

# On the 2-Independence Number of Connected Graphs

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## Abstract

The distance between two vertices  $u$  and  $v$  in a graph  $G$  equals the length of a shortest path from  $u$  to  $v$ . A set  $S$  of vertices is a 2-independent set if the distance between any two elements in  $S$  is greater than two in  $G$ . The 2-independence number of a graph  $G$ , denoted by  $\alpha_2(G)$ , is the maximum size of a 2-independent set in  $G$ . In this paper, we determine a sharp upper bound for the 2-independence number in a connected graph and provide a characterization of the connected graphs achieving this sharp upper bound.

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## 1 Introduction

All graphs considered in this paper are finite, loopless, and without multiple edges. For a graph  $G$ ,  $V(G)$  and  $E(G)$  denote the *vertex set* and the *edge set* of  $G$ , respectively. A  $u$ - $v$  path  $P : u = v_1, v_2, \dots, v_k = v$  of  $G$  is a sequence of  $k$  vertices in  $G$  such that  $v_i v_{i+1} \in E(G)$  for  $i = 1, 2, \dots, k - 1$ . Denote by  $P_n$  a  $n$ -path with  $n$  vertices. The *length* of  $P_n$  is  $n-1$ . For any two vertices  $u$  and  $v$  in  $G$ , the *distance between  $u$  and  $v$* , denoted by  $\text{dist}_G(u, v)$ , is the minimum length of all  $u$ - $v$  paths in  $G$ . A set  $S$  of vertices is a  $k$ -independent set if the distance between any two elements in  $S$  is greater than  $k$  in  $G$ . The  $k$ -independence number of a graph  $G$ , denoted by  $\alpha_k(G)$ , is the maximum size

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of a  $k$ -independent set in  $G$ . The study of the number of independent sets in a graph has a rich history. Finding a  $k$ -independent set of a graph is NP-hard (see [6], [7]). A. Abiad, G. Coutinho and M.A. Fiol [1] found the spectral bounds on the  $k$ -independence number of a graph. For some cases, they also showed that the bounds are sharp. Jou [3] determined the  $k$ -th largest number of 2-independent sets among all extra-free forest of order  $n \geq 2$ , where  $k = 1, 2$  and 3. Extremal graphs achieving these values are also given. Min-Jen Jou and Jenq-Jong Lin [4] considered the problem of determining the small numbers of maximal 2-independent sets among all trees of order  $n$ . Extremal graphs achieving these values are also given. Min-Jen Jou, Jenq-Jong Lin and Qian-Yu Lin [5] determined a sharp upper bound for the 2-independence number in a tree. We also provided a constructive characterization of the extremal trees achieving this sharp upper bound. In this paper, we determine a sharp upper bound for the 2-independence number in a connected graph and provide a characterization of the connected graphs achieving this sharp upper bound.

## 2 A sharp upper bound

In this section, we determine a sharp upper bound for the 2-independence number in a connected graph. First, we introduce some notations.

