, other than K_1 and K_2 , are either themselves terminal trees or contain at least two terminal subtrees. Thus, for any pruned tree T with diameter at least five, there exist adjacent nodes u and v permitting T to be drawn in one of the two forms of Figure 2, where u is the root of a terminal subtree and v is in the subtree T' .

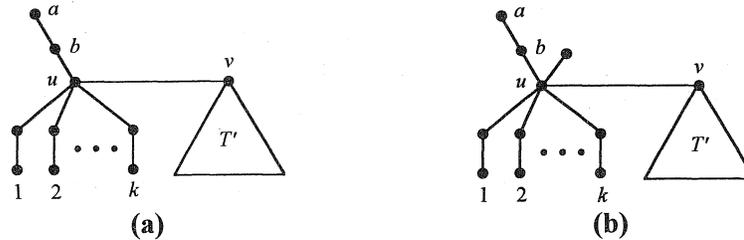


FIGURE 2

The structure of the graphs in Figure 2 corresponds to the structure in Figure 2 of Wilf's paper [4]. From this we see that Wilf's equation (2), a recursive equation solving $\mu(T)$, has a simpler form because of the pruning permitted by Lemma 2. We include it here, along with the conclusions of Lemma 2, where $\beta_1 = \beta_1(T)$ and k , a , and b are as in Figure 2.

$$(1) \quad \mu(T) = \begin{cases} 2^{\beta_1-1} + 1 & \text{if } T \in T_e \cup \{K_2\}, \\ 2^{\beta_1} & \text{if } T \in T_o \cup \{K_1\}, \\ \mu(T - \{a, b\}) + 2^k \mu(T') & \text{otherwise.} \end{cases}$$

Part three applies when the diameter is at least five, and then $\beta_1(T - \{a, b\}) = \beta_1 - 1$ and $\beta_1(T')$ is either $\beta_1 - k - 2$ or $\beta_1 - k - 1$. In either case, the subtree T' has at least three nodes.

We use this result to obtain a lower bound on the number of MIS in a tree. Then we use another tree-reduction operation to determine new lower bounds, and also new upper bounds which normally improve those given by Wilf. Finally, we obtain bounds on the number of independent sets (including nonmaximal) of nodes in an arbitrary tree.

2. IMPROVED BOUNDS

Since $\mu(T)$ is essentially independent of the number of nodes in T , we look for bounds with respect to the edge independence number $\beta_1(T)$. The first, Theorem 1, is a lower bound for $\mu(T)$ that appeals to Lemma 1 and the Fibonacci numbers F_n .

Sanders [3] exhibits a tree on $2n$ nodes and proves it has F_{n+2} maximal independent sets of nodes. The tree, called an extended path, is formed by appending a single degree-one node to each node of a path on n nodes. In terms of their edge independence number, we have for such trees T that $\mu(T) = F_{\beta_1+2}$, where $\beta_1 = \beta_1(T) = n$. We show next that, for a given value of β_1 , no tree T with $\beta_1(T) = \beta_1$ has a smaller number of maximal independent sets of nodes. Therefore, because of Lemma 1, extended paths actually represent, for each value of β_1 , an infinite class of trees satisfying the bound.

Theorem 1: Let T be any tree with $\beta_1 = \beta_1(T)$. Then $\mu(T) \geq F_{\beta_1+2}$.

Proof: If $T \in T_e \cup T_o \cup \{K_1, K_2\}$, then the result follows because F_{β_1+2} is bounded above by the appropriate $2^{\beta_1-1} + 1$ or 2^{β_1} value indicated in equation (1). Otherwise, we can use the recurrence formula in equation (1) inductively to conclude that $\mu(T) \geq F_{\beta_1+1} + 2^k F_{\beta_1-k}$. It is straightforward to show, by another induction argument, that $2^k F_{\beta_1-k} \geq F_{\beta_1}$. Therefore, $\mu(T) \geq F_{\beta_1+1} + F_{\beta_1} = F_{\beta_1+2}$. \square

Terminal subtrees can be removed from a tree T , one at a time, until T is empty providing, in some sense, a count of the number of terminal subtrees in T . Since the order of removal is not unique, one might suspect that the subtrees obtained in such a removal scheme also may not be unique. This is indeed the case and can be verified by examining a few small examples. It also would seem the number found could vary depending upon the order of removal. We now show that this does not occur.

Lemma 3: For any tree, every order of terminal subtree removal results in the same number of removed subtrees.

