The number of independent sets intersecting the set of leaves in trees

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Abstract

A subset $S \subseteq V(G)$ is independent if no two vertices of S are adjacent in G. In this paper we study the number of independent sets which meets the set of leaves in a tree. In particular we determine the smallest number and the largest number of these sets among n-vertex trees. In each case we characterize the extremal graphs.

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1 Introduction

In general we use the standard terminology and notation of graph theory, see [1]. Only simple undirected graphs are considered. By P_n, $n \geq 2$ we mean a graph with the vertex set $V(P_n) = \{x_1, ..., x_n\}$ and the edge set $E(P_n) = \{\{x_i, x_{i+1}\}; i = 1, ..., n-1\}$. Moreover P_1 is a graph with one vertex and P_0 is a graph with $V(P_0) = \emptyset$. By the *subdivision of an edge* $e = \{x, y\}$ of G we mean inserting a new vertex of degree 2 into the edge e. We denote it by $sub_{\{x,y\}}(G)$. If $\{x, y\} \in E(G)$ then we say that x is a *neighbor* of y. The set of all neighbors of x is called the *open neighborhood* of x and is denoted by $N(x)$. The set $N(x) \cup \{x\}$ we call the *closed neighborhood* and we write $N[x]$. For a subset $X \subseteq V(G)$ we put $N(X)$ and $N[X]$ instead of $\bigcup_{x \in X} N(x)$ and $\bigcup_{x \in X} N[x]$, respectively. Let $X \subset V(G) \cup E(G)$. By $G \setminus X$ we denote the graph obtained from G by deleting the set X and all edges incident with a vertex in X. The *Fibonacci numbers* are defined recursively by $F_0 = F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$, for $n \geq 2$.

A subset $S \subset V(G)$ is an *independent set* of G if no two vertices of S are adjacent in G. Moreover the empty set and a subset containing exactly one vertex also are independent in G.

The number of independent sets in G is denoted by $NI(G)$. For graph G on $|V(G)| = \emptyset$ we put $NI(G) = 1$. Let x be an arbitrary vertex of $V(G)$. By $\mathcal{F}_x$ we denote the family of all independent sets S of G such that $x \in S$. By $\mathcal{F}_{-x}$ we denote the family of all independent sets S of G such that $x \notin S$. Of course $\mathcal{F} = \mathcal{F}_x \cup \mathcal{F}_{-x}$ is the family of all independent sets in G and $NI(G) = |\mathcal{F}| = |\mathcal{F}_x| + |\mathcal{F}_{-x}|$. In the chemical literature the graph parameter $NI(G)$ is referred to as the Merrifield-Simmons index, see [7]. The study of the number $NI(G)$ of independent sets in a graph was initiated in [9]. The problem of counting the number of independent sets in a graph is NP-complete (see for instance [10]). However for certain types of graphs, the problem of determining their number of independent subsets is polynomial. For instance Prodinger and Tichy [9] proved that $NI(P_n)$ is the sequence of Fibonacci numbers. It is interesting to know that

$$NI(P_n) = F_{n+1} \qquad (1)$$

They also named the number $NI(G)$ as the Fibonacci number of graph. The literature includes many papers dealing with the theory of counting of independent sets in graphs, see [2, 3, 4, 6, 8]. In particular characterization of extremal trees with some independence properties has been considered in a number of papers, for instance [5, 11, 12, 13, 14]. In what follows T stands for a tree with the vertex set $V(T)$, $|V(T)|$ denotes the cardinality of $V(T)$. It has been proved:

Theorem 1 *[9] Let T be an n-vertex tree. Then $F_{n+1} \leq NI(T) \leq 2^{n-1}+1$.*

In [5] Lin and Lin proved that $NI(T) = F_{n+1}$ if and only if $T = P_n$ and $NI(T) = 2^{n-1} + 1$ if and only if $T = K_{1,n-1}$.
Recall that a vertex of degree 1 is called a *leaf.* For $x \in V(T)$ denote by $L(x)$ the set of leaves attached to the vertex x. Further we let $|L(x)| = l(x)$. The vertex $x \in V(T)$ with $L(x) \neq \emptyset$ is called a *support vertex.* If $l(x) \geq 2$ then x is named as a *strong support vertex.* If $l(x) = 1$ then x is named a *weak support vertex* and the unique leaf attached to the weak support vertex we call a *single-leaf.* The set of all support vertices in T we denote by $S(T)$ and the set of leaves in T we denote by L.

