The complete inclusion structure of leaf power classes

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A B S T R A C T

Let \( k \geq 2 \) be an integer and \( G = (V, E) \) be a finite simple graph. A tree \( T \) is a \( k \)-leaf root of \( G \), if \( V \) is the set of leaves of \( T \) and, for any two distinct \( x, y \in V \), the distance between \( x \) and \( y \) in \( T \) is at most \( k \) if and only if \( xy \in E \). We say that \( G \) is a \( k \)-leaf power if there is a \( k \)-leaf root of \( G \). The main result of this paper is that, for all \( 2 \leq k < k' \), the classes of \( k \) - and \( k' \)-leaf powers are inclusion-incomparable, if and only if \( k' \leq 2k - 3 \) and \( k' - k \) is an odd number. With this result, an open problem from the literature about the inclusion structure of these graph classes is solved completely. In addition, the intersection of the smallest pair of inclusion-incomparable classes is studied.

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1. Introduction

A fundamental problem in computational biology is the reconstruction of the evolutionary history of a set of species or genes, typically represented as a phylogenetic tree. The species occur as leaves of the phylogenetic tree. Motivated by the search for underlying phylogenetic trees, Nishimura, Ragde and Thilikos [15] introduced the concept of \( k \)-leaf powers and \( k \)-leaf roots. Let \( k \geq 2 \) be an integer and \( G = (V, E) \) be a finite simple graph. A tree \( T \) is a \( k \)-leaf root of \( G \), if \( V \) is the set of leaves of \( T \) and, for any two distinct \( x, y \in V \), the distance between \( x \) and \( y \) in \( T \) is at most \( k \) if and only if \( xy \in E \). The graph \( G \) is called a \( k \)-leaf power if there is a \( k \)-leaf root of \( G \).

Leaf powers have attracted a considerable amount of interest in recent years. We refer to [1–4,8,9,12–14,16] for recent work on leaf powers, and to [11] for the related notions of phylogenetic root and Steiner root. For \( k = 3 \) and \( k = 4 \), characterisations of and linear time recognition algorithms for \( k \)-leaf powers are known. Also, a linear time recognition algorithm for \( 5 \)-leaf powers has been found. For \( k \geq 5 \), no characterisation of \( k \)-leaf powers and, for \( k \geq 6 \), no efficient recognition is known.

On the structural side, it has been established that every \( 2 \)-leaf power is a \( 3 \)-leaf power and every \( 3 \)-leaf power is a \( 4 \)-leaf power,

\[
L(2) \subset L(3) \subset L(4).
\]

By subdividing all edges containing a leaf in a \( k \)-leaf root, it is easy to see that every \( k \)-leaf power is a \((k + 2)\)-leaf power,

\[
L(4) \subset L(6) \subset L(8) \ldots \quad \text{and} \quad L(3) \subset L(5) \subset L(7) \ldots.
\]

Finally, by subdividing all edges not containing a leaf in a \( k \)-leaf root, it is straightforward to see that, for any \( k \geq 2 \), every \( k \)-leaf power is both a \((2k - 2)\)- and \((2k - 1)\)-leaf power,

\[
L(k) \subset L(2k - 2) \quad \text{and} \quad L(k) \subset L(2k - 1).
\]
The first negative result about leaf power class inclusions was obtained in a paper by Fellows et al. [10] containing an example of a 4-leaf power which is not a 5-leaf power, 
\[ L(4) \not\subset L(5). \]

In this paper the question about the inclusion structure of the graph classes of leaf powers is solved completely. The main result is that, for all \( 2 \leq k < k' \), the classes of \( k \)- and \( k' \)-leaf powers are inclusion-incomparable, that is

\[ L(k) \not\subset L(k') \quad \text{and} \quad L(k') \not\subset L(k), \]

if and only if \( k' \leq 2k - 3 \) and \( k' - k \) is an odd number. In addition, a partial structural characterisation for the intersection of the smallest pair of inclusion-incomparable classes \( L(4) \cap L(5) \) is given.