The (open) *neighborhood*  $N_G(v)$  of a vertex  $v$  is the set of vertices adjacent to  $v$  in  $G$ , and the *closed neighborhood*  $N_G[v]$  is  $N_G[v] = N_G(v) \cup \{v\}$ . The *degree* of  $v$  is the cardinality of  $N_G(v)$ , denoted by  $\deg_G(v)$ . A vertex  $x$  is said to be a *leaf* if  $\deg_G(x) = 1$ . A vertex of  $G$  is a *support vertex* if it is adjacent to a leaf in  $G$ . We denote by  $L(G)$  and  $U(G)$  the collections of the leaves and support vertices of  $G$ , respectively. Two leaves  $x$  and  $x'$  are called *duplicated leaves* in a graph  $G$  if they are adjacent to the same support vertex. The *closed 2-neighborhood*  $N_G^2[v]$  of a vertex  $v$  is the set of the vertices  $u$  satisfying  $\text{dist}_G(u, v) \leq 2$  and the (open) *2-neighborhood* is  $N_G^2(v) = N_G^2[v] - \{v\}$ . For any subset  $A$ , denote  $N_G^2[A] = \bigcup_{v \in A} N_G^2[v]$  and  $N_G^2(A) = \bigcup_{v \in A} N_G^2(v)$ . Let  $L^*(G) = \{x : x \in L(G), |N_G^2[x] \cap L(G)| = 1\}$ . A connected graph is said to be *fresh* if  $L(G) = L^*(G)$ . A 2-independent set  $S$  of  $G$  is called a  $\alpha_2$ -*set* if  $|S| = \alpha_2(G)$ . For a subset  $A \subseteq V(G)$ , the *induced subgraph*  $\prec A \succ_G$  of a graph  $G$  is a subgraph  $G' = (A, E(G'))$ , where  $E(G') = \{uv : u, v \in A, uv \in E(G)\}$ . For a subset  $A \subseteq V(G)$ , the *deletion of  $A$  from  $G$*  is the graph  $G - A$  obtained by removing all vertices in  $A$  and all edges incident to these vertices. For a subset  $B \subseteq E(G)$ , the *edge-deletion of  $B$  from  $G$*  is the graph  $G - B$  obtained by removing all edges of  $B$ . For two different sets  $A$  and  $B$ , written  $A - B$ , is the set of all elements of  $A$  that are not elements of  $B$ . A *forest* is a graph with no cycles, and a *tree* is a connected forest. For other undefined notations, the reader is referred to [2] for graph theory.

The following are the useful lemmas.

**Lemma 2.1.** *Let  $H$  be a deletion of a connected graph  $G$ . If  $H$  is connected, then  $\alpha_2(H) \leq \alpha_2(G)$ .*

*Proof.* Let  $S$  be a  $\alpha_2$ -set of  $H$ . Thus  $S$  is a 2-independent set of  $G$ . Hence  $\alpha_2(H) = |S| \leq \alpha_2(G)$ , which completes the proof.  $\square$

**Lemma 2.2.** *Let  $G'$  be an edge-deletion of a connected graph  $G$ . If  $G'$  is connected, then  $\alpha_2(G) \leq \alpha_2(G')$ .*

*Proof.* Let  $S$  be a  $\alpha_2$ -set of  $G$ . For two distinct vertices  $u$  and  $v$  of  $S$ ,  $\text{dist}_{G'}(u, v) \geq \text{dist}_G(u, v) \geq 3$ . Thus  $S$  is a 2-independent set of  $G'$ . Hence  $\alpha_2(G) = |S| \leq \alpha_2(G')$ , which completes the proof.  $\square$

**Lemma 2.3.** *Let  $G$  be a connected graph. Then there exists a  $\alpha_2$ -set  $S$  satisfying  $L^*(G) \subseteq S$ .*

*Proof.* Let  $S$  be a  $\alpha_2$ -set of  $G$ . If  $L^*(G) \subseteq S$ , then we are done. So we assume that  $L^*(G) - S = \{x_1, \dots, x_t\}$ , where  $t \geq 1$ . Let  $u_i$  be a vertex of  $S$  such that  $\text{dist}_G(u_i, x_i)$  is as small as possible. Then  $\text{dist}_G(x_i, u_i) \leq 2$  for all  $i$ . Let  $S^* = (S - \{u_1, \dots, u_t\}) \cup \{x_1, \dots, x_t\}$ . So  $|S^*| \geq |S| = \alpha_2(G)$ . We can see that  $\text{dist}_G(x_i, x_j) \geq 3$  for all  $i \neq j$ . For  $w \in S^*$  and  $w \neq x_i$ ,  $\text{dist}_G(x_i, w) \geq \text{dist}_G(u_i, w) \geq 3$ . Hence  $S^*$  is a  $\alpha_2$ -set of  $G$  satisfying  $L^*(G) \subseteq S^*$ .  $\square$

**Lemma 2.4.** *Let  $G$  be a connected graph of order  $|G| \geq 3$ . If  $x$  and  $x'$  are duplicated leaves of  $G$  and  $N_G(x) = N_G(x')$ , then  $\alpha_2(G - \{x'\}) = \alpha_2(G)$ .*

*Proof.* Let  $x \in L^*(G)$ . By Lemma 2.3, there exists a  $\alpha_2$ -set  $S$  of  $G$  satisfying  $x \in S$ . So  $S$  is a  $\alpha_2$ -set of  $G - \{x'\}$ . Hence  $\alpha_2(G - \{x'\}) = |S| = \alpha_2(G)$ , which completes the proof.  $\square$