A vertex $x \in V(T)$ is penultimate if x is not a leaf and x is adjacent to at least $deg_T x - 1$ leaves. Note that x is adjacent to $deg_T x$ leaves if and only if x is the center of a star $K_{1,n-1}$. Every n-vertex tree T with $n \geq 3$ has a penultimate vertex.
Let $\widetilde{T}$ be an arbitrary tree. From now on for a tree T with $|V(T)| \geq 3$ by *$\widetilde{T}$-addition* we mean a local augmentation which is the operation $T \mapsto ad_{\widetilde{T}(x,y)}(T)$ of adding to the vertex $x \in V(T)$ a graph $\widetilde{T}$ so that a vertex x is identified with a fixed vertex $y \in V(\widetilde{T})$.
In this paper we consider independent sets intersecting the set of leaves. In particular we study independent sets S of T such that for every $x \in S(T)$, $S \cap L(x) \neq \emptyset$ i.e., S contains for each support vertex at least one leaf. Next we calculate the number of all independent sets which contain L as a subset. In each case we characterize extremal trees.

2 The number of independent sets intersecting the set L(x) for each x ∈ S(T)

By $NI_l(T)$ we denote the total number of independent sets in T such that for every $x \in S(T)$, $S \cap L(x) \neq \emptyset$. It is obvious that every n-vertex tree, $n \geq 3$ has such independent sets. The following Theorem gives the basic rule for counting these independent sets.

Theorem 2 *Let T be an n-vertex tree, $n \geq 3$. Then*

$$NI_l(T) = \prod_{x \in S(T)} (2^{l(x)} - 1) NI(T \setminus N[L]).$$

P R O O F: Let $S(T)$ be the set of all support vertices of the tree T. Assume that $\mathcal{F}$ is a family of all independent sets such that if $S \in \mathcal{F}$ then for every $x \in S(T)$, $S \cap L(x) \neq \emptyset$. Let $l(x)$ be the number of leaves attached to the vertex x in T. Assume that $L(x) = \{z_1, .., z_{l(x)}\}$, $l(x) \geq 1$. Then for every $\emptyset \neq L'(x) \subseteq L(x)$ there is an independent set $S \in \mathcal{F}$ such that $L'(x) \subset S$. Consequently we have $2^{l(x)} - 1$ such subsets for every $x \in S(T)$. Since at least one vertex from $L(x)$ belongs to S, it is easily seen that $x \notin S$. So $S = S^* \cup \bigcup_{x \in S(T)} L'(x)$ where S^* is an arbitrary independent set of the graph $T \setminus N[L]$. Hence by the fundamental combinatorial statements we have that $NI_l(T) = \prod_{x \in S(T)} (2^{l(x)} - 1) NI(T \setminus N[L])$.

Thus the Theorem is proved. □

From Theorem 2 immediately follows:

Corollary 1 *Let T be an n-vertex tree, $n \geq 3$. Then $NI_l(T) = \prod_{x \in S(T)} (2^{l(x)} - 1)$ if and only if every vertex from $V(T)$ is either a leaf or a support vertex.*

Theorem 3 *Let T be an n-vertex tree, $n \geq 3$. Then $1 \leq NI_l(T) \leq 2^{n-1} - 1$. Furthermore $NI_l(T) = 1$ if and only if every vertex from $V(T)$ is either a single-leaf or a weak support vertex and $NI_l(T) = 2^{n-1} - 1$ if and only if $T = K_{1,n-1}$.*

P R O O F: Let T be an n-vertex tree with $n \geq 3$. The lower bound for the number $NI_l(T)$ immediately follows from Corollary 1. If $T = K_{1,n-1}$ then it is obvious that $NI_l(T) = 2^{n-1} - 1$. We shall prove that for every $T \neq K_{1,n-1}$, $NI_l(T) < 2^{n-1} - 1$. Let $T \neq K_{1,n-1}$. Then $|S(T)| \geq 2$. Assume that $|S(T)| = s$, $s \geq 2$ and for $x_i \in S(T)$, $i = 1, ..., s$, $|L(x_i)| = l(x_i)$. It is clear that $n = s + \sum_{i=1}^{s} l(x_i) + p$ where $p = |V(T)| - (|S(T)| + |L|)$. Let $\mathcal{F}^*$