The paper is organized as follows. The main results are given in Section 2. Some auxiliary material is provided in Section 3. The result about the intersection \( L(4) \cap L(5) \) is proved in Section 4. The proof of the main theorem is given in Section 5. Some conclusions are provided in Section 6.

2. Main results

2.1. The inclusion structure of leaf power classes

**Theorem 1.** Let \( L(k), k \geq 2 \), denote the class of \( k \)-leaf powers. Then, for all \( l \geq 1 \),

(i) \( L(k + l) \not\subset L(k) \) and 
(ii) \( L(k) \not\subset L(k + l) \iff \) \( l \) is odd and \( l \leq k - 3 \).

As a consequence of the proof of Theorem 1, we obtain a further characterisation of the pairs of leaf power classes for which inclusion holds. We call an edge of a tree external if it contains a leaf. Otherwise, we call it internal.

**Corollary 1.** For all \( 2 \leq k < k' \), the inclusion \( L(k) \subset L(k') \) holds if and only if every \( k \)-leaf root of every element \( G \) of \( L(k) \cap L(k') \) can be transformed into a \( k' \)-leaf root of \( G \) by the two simple operations of first possibly subdividing all internal edges exactly once and then possibly subdividing all external edges a fixed number of times.

The following result was published without proof in [6].

**Corollary 2.**
\[ L(k) \not\subset L(k + 1) \iff k \geq 4. \]

2.2. The intersection of the 4- and 5-leaf power classes

According to Theorem 1, the smallest indices \( k, l \) such that 
\[ L(k + l) \not\subset L(k) \quad \text{and} \quad L(k) \not\subset L(k + l) \]
are \( k = 4 \) and \( l = 1 \). Here we study the intersection of the “smallest” pair of inclusion-incomparable classes, 
\[ L(4) \cap L(5). \]

A tree is called basic if no two of its leaves have the same parent vertex; that is, have the same neighbour. A \( k \)-leaf power is called basic if it has a basic \( k \)-leaf root. Let a vertex of a tree be called a branching vertex, if its degree is 3 or greater. Let a subpath of a tree be called a degree-2 path, if only its endvertices are not of degree 2 in the tree.

**Theorem 2.** Let \( S \) be a basic tree. Then \( S^2 \not\in L(4) \cap L(5) \) if and only if there is a subtree of \( S \) such that

(i) all its degree-2 paths have length 1, 2 or 4, 
(ii) it contains two (unordered) pairs of adjacent branching vertices.

**Corollary 3.** Let \( S \) be a basic tree with three consecutive branching vertices. Then \( S^2 \) is not a 5-leaf power.

**Proof.** Suppose that \( S \) is a basic tree with three consecutive branching vertices. Then \( S \) evidently contains a subtree satisfying conditions (i) and (ii) of Theorem 2. Hence, by Theorem 2, \( S^2 \not\in L(4) \cap L(5) \), and, since the square of any tree is a 4-leaf power, \( S^2 \not\in L(5) \). \( \square \)

By Corollary 3, for the trees shown in Figs. 1 and 2, we have \( S^2 \not\in L(5) \) and, equivalently, \( S^2 \in L(4) \setminus L(5) \).

Fig. 1 shows the example on 13 vertices found by Fellows et al. [10]. Their indirect proof makes use of the symmetry of the example and is based on a case analysis for distances of vertices in an assumed 3-Steiner root.

Fig. 2 shows an example on ten vertices. Among squares of basic trees there are obviously no examples with fewer vertices.
Remark 1. In fact, it is readily seen that, by Theorem 2, among basic trees on ten vertices, the tree in Fig. 2 is the only one whose square is not a 5-leaf power. Finally, among trees on at most ten vertices, which are not basic, every tree has its square in $L(5)$. Indeed, for a proof sketch, suppose that $T$ is a tree on at most ten vertices, which is not basic. Then let $T'$ be obtained from $T$ by deleting, for each set of leaves with the same parent vertex, all but one leaves. Now $T'$ is a basic tree on at most nine vertices. It follows from the proof of Theorem 2 that there is a $3$-Steiner-root $T''$ of $(T')^2$ obtained from $T'$ by subdividing some of its edges exactly once. Finally, we get a $3$-Steiner-root of $T^2$ by appropriately adding back to $T''$ the leaves we deleted from $T$, so that $T^2 \in L(5)$.