**Theorem 2.5.** [5] *Let  $T$  be a tree of order  $|T| \geq 2$ . Then  $\alpha_2(T) \leq \lfloor \frac{|T|}{2} \rfloor$  and the upper bound is sharp.*

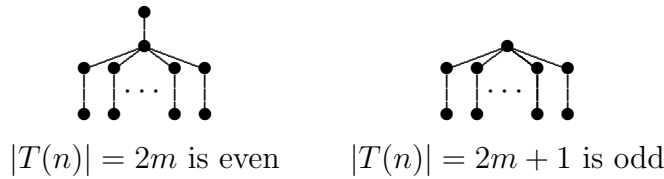


Figure 1: The tree  $T(n)$ , where  $\lfloor \frac{n}{2} \rfloor = m \geq 1$ .

Let  $T(n)$  be as in Figure 1, where  $\lfloor \frac{n}{2} \rfloor = m$ . We can see that  $\alpha_2(T(n)) = m$ , as a result, the upper bound in Theorem 2.6 is sharp.

**Theorem 2.6.** *Let  $G$  be a graph of order  $|G| \geq 2$ . Then  $\alpha_2(G) \leq \lfloor \frac{|G|}{2} \rfloor$  and the upper bound is sharp.*

*Proof.* Let  $T$  be a spanning tree of  $G$ . Then  $|T| = |G|$ . By Lemma 2.2 and Theorem 2.5,  $\alpha_2(G) \leq \alpha_2(T) \leq \lfloor \frac{|T|}{2} \rfloor = \lfloor \frac{|G|}{2} \rfloor$ , which completes the proof.  $\square$

### 3 Characterization

In this section, we provide a characterization of the connected graphs achieving this sharp upper bound in Theorem 2.6. For the convenience of the characterization, let  $\mathcal{G}(m)$  be the set of connected graph  $G$  satisfying  $\alpha_2(G) = \lfloor \frac{|G|}{2} \rfloor = m$ , where  $m \geq 1$ . Then  $|G| = 2m$  or  $2m + 1$  for every  $G \in \mathcal{G}(m)$ . We want to construction  $\mathcal{G}(m)$  for all  $m \geq 1$ . Due to the construction, we first mention two sets  $\mathcal{H}_1(m)$  and  $\mathcal{H}_2(m)$ . They are collections of some connected graphs  $G$ .

(I)  $\mathcal{H}_1(m) = \{G : G \text{ hold the following properties } a \text{ and } b\}$ .

(a)  $|L^*(G)| = m$ .

(b)  $\prec V(G) - L^*(G) \succ_G$  is connected.

(II)  $\mathcal{H}_2(m) = \{G : G \text{ hold the following properties } c, d \text{ and } e\}$ .

(c)  $|L^*(G)| = m - 1$ .

(d)  $\prec V(G) - L^*(G) \succ_G$  is connected.

(e)  $C = \{w_1, w_2, w_3\} = V(G) - N_G[L^*(G)]$  and  $N_G(w_1) = \{w_2, w_3\}$ .

The following Theorem is the main theorem.

**Theorem 3.1.** *For  $m \geq 1$ ,  $\mathcal{G}(m) = \bigcup_{i=1}^2 \mathcal{H}_i(m)$ .*

Suppose that  $G \in \mathcal{H}_i(m)$  for some  $i$ , where  $m \geq 1$ , we can see that  $G$  is a connected graph satisfying  $\alpha_2(G) = \lfloor \frac{|G|}{2} \rfloor = m$ . Hence we obtain that  $\mathcal{H}_i(m) \subseteq \mathcal{G}(m)$  for  $i = 1, 2$ . On the other hand, we will prove  $\mathcal{G}(m) \subseteq \bigcup_{i=1}^2 \mathcal{H}_i(m)$  and we prove it through a sequence of lemmas.