be the family of all independent sets S of T such that for every $x \in S(T)$, $S \cap L(x) \neq \emptyset$. Let $S \in \mathcal{F}^*$. Then it is obvious that $S \cap S(T) = \emptyset$. Hence $S = \bigcup_{i=1}^{s} S_i \cup S'$ where S_i is an arbitrary nonempty subset of $L(x_i)$ for every $i = 1, ..., s$ and S' is an arbitrary independent set of the graph $T \setminus (S(T) \cup L)$. Denote $T' = T \setminus (S(T) \cup L)$. By previous assumptions $|V(T')| = p$ hence there are at most 2^p independent sets in the graph T'. By the Theorem 2 we have that $NI_l(T) = \prod_{i=1}^{s} (2^{l(x_i)} - 1) NI(T') < \prod_{i=1}^{s} 2^{l(x_i)} 2^p = 2^{p + \sum_{i=1}^{s} l(x_i)} = 2^{n-s}$. By $s \geq 2$ immediately follows that $2^{n-s} < 2^{n-1} - 1$ what gives that $NI_l(T) < NI_l(K_{1,n-1}) = 2^{n-1} - 1$.

Thus the Theorem is proved. □

Theorem 4 *Let $n \geq 3$ be integer. Then $NI_l(P_n) = F_{n-3}$.*

P R O O F: Let $V(P_n) = \{x_1, ..., x_n\}$, $n \geq 3$ and vertices be numbered in the natural fashion. Then $S(T) = \{x_2, x_{n-1}\}$. Let $S \subset V(P_n)$ be an arbitrary independent set of P_n such that for every $x \in S(T)$, $L(x) \cap S \neq \emptyset$. Hence $x_1, x_n \in S$. This means that $S = S' \cup \{x_1, x_n\}$, where S' is an arbitrary independent set of the graph $P_n \setminus \{x_1, x_2, x_{n-1}, x_n\}$ which is isomorphic to P_{n-4}. Since (1) gives exactly F_{n-3} sets S' we have $NI_l(P_n) = F_{n-3}$, that completes the proof. □

3 The total number of independent sets containing L as a subset

In this section we study the number of all independent sets including all leaves. By $NI_L(T)$ we denote the total number of independent sets in T including the set L. It is easily seen that $NI_L(T) = NI(T \setminus N[L])$. Let $\mathcal{F}_L$ be the family of all independent sets of T including L. Then $|\mathcal{F}_L| = |\mathcal{F}'|$, where $\mathcal{F}'$ is the family of all independent sets in $T \setminus N[L]$

Let x be an arbitrary vertex of $V(T)$. By $\mathcal{F}_{L,x}$ we denote the family of all independent sets including L such that $x \in S$. By $\mathcal{F}_{L,-x}$ we denote the family of all independent sets including L such that $x \notin S$. Evidently $\mathcal{F}_{L,x} \cup \mathcal{F}_{L,-x} = \mathcal{F}_L$ is the family of all independent sets including L in T. Then the basic rule for counting independent sets including L in T is as follows $NI_L(T) = |\mathcal{F}_L| = |\mathcal{F}_{L,x}| + |\mathcal{F}_{L,-x}|$.

Theorem 5 *Let T be an arbitrary n-vertex tree, $n \geq 3$. Then $NI_L(T) \geq 1$ with equality if and only if each vertex of $V(T)$ is either a leaf or a support vertex.*

P R O O F: Let T be an arbitrary tree with $n \geq 3$ and $L \subset V(T)$ be the set of leaves of T. The inequality is obvious. Denote $T' = T \setminus N[L]$. Of course

$N[L] = S(T) \cup L$. Assume that $V(T) = S(T) \cup L$. Let S be an arbitrary independent set including L in T. Then $L \subseteq S$. Moreover by the definition of independent set $S(T) \cap S = \emptyset$. By the assumption of T we deduce that T' is the empty graph. Consequently $S = L$ is the unique independent set including L in T. Conversely assume now that $NI_L(T) = 1$ and let S be the unique independent set including the set L in T. Of course $S = L \cup S^*$ where S^* is the unique independent set of T'. Assume on the contrary that there is a vertex $x \in V(T) \setminus (S(T) \cup L)$. This gives that $N[L] \cap \{x\} = \emptyset$. Consequently $x \in V(T')$. Let $\mathcal{F}'$ be a family of all independent sets of T'. Then it is obvious that the empty set and a subset containing the vertex x belong to the family $\mathcal{F}'$. Hence $|\mathcal{F}'| \geq 2$ so $NI_L(T) \geq 2$ what gives a contradiction that S is the unique independent set including L in T.