So, among trees on at most ten vertices, the tree in Fig. 2 is the only one whose square is not a 5-leaf power. We have made no major effort here to carefully analyse those elements of $L(4) \cap L(5)$, which are not squares of trees, but we believe that such elements on at most ten vertices do not exist.

Remark 2. It follows from a result of [4], that a 2-connected graph is a basic 4-leaf power if and only if it is the square of some tree. Hence, since the square of any tree is 2-connected, the 2-connected basic 4-leaf powers are precisely the squares of trees. Two vertices, say $x$ and $y$, of a graph $G = (V, E)$ are called true twins if they have the same set of neighbours in $V \setminus \{x, y\}$ and $xy \in E$. Now it is readily shown that the 2-connected 4-leaf powers without true twins are precisely the squares of basic trees. Indeed, suppose $G$ is a 2-connected 4-leaf power without true twins. Let $T$ be a 4-leaf root of $G$. If $T$ is not basic, then it has two leaves sharing the same neighbour, and those leaves correspond to two true twins of $G$, a contradiction. Hence $G$ is a 2-connected basic 4-leaf power, and thus $G$ is the square of some tree, which, analogously to the argument for $T$, must be basic. Conversely, suppose $G$ is the square of some basic tree $T$. Then $G$ is clearly a 2-connected 4-leaf power. It is an easy check that, assuming $T$ has at least five vertices, $G$ does not have a pair of true twins.

So, Theorem 2 covers precisely those elements of $L(4) \cap L(5)$ that are 2-connected and have no true twins, by giving a necessary and sufficient condition for a basic tree $S$ to satisfy $S^2 \notin L(4) \cap L(5)$.

For some comments on the general connected case see [6].

3. Basic notions

A finite simple graph is an undirected graph with a finite vertex set without loops or multiple edges.

For a finite simple graph $G = (V, E)$ and some vertex $v$ we sometimes write $v \in G$, respectively $v \notin G$, to mean $v \in V$, respectively $v \notin V$. Also, we sometimes use component of $G$ to mean connected component (maximal connected subgraph) of $G$.

For a finite simple graph $G = (V, E)$ and $x, y \in V$, let the distance $d_G(x, y)$ of $x$ and $y$ be the length, i.e., number of edges, of a shortest path in $G$ between $x$ and $y$. For $k \geq 1$, let $G^k = (V, E^k)$ with $xy \in E^k$ if and only if $d_G(x, y) \leq k$ denote the $k$th power of $G$.

For two sets $X$ and $Y$, we use $X \subset Y$ to mean set inclusion, with $X$ not necessarily being properly included in $Y$.

For a tree $T = (V, E)$ and a set $\emptyset \neq X \subset V$, we denote the smallest (with respect to vertex deletion) subtree of $T$ containing $X$ in its vertex set as the subtree $T[X]$ of $T$ spanned by the vertices in $X$.

For $k \geq 2$, let $P_k$ be the chordless path with $k$ vertices $v_0, v_1, \ldots, v_{k-1}$ and $k - 1$ edges $v_0v_1, \ldots, v_{k-2}v_{k-1}$.

Definition 1. Let $T$ be a tree with more than two vertices. The first derivative $T^{(1)}$ of $T$ is the tree obtained from $T$ by deleting its leaves. For $k \geq 2$, the $k$th derivative $T^{(k)}$ of $T$ is the first derivative of $T^{(k-1)}$, if $T^{(k-1)}$ exists and has more than two vertices.

Let $G = (V, E)$ be a finite simple graph and $k \geq 1$. A tree $T$ is a $k$-Steiner root of the graph $G$, if $V$ can be identified as a subset of the vertices of $T$ and, for all distinct $x, y \in V$, $xy \in E$ if and only if $d_T(x, y) \leq k$. $G$ is a $k$-Steiner power if it has a $k$-Steiner root. The vertices of the $k$-Steiner root corresponding to the vertices of the $k$-Steiner power are called the real vertices. The other vertices, if they exist, are called the Steiner vertices. Now, by definition, $G$ is the subgraph of $T^k$ induced by the real vertices of $T$, and we write $G \leq T^k$ for short.