Proof: Let $t_{\min}(T)$ and $t_{\max}(T)$ be the minimum and maximum number of terminal subtrees that can be removed from a tree T , under any order of removal. If T is itself a terminal tree, the result holds since there is no option but to remove the entire tree. This also implies $t_{\min}(T) = 2$ whenever $t_{\max}(T) = 2$. Now, letting $t_{\max}(T) = m \geq 3$, we show by induction that $t_{\min}(T)$ also must equal m . For some k , $2 \leq k \leq t_{\max}(T)$, there exist terminal subtrees S_1, S_2, \dots, S_k of T , any one of which can be an initial subtree removed from T . There exist indices i and j , $1 \leq i \neq j \leq k$, for which $t_{\max}(T - S_i) = t_{\max}(T) - 1 = m - 1$ and $t_{\min}(T - S_j) = t_{\min}(T) - 1 < m - 1$. By the induction hypothesis, terminal subtrees can be removed in any order from $T - S_i$ and $T - S_j$ without affecting the number of such removals. Furthermore, S_j is a terminal subtree of $T - S_i$ and S_i is one of $T - S_j$. Thus, $t_{\max}(T - S_i - S_j) = t_{\max}(T) - 2 = m - 2$ and $t_{\min}(T - S_j - S_i) = t_{\min}(T) - 2 < m - 2$, a contradiction implied by the induction hypothesis since $T - S_j - S_i = T - S_i - S_j$. Hence, $t_{\min}(T) = m$. \square

In view of Lemma 3, it is now possible to define, for any tree T , a new invariant $t(T)$ to be the number of terminal subtrees removable from T . It is convenient to let $t(K_1) = t(K_2) = 0$.

Theorem 2: Let T be a tree with $\beta_1 = \beta_1(T)$ and $t = t(T)$. Then $2^{\beta_1-t} + 2^t - 1 \leq \mu(T) \leq 2^{\beta_1}$.

Proof: If $t(T) \leq 1$, then T is in $T_e \cup T_0 \cup \{K_1, K_2\}$ and both bounds follow from the first two cases of equation (1). Now consider the case in which $\beta_1 = 2t$. Then the lower bound is $2^{t+1} - 1$. A straightforward induction argument shows $2^{t+1} - 1 \leq F_{2t+2}$; then Theorem 1 establishes that such trees satisfy the lower bound of the theorem. Now, assume T is a tree with $t(T) = t \geq 2$ and that the lower bound is satisfied by all trees with either fewer than t terminal subtrees or with t terminal subtrees and $2t$ independent edges. Then, we can invoke the third part of equation (1) inductively and have, referring to Figure 2,

$$\begin{aligned} \beta_1(T - \{a, b\}) &= \beta_1 - 1; \quad t - 1 \leq t(T - \{a, b\}) \leq t; \\ \beta_1 - k - 2 &\leq \beta_1(T') \leq \beta_1 - k - 1; \quad t(T') = t - 1. \end{aligned}$$

The lower bound decreases as β_1 decreases and, when t decreases, the lower bound decreases if and only if $\beta_1 < 2t$. Thus, we must consider two cases:

Case 1. $\beta_1 < 2t$ and $t(T - \{a, b\}) = t - 1$. Then

$$\begin{aligned} \mu(T) &\geq \{2^{\beta_1 - t} + 2^{t-1} - 1\} + 2^k \{2^{\beta_1 - k - t - 1} + 2^{t-1} - 1\} \\ &= 2^{\beta_1 - t} + 2^{t-1} - 1 + 2^{\beta_1 - t - 1} + 2^k (2^{t-1} - 1) \geq 2^{\beta_1 - t} + 2^t - 1. \end{aligned}$$

Case 2. $\beta_1 > 2t$ and $t(T - \{a, b\}) = t$. The result when $\beta_1 = 2t$ has already been established. We again use the recursive part of equation (1), where $t(T - \{a, b\}) = t$ and $\beta_1(T - \{a, b\}) = \beta_1 - 1$, and proceed by induction on the value of β_1 . It follows that

$$\begin{aligned} \mu(T) &\geq \{2^{\beta_1 - 1 - t} + 2^t - 1\} + 2^k \{2^{\beta_1 - k - t - 1} + 2^{t-1} - 1\} \\ &= 2^{\beta_1 - t - 1} + 2^t - 1 + 2^{\beta_1 - t - 1} + 2^k (2^{t-1} - 1) > 2^{\beta_1 - t} + 2^t - 1. \end{aligned}$$

establishes the lower bound.