**Lemma 3.2.** *For  $n \geq 3$ ,  $\alpha_2(C_n) = \lfloor \frac{n}{3} \rfloor$ .*

*Proof.* Let  $V(C_n) = \{v_1, v_2, \dots, v_n\}$  and  $\lfloor \frac{n}{3} \rfloor = k$ . Then  $S = \{v_3, \dots, v_{3k}\}$  is a 2-independent set of  $C_n$ , so  $\alpha_2(C_n) \geq |S| = k$ . Suppose, by contradiction,  $\alpha_2(C_n) \geq k + 1$  and  $S^* = \{v_{s_1}, \dots, v_{s_{k+1}}\}$  is a 2-independent set of  $C_n$ , where  $s_1 < s_2 < \dots < s_{k+1}$ . Then  $\text{dist}_{C_n}(v_{s_i}, v_{s_{i+1}}) \geq 3$  for  $i = 1, \dots, k$  and  $\text{dist}_{C_n}(v_{s_1}, v_{s_{k+1}}) \geq 3$ . Then  $|C_n| \geq 3k + 3 > n$ . This is a contradiction, so  $\alpha_2(C_n) \leq k$ . Thus  $\lfloor \frac{n}{3} \rfloor = k \leq \alpha_2(C_n) \leq k = \lfloor \frac{n}{3} \rfloor$ , which completes the proof.  $\square$

**Lemma 3.3.** *Let  $G \in \mathcal{G}(m)$  and  $|G| = 2m$ , where  $m \geq 1$ . Then the following hold.*

(i)  $|L(G)| = |L^*(G)| = m$ .

(ii) *The induced subgraph  $\prec V(G) - L(G) \succ_G$  is connected.*

*Proof.* If  $L(G) = \emptyset$ , by Lemma 2.2 and Lemma 3.2,  $m \leq \alpha_2(G) \leq \alpha_2(C_{2m}) = \lfloor \frac{2m}{3} \rfloor < m$ . This is a contradiction, so  $L(G) \neq \emptyset$ .

**Claim 1.**  $L(G) = L^*(G)$ . Suppose, by contradiction,  $x$  and  $x'$  are duplicated leaves of  $G$  and  $N_G(x) = N_G(x')$ . By Lemma 2.4 and Theorem 2.6,  $m = \alpha_2(G) = \alpha_2(G - \{x'\}) \leq \lfloor \frac{2m-1}{2} \rfloor = m - 1$ . This is a contradiction, so  $L(G) = L^*(G)$ .

(i) We prove it by induction on  $m$ . We can see that  $\mathcal{G}(1) = \{P_2, P_3, C_3\}$ . If  $|G| = 2$  is even, this means that  $G = P_2$ . So it's true for  $m = 1$ . Assume that it's true for  $m - 1$ , where  $m \geq 2$ . Let  $G \in \mathcal{G}(m)$  and  $|G| = 2m$ . Let  $u_0 \in L(G)$  and  $u'_0 \in N_G(u_0)$ . Suppose  $G' = G - \{u_0, u'_0\}$ , by Claim 1, then  $G'$  is a connected graph of order  $|G'| = 2(m - 1)$ . By Theorem 2.6,  $m - 1 \leq \alpha_2(G') \leq \lfloor \frac{|G'|}{2} \rfloor = \lfloor \frac{|G|}{2} \rfloor - 1 = m - 1$ . The equalities hold, so  $\alpha_2(G') = \lfloor \frac{|G'|}{2} \rfloor = m - 1$ . Hence  $G' \in \mathcal{G}(m - 1)$ , by the induction hypothesis,  $|L(G')| = |L^*(G')| = m - 1$ . Let  $L_1 = L^*(G') = L(G') = \{u_1, \dots, u_{m-1}\}$  and  $U_1 = \{u'_1, \dots, u'_{m-1}\}$ , where  $u'_i \in N_{G'}(u_i)$  for  $i = 1, \dots, m - 1$ . So  $V(G') = L_1 \cup U_1$ .