Note that, for any tree $T$ and $k \geq 1$, by definition, $T$ is a $k$-Steiner root of $T^k$. Note further that the tree $T'$ obtained from $T$ by adding exactly one leaf to every vertex is a basic $(k + 2)$-leaf root of $T^k$. Since every $k$-Steiner power $G$ is the subgraph of $T^k$, for some tree $T$, we see that $G$ is also a basic $(k + 2)$-leaf power. By deleting the leaves of a basic $(k + 2)$-leaf root of $G$, we obtain a $k$-Steiner root of $G$. The equivalence of $G$ being a $k$-Steiner power and $G$ being a basic $(k+2)$-leaf power is used throughout this paper.

4. Proof of Theorem 2

The proof is divided into two parts, corresponding to the two directions of the equivalence result.

In the first part, we show that, if a basic tree $S$ has a subtree satisfying (i) and (ii) of Theorem 2, then $S^2$ is not a 5-leaf power.
The other direction is handled by proving the contraposition of the statement. That is, we prove that, if a basic tree $S$ has no subtree satisfying (i) and (ii) of Theorem 2, then $S^2$ is a 5-leaf power. Note that, since the square of any tree is a 4-leaf power, $S^2 \in L(4)$ is equivalent to $S^2 \in L(4) \cap L(5)$.

To do this, roughly speaking, we will construct 3-Steiner roots for all subtrees of $S^2$ satisfying (i) (and, therefore, not satisfying (ii)) (see Lemma 7) and join them together to form a 3-Steiner root of $S^2$ (see Theorem 4). Note that any 3-Steiner power is a 5-leaf power.

4.1 First part of the proof

A well-known fact for distances in trees found by Buneman [7] is the following characterisation in terms of a four-point condition:

**Theorem 3.** Let $G = (V, E)$ be a connected graph. Then $G$ is a tree if and only if $G$ contains no triangles and $G$ satisfies the following four-point condition: For all $u, v, x, y \in V$,

$$d_G(u, v) + d_G(x, y) \leq \max\{d_G(u, x) + d_G(v, y), d_G(u, y) + d_G(v, x)\}.$$  

**Lemma 1.** Let $p \geq 1$ and let $P$ be the path $P_{2p+1}$. Suppose that $P^p$ is an induced subgraph of $T^k$, for some tree $T$ and $k \geq 1$. Then, for distances in $T$, we have $\max_{p+1 \leq i \leq j \leq p+1} d_T(v_i, v_j) = d_T(v_{p+1-i}, v_{p+1})$, and the maximum is attained exclusively at $(i, j) = (p + 1, l, p + 1)$.

**Proof.** Let $X = \{v_{p+1-i}, v_{p+2-i}, \ldots, v_{p+1}\}$. Note that $X$ is a clique in $P^p$, and thus the mutual $T$-distance of vertices in $X$ is at most $k$. Let $a, b \in X$ be two vertices with maximal $T$-distance in $X$; that is, $d_T(a, b) = \max_{a, b \in X} d_T(u, v)$. Suppose that $v \in V_P \setminus \{a, b\}$ is such that the $P$-distance of $v$ to $a$ and $b$ is at most $p$; that is, $d_P(a, v) \leq k$ and $d_P(b, v) \leq k$. Suppose further that $c \in X \setminus \{a, b, v\}$. Then, by Theorem 3, we have $d_T(c, v) + d_T(a, b) \leq \max\{d_T(a, v) + d_T(b, c), d_T(b, v) + d_T(a, c)\} \leq k + d_T(a, b)$ and hence also $d_T(c, v) \leq k$; that is, the $P$-distance of $c$ and $v$ does not exceed $p$. Now we must have $\{a, b\} = \{v_{p+1-i}, v_{p+1}\}$, since if $v_{p+1-i} \notin \{a, b\}$, then considering $v = v_{2p+2-i}$ and $c = v_{p+1-i}$ yields a contradiction ($v$ and $c$ as supposed above, $d_T(c, v) = p + 1$, and if $v_{p+1} \notin \{a, b\}$, then considering $v = v_0$ and $c = v_{p+1}$ gives a contradiction ($v$ and $c$ as supposed above, $d_T(c, v) = p + 1$). \qed