To verify the right inequality, we again use equation (1) inductively. The result was shown above for all trees with $t(T) \leq 1$. Assume T is a tree with $t(T) \geq 2$ and that the result holds for all trees with edge independence number less than β_1 . Then $\beta_1 = \beta_1(T) \geq 3$ and $\mu(T) \leq 2^{\beta_1 - 1} + 2^k 2^{\beta_1 - k - 1} = 2^{\beta_1}$. \square

When $t(T) \leq 1$, regardless of the value of $\beta_1(T)$, equation (1) shows that equality holds on the right in the n odd cases of Figure 1 and on the left in the n even cases. Other trees can be obtained by appending an arbitrary number of degree-one neighbors to the degree-two nodes in either of the trees in Figure 1. This process produces all trees T for which $t(T) =$

The upper bound also is achievable, for any β_1 and $t \geq 2$, by an infinite number of trees. Consider the tree in Figure 2(a). The recurrence in equation (1) can be iterated k times, on the first term, to give the equation $\mu(T) = \mu(T'') + (2^{k+1} - 1)\mu(T')$, where T' is the same as in Figure 2, and T'' is T' with node v having node u as a degree-one neighbor. We call this the **iterated recurrence formula**. From Lemma 1, if node v already has a degree-one neighbor, $\mu(T'') = \mu(T')$ and the recurrence formula simplifies to $\mu(T) = 2^{k+1}\mu(T')$. We now construct a tree T that has this property at each step of the iterated recurrence. Let T_1 be any tree in T_0 . For $t \geq 2$, let S_t be any tree in T_0 with its identified root node u . Now, form T_t by adding an edge between node u in S_t and any node in T_{t-1} having a degree-one neighbor. Clearly, $\beta_1(T_t) = \beta_1(S_t) + \beta_1(T_{t-1})$, and an induction argument with $\mu(T_t) = 2^{k+1}\mu(T_{t-1})$ shows that $\mu(T_t) = 2^{\beta_1(T_t)}$. The lower bound is also achieved, when $t = 2$, by any tree that can be pruned to P_6 , the path on six nodes.

We conclude this section with an upper bound on $\mu(T)$ for a restricted class of trees that will prove useful in the next section. Let T^* be the collection of trees with every node being a degree-one node or having a degree-one neighbor. First, an upper bound independent of $t(T)$ is given.

Theorem 3: Let $T \in T^*$ with $\beta_1 = \beta_1(T)$. Then $\mu(T) \leq 2^{\beta_1-1} + 1$.

Proof: If $t(T) \leq 1$, then $T \in \mathcal{T}_e \cup \{K_2\}$ and equality follows from equation (1). Now, assume that $T \in T^*$, $t(T) \geq 2$, $\beta_1(T) = \beta_1 = m \geq 3$, and that the result holds for trees in T^* with fewer independent edges. Identify a terminal subtree, as in Figure 2(b), and use the recurrence in equation (1). We have $T - \{a, b\}$ and T' both in T^* and $\beta_1(T - \{a, b\}) = \beta_1 - 1$. Here, we are guaranteed that $\beta_1(T') = \beta_1 - k - 2$. Therefore, by the induction hypothesis,

$$\mu(T) \leq 2^{\beta_1-2} + 1 + 2^k (2^{\beta_1-k-3} + 1) = 2^{\beta_1-2} + 1 + 2^{\beta_1-3} + 2^k.$$

Since $1 \leq \beta_1(T') = \beta_1 - k - 2$, we have $k \leq \beta_1 - 3$ and then $\mu(T) \leq 2^{\beta_1-1} + 1$. \square

Lemma 4: Let $T \in T^*$ with $\beta_1 = \beta_1(T)$ and $t = t(T)$. Then $\beta_1 \geq 2t$.

Proof: If $T = K_2$, then $t(T) = 0$ and the conclusion follows. If $t = 1$, then $T \in \mathcal{T}_e$ and, for all such trees, $\beta_1(T) \geq 2 = 2t$. Assume $t > 1$ and that the result holds for all trees with fewer terminal subtrees. Now, let $T \in T^*$ with $t(T) = t$. From previous discussions and Figure 2(b), we know that $t(T') = t - 1$, $\beta_1(T') = \beta_1 - k - 2$, and $T' \in T^*$. Therefore, by the induction hypothesis,

$$\beta_1 - k - 2 \geq 2(t - 1).$$

Since $k \geq 0$, the result follows. \square

The bound of Theorem 3 can be improved when $t(T)$ is known. We will again make use of the iterated form of the recurrence formula described after Theorem 2.