**Claim 2.**  $u'_0 \notin N_G(L_1)$ . Suppose, by contradiction,  $A = N_G(u'_0) \cap L_1 \neq \emptyset$  and  $B = L_1 - A$ . Let  $A' = N_{G'}(A)$  and  $B' = N_{G'}(B)$ , where  $|A| = |A'| = a$  and  $|B| = |B'| = b$ . By Lemma 2.3, there exists a  $\alpha_2$ -set  $S$  of  $G$  satisfying  $L(G) \subset S$ . Then  $u_0 \in S$  and  $A \cap S = \emptyset$ . Since  $G$  is connected,  $N_{G'}^2(A') \cap B \neq \emptyset$ . Then  $|A' \cap S| \leq a - 1$  and  $m = \alpha_2(G) = |\{u_0\}| + |A' \cap S| + |B| \leq 1 + (a - 1) + b = a + b = m - 1$ . This is a contradiction, so  $u'_0 \notin N_G(L_1)$ .

By Claim 2, we have that  $L(G) = L^*(G) = \{u_0, u_1, \dots, u_{m-1}\}$  and  $|L(G)| = |L^*(G)| = m$ .

(ii) Since  $G$  is connected, this implies that  $\prec V(G) - L(G) \succ_G$  is connected.  $\square$

**Lemma 3.4.** Let  $G \in \mathcal{G}(m)$  and  $|G| = 2m + 1$ , where  $m \geq 1$ . If  $G$  have duplicated leaves, then  $|L^*(G)| = |L(G)| - 1 = m$ .

*Proof.* By lemma 2.4, suppose  $G'$  is a fresh graph, where  $G'$  is a subgraph of  $G$  and  $|G'| = |G| - a$ , such that  $\alpha_2(G') = \alpha_2(G) = m$ . By Theorem 2.6,  $m = \alpha_2(G') \leq \lfloor \frac{|G'|}{2} \rfloor = \lfloor \frac{|G| - a}{2} \rfloor \leq \lfloor \frac{2m}{2} \rfloor = m$ . The equalities hold, so  $a = 1$  and  $G' \in \mathcal{G}(m)$ . By Lemma 3.3,  $|L(G')| = |L^*(G')| = m$ . Hence  $|L^*(G)| = |L(G)| - 1 = m$ .  $\square$

**Lemma 3.5.** If  $G \in \mathcal{G}(m)$  and  $|G| = 2m + 1$ , where  $m \geq 1$ , then  $|L^*(G)| = m$  or  $m - 1$ .

*Proof.* We prove it by induction on  $m$ . We can see that  $\mathcal{G}(1) = \{P_2, P_3, C_3\}$ . If  $|G| = 3$  is odd, this means that  $G = P_3$  or  $C_3$ . So it's true for  $m = 1$ . Assume that it's true for  $m - 1$ , where  $m \geq 2$ . Let  $G \in \mathcal{G}(m)$  and  $|G| = 2m + 1$ . If  $L(G) = \emptyset$ , by Lemma 2.2 and lemma 3.2, then  $m = \alpha_2(G) \leq \alpha_2(C_{2m+1}) = \lfloor \frac{2m+1}{3} \rfloor < m$ , where  $m \geq 2$ . This is a contradiction, so  $L(G) \neq \emptyset$ .

If  $L^*(G) \neq L(G)$ . By Lemma 3.4,  $|L^*(G)| = |L(G)| - 1 = m$ . So we assume that  $L^*(G) = L(G)$ . Let  $u_0 \in L(G)$  and  $u'_0 \in N_G(u_0)$ . Suppose  $G' = G - \{u_0, u'_0\}$ , then  $G'$  is a connected graph of order  $|G'| = 2(m-1) + 1$ . By Theorem 2.6,  $m-1 \leq \alpha_2(G') \leq \lfloor \frac{|G'|}{2} \rfloor = \lfloor \frac{|G|}{2} \rfloor - 1 = m-1$ . The equalities hold, so  $\alpha_2(G') = \lfloor \frac{|G'|}{2} \rfloor = m-1$ . Thus  $G' \in \mathcal{G}(m-1)$ , by the induction hypothesis,  $|L^*(G')| = m-1$  or  $m-2$ . Let  $L_1 = L^*(G') = \{u_1, \dots, u_k\}$ , where  $m-2 \leq k \leq m-1$ , and  $U_1 = N_{G'}(L_1) \cap U(T) = \{u'_1, \dots, u'_k\}$ . If  $N_G(u'_0) \cap L_1 = \emptyset$ , then  $|L^*(G)| = k+1$  and  $|L^*(G)| = m$  or  $m-1$ . So we assume that  $A = N_G(u'_0) \cap L_1 \neq \emptyset$  and  $B = L_1 - A$ . Let  $A' = N_{G'}(A)$  and  $B' = N_{G'}(B)$ , where  $|A| = |A'| = a$  and  $|B| = |B'| = b$ . By Lemma 2.3, there exists a  $\alpha_2$ -set  $S$  of  $G$  satisfying  $L^*(G) \subset S$ . Then  $u_0 \in S$  and  $A \cap S = \emptyset$ . Since  $a+b = k \leq m-1$ ,  $C = V(G') - (A \cup A' \cup B \cup B')$  and  $|C| = 1$  or  $3$ .