**Lemma 2.** Let $p \geq 2$ and let $P$ be the path $P_{2p+1}$. Suppose that $P^p$ is an induced subgraph of $T^k$, for some tree $T$ and $k \geq 1$. Then, for all $1 \leq m \leq p$, we have $d_T(v_{p-1}, v_{1-m}) \leq k - p + m$.

**Proof.** We will prove the claim by induction on $m$. For $m = p$, since $d_T(v_{p-1}, v_{p-1}) = p$ and $P^p \leq T^k$, we have $d_T(v_{p-1}, v_{p-1}) \leq k$. Suppose now that, for $2 \leq m \leq p$, we have shown $d_T(v_{p-1}, v_{p-1+m}) \leq k - p + m$. Then, by Lemma 1 (with $l = m$ and noting that $p + 1 - l \leq p - 1$), we have, in particular, $d_T(v_{p-1}, v_{1-m+1}) < d_T(v_{p-1}, v_{1-m+1}) \leq k - p + m$, which concludes the proof. \qed

See Fig. 3 for the paths $P_{2p+1}$ and $P_{2p+1}$ in Lemma 1 and Lemma 2, respectively.

**Lemma 3.** Let $k \geq 4$, and let $P$ be the path $P_{2k-3}$. Suppose that the $k$-leaf power $P_k^{k-2}$ without true twins is a $(k + 1)$-leaf power, and let $T$ be a $(k - 1)$-Steiner root of $P_k^{k-2}$. Then the subtree $T'$ of $T$ spanned by the three real vertices corresponding to $v_{k-3}, v_{k-2}$ and $v_{k-1}$, is obtained from the subpath $v_{k-3}v_{k-2}v_{k-1}$ of $P$ by a subdivision of at most one of its edges by exactly one vertex.

**Proof.** By Lemma 2 (with $m, p$ and $k$ in the lemma being $2, k - 2$ and $k - 1$, respectively), we have $d_T(v_{k-3}, v_{k-1}) \leq (k - 1) - (k - 2) + 2 = 3$. By Lemma 1 (with $l, p$ and $k$ in the lemma being $2, k - 2$ and $k - 1$, respectively), we have $1 \leq d_T(v_{k-3}, v_{k-1}) < d_T(v_{k-3}, v_{k-1})$ and $1 \leq d_T(v_{k-2}, v_{k-3}) < d_T(v_{k-3}, v_{k-1})$, and hence $2 \leq d_T(v_{k-3}, v_{k-1}) \leq 3$. If $d_T(v_{k-3}, v_{k-1}) = 2$, then $d_T(v_{k-2}, v_{k-1}) = 1$ and $d_T(v_{k-2}, v_{k-3}) = 1$, and $T'$ is the path $v_{k-3}v_{k-2}v_{k-1}$. If $d_T(v_{k-3}, v_{k-1}) = 3$, then $d_T(v_{k-2}, v_{k-3}) = 2$ and $d_T(v_{k-2}, v_{k-1}) = 2$. As the three $T$-distances add up to an even number, we have either $d_T(v_{k-3}, v_{k-1}) = 2$, or $d_T(v_{k-3}, v_{k-1}) = 1$, or $d_T(v_{k-3}, v_{k-1}) = 2$, in which case $T'$ is obtained from the subpath $v_{k-3}v_{k-2}v_{k-1}$ by subdividing the edge $v_{k-2}v_{k-1}$ exactly once. If $d_T(v_{k-3}, v_{k-2}) = 2$ and $d_T(v_{k-2}, v_{k-1}) = 1, 1$, in which case $T'$ is obtained from $v_{k-2}v_{k-1}$ by subdividing the edge $v_{k-2}v_{k-1}$ exactly once. \qed