Thus the Theorem is proved. □

Theorem 6 *Let T be an arbitrary n-vertex tree, $n \geq 3$. Then $NI_L(T) \leq F_{n-3}$ with equality for $T = P_n$.*

P R O O F: Firstly we shall prove that $NI_L(P_n) = F_{n-3}$. Let $V(P_n) = \{x_1, ..., x_n\}$, $n \geq 3$ and vertices are numbered in natural fashion. Let $S \subset V(P_n)$ be an arbitrary independent set of P_n such that $x_1, x_n \in S$. Hence by Theorem 4 we obtain that $NI_L(P_n) = NI^*(P_n) = F_{n-3}$. Now we prove that for every n-vertex tree $NI_L(T) \leq NI_L(P_n)$. If $T = K_{1,p}$, $p \geq 2$, then the inequality is obvious. Let $T \neq K_{1,p}$, $p \geq 2$. To avoid trivialities assume that $n \geq 5$ and $T \neq P_n$. Let $X \subseteq S(T)$ be the set of strong support vertices of T and $L(x) = \{z_1, ..., z_{l(x)}\}$, $l(x) \geq 2$ be the set of leaves attached to the vertex x. Assume that z_i, $1 \leq i \leq l(x)$ be a fixed vertex of $L(x)$. Then it is easy to observe that $NI_L(T) = NI_L(T \setminus \{z_i\})$. Let u be a penultimate vertex of T and $v \in N(u) \setminus L(u)$. The existence of the vertex v gives the fact that $T \neq K_{1,n-1}$.

Claim (1). $NI_L(T) \leq NI_L(sub_{\{u,v\}}(T \setminus \{z_i\})$.

Denote $T' = sub_{\{u,v\}}(T \setminus \{z_i\})$ and let $\mathcal{F}_L$ and $\mathcal{F}'_L$ be the families of all independent sets including the set of leaves in T and in T', respectively. By the basic rule for counting independent sets including L we have that $NI_L(T') = |\mathcal{F}'_L| = |\mathcal{F}'_{L,u}| + |\mathcal{F}'_{L,-u}|$. Since u is the penultimate vertex in T hence by the definition of the subdivision of edge $\{u, v\}$ it follows that u is the penultimate vertex in T', too. Let $S \in \mathcal{F}'_L$. Then it is obvious that $u \notin S$. This implies that $NI_L(T') = |\mathcal{F}'_{L,-u}|$. Let z be a vertex inserted into edge $\{u, v\}$. Of course $|\mathcal{F}'_{L,-u}| = |\mathcal{F}'_{L,z}| + |\mathcal{F}'_{L,-z}| = |\mathcal{F}'_{L,z}| + NI_L(T)$, which ends the proof of this claim.

From the above it is clear that there is an n-vertex tree $\widetilde{T}$ such that $NI_L(\widetilde{T}) \geq NI_L(T)$ and for every $x \in S(\widetilde{T})$, x is a weak support vertex. Let $Y \subset S(\widetilde{T})$ be the set of week support vertices and every $y \in Y$ is not penultimate. Assume that $y \in Y$ and $L(y) = \{w\}$. Let u' be a penultimate vertex in $\widetilde{T}$ and $v' \in N(u') \setminus L(u')$.

Claim (2). $NI_L(\widetilde{T}) \leq NI_L(sub_{\{u',v'\}}(\widetilde{T} \setminus \{w\}))$.

We prove this claim analogously as Claim (1).

Consequently we can construct an n-vertex tree T^* with $NI_L(T^*) \geq NI_L(\widetilde{T})$ such that T^* does not have strong support vertices and every week support vertex is penultimate. If $T^* \neq P_n$, then there is $x' \in V(T^*)$ and P_t, P_m, for $t, m \geq 3$ are subgraphs of T^* attached to the vertex x'.

Claim (3). $NI_L(T^*) \leq NI_L(ad_{P_t(w',x')}(T^* \setminus (P_t \setminus \{x'\}))$ where w' is the end vertex of P_m which is identified with the initial vertex x' of P_t.