**Claim.**  $|S \cap A'| \leq 1$ . Suppose, by contradiction,  $|S \cap A'| \geq 2$ . Since  $G$  is connected,  $\prec A' \succ_{G'}$  is connected or  $N_{G'}^2(A') \cap (C \cup B') \neq \emptyset$ . Then we have that  $2 \leq |S \cap A'| \leq a-1$  and  $m = \alpha_2(G) = |\{u_0\}| + |A' \cap S| + |B| \leq 1 + (a-1) + b = a+b = m-1$ . This is a contradiction, so  $|S \cap A'| \leq 1$ .

Since  $\alpha_2(G) = \alpha_2(G') + 1$ , by Claim,  $|A| = a = 1$ , say  $A = \{u_1\}$ . If  $k = m-2$ , then  $C = \{w_1, w_2, w_3\}$ , where  $N_{G'}(w_1) = \{w_2, w_3\}$ , and  $C \cap L^*(G) = \emptyset$ . Since  $G'$  is connected,  $u'_1 \in N_{G'}(\{w_2, w_3\} \cup B')$ . Thus  $\text{dist}_{G'}(u'_1, w_1) = 2$  or  $\text{dist}_{G'}(u'_1, u_i) = 2$  for some  $u_i \in B$ . Then  $u'_1 \notin S$  and  $m = |S| = |\{u_0, w_1\}| + |B| = 2 + (m-2-1) = m-1$ . This is a contradiction, so  $k = m-1$ . So  $m \geq |L^*(G)| \geq |B| + 1 = m-2+1 = m-1$ .  $\square$

**Lemma 3.6.** For  $m \geq 1$ ,  $\mathcal{G}(m) \subseteq \bigcup_{i=1}^2 \mathcal{H}_i(m)$ .

*Proof.* Let  $G \in \mathcal{G}(m)$ . Then  $|G| = 2m$  or  $2m+1$ . If  $|G| = 2m$ , by Lemma 3.3,  $|L(G)| = |L^*(G)| = m$  and  $|G - L^*(G)| = m$ , where  $V(G) = L^*(G) \cup U(G)$ . By Lemma 2.3,  $L^*(G)$  is a  $\alpha_2$ -set of  $G$ . Since  $G$  is connected, this implies that  $G' = G - L^*(G)$  is connected. Hence  $G \in \mathcal{H}_1(m)$ . So we assume that  $|G| = 2m+1$ . By Lemma 3.4,  $|L^*(G)| = m$  or  $m-1$ .

**Case 1.**  $|L^*(G)| = m$ . Then  $L^*(G)$  is a  $\alpha_2$ -set of  $G$ . Since  $G$  is connected, this implies that  $G' = G - L^*(G)$  is connected. Hence  $G \in \mathcal{H}_1(m)$ .

**Case 2.**  $|L^*(G)| = m-1$ . Let  $C = V(G) - N_G[L^*(G)]$ . Then  $|C| = 3$ , say  $C = \{w_1, w_2, w_3\}$  and  $C \cap L(G) = \emptyset$ . This means that  $N_G(w_1) = \{w_2, w_3\}$ . Hence  $G \in \mathcal{H}_2(m)$ .

By Cases 1 and 2,  $G \in \mathcal{H}_1(m)$  or  $G \in \mathcal{H}_2(m)$ .  $\square$

As an immediate consequence of Lemma 3.6, we obtain the Theorem 3.1. Hence we provide a characterization of  $\mathcal{G}(m)$  for all  $m \geq 1$ .

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