Theorem 4: Let $T \in T^* - \{K_2\}$ with $\beta_1 = \beta_1(T)$ and $t = t(T)$. Then $\mu(T) \leq 3^{t-1} 2^{\beta_1-2t+1} + 2^{t-1}$.

Proof: When $t = 1$, the right-hand side reduces to $2^{\beta_1-1} + 1$, the bound given in Theorem 3. Suppose $T \in T^*$ with $t(T) = t \geq 2$ and that the result holds for all trees with fewer terminal subtrees. The iterated form of the recurrence in equation (1) is $\mu(T) = \mu(T'') + (2^{k+1} - 1)\mu(T')$, where T'' is as described in the discussion following Theorem 2. Then $\beta_1(T'') = \beta_1 - k - 1$ and $t - 1 \leq t(T'') \leq t$ and, since the bound increases as t decreases, we have by the induction hypothesis that

$$\mu(T'') \leq 3^{t-2} 2^{\beta_1-k-2t+2} + 2^{t-2} \quad \text{and} \quad \mu(T') \leq 3^{t-2} 2^{\beta_1-k-2t+1} + 2^{t-2}.$$

This gives

$$\begin{aligned} \mu(T) &\leq 3^{t-2} 2^{\beta_1-k-2t+2} + 2^{t-2} + (2^{k+1} - 1)(3^{t-2} 2^{\beta_1-k-2t+1} + 2^{t-2}) \\ &= 3^{t-2} 2^{\beta_1-k-2t+2} + 3^{t-2} 2^{\beta_1-2t+2} - 3^{t-2} 2^{\beta_1-k-2t+1} + 2^{k+1} 2^{t-2} \\ &= 3^{t-2} 2^{\beta_1-k-2t+1} + 3^{t-2} 2^{\beta_1-2t+2} + 2^{k+1} 2^{t-2} \end{aligned}$$

Suppose this bound is greater than $3^{t-1} 2^{\beta_1-2t+1} + 2^{t-1}$. Then we have

$$\begin{aligned} 2^{k+1} 2^{t-2} - 2^{t-1} &> 3^{t-1} 2^{\beta_1-2t+1} - (3^{t-2} 2^{\beta_1-2t+2} + 3^{t-2} 2^{\beta_1-k-2t+1}) \quad \text{or} \\ 2^{t-1} (2^k - 1) &> 3^{t-2} 2^{\beta_1-2t+1} (1 - 2^{-k}) \quad \text{or} \quad 2^{t-1} 2^k > 3^{t-2} 2^{\beta_1-2t+1}. \end{aligned}$$

Since $k \leq \beta_1 - 2t$, from the proof of Lemma 4, $2^{t-1} 2^{\beta_1-2t} > 3^{t-2} 2^{\beta_1-2t+1}$ or $2^{t-2} > 3^{t-2}$, a contradiction. \square

Trees achieving this bound are presented at the end of the next section.

3. NUMBER OF INDEPENDENT SETS

Now consider the number of independent sets of nodes in a tree. The counted sets must be distinct, but they need not be maximal, and we count the empty set. For example, the star $K_{1,n}$ has $2^n + 1$ independent sets of nodes. Denote this number by $\mu^*(T)$. Prodinger & Tichy [2] have shown, for an arbitrary tree on n nodes, that $F_{n+2} \leq \mu^*(T) \leq 2^{n-1} + 1$. The left inequality holds for a path on n nodes and the right for the star $K_{1,n-1}$. We shall derive these bounds in a manner which also exhibits a relationship between this and the original problem of counting the number of maximal independent sets of nodes.

In this section, let T^* be the tree obtained from the tree T by appending a single pendant edge to each node of T .

Lemma 5: For any tree T , $\mu(T^*) = \mu^*(T)$.

Proof: Let T have nodes $V(T) = \{v_1, v_2, \dots, v_n\}$ and T^* have additional nodes $\{w_1, w_2, \dots, w_n\}$, where w_i has v_i as its only neighbor, for $1 \leq i \leq n$. For any set of nodes S , it is immediate that S is an independent set of nodes in T if and only if $S^* = S \cup \{w_i | v_i \notin S\}$ is a maximal independent set of nodes in T^* . \square

If terminal subtrees are systematically removed from T^* until it is empty, one finds, as will be shown in Lemma 6, that the collection of identified root nodes forms a minimum node cover of the original tree T . The number of these covering nodes is equal to $\beta_1(T)$, a relationship that holds for any triangle-free graph [1, p. 171]. Let $\beta_0(T)$ be the node independence number of the tree T . Then, if T has n nodes, $n - \beta_0(T) = \beta_1(T)$ is the size of a smallest node cover of T .