Denote $T'' = ad_{P_t(w',x')}(T^* \setminus (P_t \setminus \{x'\}))$. Let $\mathcal{F}_L^*$ and $\mathcal{F}_L''$ are families of all independent sets including the set of leaves in T^* and in T'', respectively. By the general rule for counting independent sets we have that $NI_L(T^*) = |\mathcal{F}^*_{L,x'}| + |\mathcal{F}^*_{L,-x'}|$. Let $S \in \mathcal{F}^*_L$. Of course $w' \in S$. Denote $S_1 = S \cap V(T^* \setminus (P_t \cup P_m))$, $S_2 = S \cap V(P_m)$ and $S_3 = S \cap V(P_t)$. Evidently if $x' \in S$ then $x' \in S_2 \cap S_3$. Since $NI_L(T'') = |\mathcal{F}''_{L,x'}| + |\mathcal{F}''_{L,-x'}|$ two possible cases should be distinguished:

(1) $x' \in S$

In this case $S_1 \cup S_2 \cup S_3$ is an independent set of T'' including the set of leaves. Hence $|\mathcal{F}^*_{L,x'}| \leq |\mathcal{F}''_{L,x'}|$.

(2) $x' \notin S$

Let $y' \in N(x') \cap V(P_t)$. If $y' \in S$ then $S_1 \cup S_2 \cup S_3 \setminus \{w'\}$ is an independent set including the set of leaves in T''. If $y' \notin S$ then $S_1 \cup S_2 \cup S_3$ is an independent set including the set of leaves in T''.

Consequently from the above possibilities and by fundamental combinatorial statements we have that $|\mathcal{F}^*_{L,-x'}| \leq |\mathcal{F}''_{L,-x'}|$.

Finally we obtain that $NI_L(T^*) = |\mathcal{F}^*_{L,x'}| + |\mathcal{F}^*_{L,-x'}| \leq |\mathcal{F}''_{L,x'}| + |\mathcal{F}''_{L,-x'}| = NI_L(T'')$.

Hence by Claim (3) we deduce that $NI_L(P_n) \geq NI_L(T'')$, which ends the proof. □

References

[1] R.Diestel, *Graph Theory*, Springer-Verleg, Heideberg, New-York. Inc., (2005).

[2] G.Hopkins, W.Staton, *Some idenities arising from the Fibonacci numbers of certains graphs*, The Fibonacci Quarterly (1984) 225-228.

[3] M.J.Chou, G.J.Chang, *Survey on counting maximal independent sets*, in; S.Tangmance, E.Schulz (Eds.), Proceedings of the Second Asian Mathematical Conference, Word Scientific, Singapore (1995) 265-275.

[4] M.Jou, G.J.Chang *Maximal independent sets in graphs with at most one cycle*, Discrete Appl. Math. 79 (1997) 67-73.

[5] S.B.Lin, C.Lin, *Trees and forests with large and small independent indices*, Chinese J. Math. 23 (3) (1995) 199-210.

[6] M.Kwaśnik, I.Włoch, *The total number of generalized stable sets and kernels of graphs*, Ars Combinatoria 55(2000), 139-146.

[7] R.E.Merrifield, H.E.Simmons, *Topological Methods in Chemistry*, John Wiley & Sons, New York, 1989.

[8] A.S.Pedersen, P.D.Vestergaard, *The number of independent sets in unicyclic graphs*, Discrete Appl. Math. 152 (2005) 246-256.

[9] H.Prodinger, R.F.Tichy, *Fibonacci numbers of graphs*, Fibonacci Quarterly 20, (1982) 16-21.

[10] D.Roth, *On the hardness of aproximate reasoning*, Artif. Intell. 82 (1996) 273-302.

[11] B.E.Sagan, *A note on independent sets in trees*, SIAM J.Alg.Discrete Math. Vol 1, No 1, February (1988) 105-108.

[12] H.Wilf, *The number of maximal independent sets in a tree*, SIAM J.Alg. Discrete Math. Vol 7, No 1, January, (1986) 125-130.

[13] I.Włoch, *Generalized Fibonacci polynomial of graphs*, Ars Combinatoria, 68(2003) 49-55.

[14] J.Zito, *The stucture and maximum number of maximum independent sets in trees*, J.Graph Theory 15(2), (1991), 207-221.