Lemma 6: For any tree T , $t(T^*) = \beta_1(T)$.

Proof: Induct on the value of $t(T^*)$, and first consider the case in which $t(T^*) = 0$. Then $T^* = K_2$ and $T = K_1$, and the base case is established. Now, suppose T is a tree with $t(T^*) = m \geq 1$ and that the lemma holds for all similarly constructed trees T^* for which $t(T^*) < m$. Let S be any terminal subtree of T^* . Then $t(T^* - S) = t(T^*) - 1$ and, by the induction hypothesis,

$$t(T^* - S) = n - |S \cap T| - \beta_0(T - S \cap T) = n - \beta_0(T) - 1.$$

The result follows. \square

The number of nodes in T is $\beta_1(T^*)$ and, from Lemma 6 and Theorems 1, 2, and 4, we have the following bounds on $\mu^*(T)$.

Theorem 5: Let T be any tree on $n \geq 2$ nodes with $\beta_1 = \beta_1(T)$. Then

$$\max\{F_{n+2}, 2^{n-\beta_1} + 2^{\beta_1} - 1\} \leq \mu^*(T) \leq 3^{\beta_1-1} 2^{n-2\beta_1+1} + 2^{\beta_1-1}.$$

It is known [2] that $\mu^*(P_n) = F_{n+2}$, where P_n is the path on n nodes. Therefore, we have $\mu(T) = F_{\beta_1+2}$ for trees T constructed from a path on $\beta_1 = \beta_1(T)$ nodes with each node having one or more degree-one neighbors appended to it. These trees were introduced in the discussion prior to Theorem 1 and were shown to be a generalization of the extended paths given in [3]. The above has given an alternate proof for the number of MIS in such trees and reaffirms that they

represent an infinite class of trees having the smallest number of MIS for a given number of maximum independent edges.

An infinite class of trees satisfying the bounds of Theorem 4 can be constructed with the aid of Lemmas 5 and 6. First, we will form a tree T for which $\mu^*(T) = 3^{\beta_1-1}2^{n-2\beta_1+1} + 2^{\beta_1-1}$, the upper bound of Theorem 5. For any positive integers t and β_1 , $2t \leq \beta_1$, construct a star on $\beta_1 - t + 1$ nodes. Next, append a degree-one node to $t - 1$ of the leaf nodes of the star, as in Figure 3, and let this tree be T . Observe that $\beta_1(T) = t$, $t(T) = 1$, and the number of nodes is β_1 .

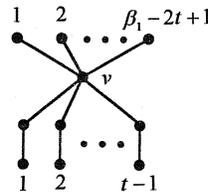


FIGURE 3

Now consider the number of independent sets of nodes in this tree. First, examine the independent sets of nodes not containing the center node v . Node v has $\beta_1 - 2t + 1$ degree-one neighbors that can be members of an independent set of nodes in 2^{β_1-2t+1} ways. It also has $t - 1$ degree-two neighbors, each with a degree-one neighbor. A degree-two node and its degree-one neighbor can contribute to an independent set of nodes in any of three ways: either node individually or neither node. Thus, there are 3^{t-1} ways to select independent sets of these nodes. Together, we have a total of $3^{t-1}2^{\beta_1-2t+1}$ ways to form independent sets of nodes not including node v . When node v is included, only the $t - 1$ nodes distance two from v can be used. There are 2^{t-1} such sets. The total now is $3^{t-1}2^{\beta_1-2t+1} + 2^{t-1}$ and, since $t = \beta_1(T)$ and β_1 is the number of nodes, T is a tree that leads to the upper bound of Theorem 5. Now, for any $n \geq 2\beta_1$, construct T^* by appending a degree-one node to every node of T . Then $\beta_1(T^*) = \beta_1$, $t(T^*) = t$, and Lemma 6 shows that the number of MIS in T^* is $3^{t-1}2^{\beta_1-2t+1} + 2^{t-1}$, the upper bound of Theorem 4. To obtain the desired number of nodes n , merely append a total of $n - 2\beta_1$ degree-one nodes to any node(s) already having at least one such neighbor.

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