**Lemma 4.** Let $k \geq 4$, and let $S$ be a tree with at least two vertices, such that $S^{k-2}$ has no true twins. Suppose that the $k$-leaf power $S^{k-2}$ is a $(k + 1)$-leaf power, and let $T$ be a $(k - 1)$-Steiner root of $S^{k-2}$; that is, $S^{k-2} \leq T^{k-1}$. Let $S'$ be the $(k - 3)^{rd}$ derivative of $S$. Then the subtree $T'\vert_{V_{S'}\setminus V_{S}}$ of $T$ spanned by the real vertices corresponding to the vertices of $S'$ is obtained from $S'$ by a subdivision of some of its edges by exactly one vertex.

**Proof.** Note that $|V(S')| \geq 3$, since otherwise $S^{k-2}$ would have two true twins. Hence every edge of $S'$ is contained in some subpath $P_3$ of $S'$. It is now sufficient to show that, for every $P_3$ in $S'$ with edges $ab$ and $bc$, $T[[a, b, c]]$ is obtained from $a$
suitable subdivision of $abc$. As $S'$ is the $(k-3)^{rd}$ derivative of $S$, for every such $abc$, there is a path $P_{2k-3}$ in $S$ with $v_{k-3} = a$, $v_{k-2} = b$ and $v_{k-1} = c$, and thus, by Lemma 3, we are done. □

Let $S$ be a basic tree with at least two vertices. Suppose that $S^2$ is a 5-leaf power, and let $T$ be a 3-Steiner root of $S^2$. Let $S'$ be the first derivative of $S$. By Lemma 4, the subtree $T[V_{S'}]$ of $T$ spanned by the real vertices corresponding to the vertices of $S'$ is obtained from $S'$ by a subdivision of some of its edges by exactly one vertex. This provides useful information about the relationship between $S$ and $T$. In our special case, we can say more.

Lemma 5. Let $S$ be a basic tree with at least two vertices. Suppose that $S^2$ is a 5-leaf power, and let $T$ be a 3-Steiner root of $S^2$. Let $v$ be a branching vertex of $S$ (i.e., of degree exceeding 2), and let $a$, $b$ and $c$ be adjacent to $v$ in $S$. Let $C$ be the claw with vertices $a$, $b$, $c$ and $v$ in $S$. Then the subtree $T[V_C]$ of $T$ spanned by the real vertices corresponding to the vertices of $C$ is obtained from $C$ by a subdivision of some (or possibly none) of its edges by exactly one vertex.

Proof. As $S$ is basic, at most one of them can be a leaf. If neither of $a$, $b$ and $c$ is a leaf of $S$, then, by Lemma 4, we are done. Without loss of generality, we may assume that $a$ is a leaf and that there is a fifth vertex $x$ adjacent to $b$ and a sixth vertex $y$ adjacent to $c$. By Lemma 4, there are two possibilities for $T$-distances between $b$, $c$ and $v$. Either $d_T(b, c) = 2$ and $d_T(b, v) = d_T(c, v) = 1$, or $d_T(b, c) = 3$ and $d_T(b, v), d_T(c, v) = \{1, 2\}$.

Let us consider the case $d_T(b, c) = 2$ first. If the claim does not hold, then $a$ must be adjacent to $b$ or $c$ in $T$. Without loss of generality, we may assume that $ab$ is an edge in $T$, so that $abcv$ is a $P_4$ in $T$. Note that $x$ must have a $T$-distance of at most 3 to both $b$ and $v$ and a $T$-distance of at least 4 to both $a$ and $c$, which is impossible to realise.

In the case $d_T(b, c) = 3$, without loss of generality, we may assume that $d_T(b, v) = 1$ and $d_T(c, v) = 2$. If the claim does not hold, then $a$ must be adjacent to both $c$ and $v$ in $T$, so that $bavc$ is a $P_4$ in $T$. Note that $y$ must have a $T$-distance of at most 3 to both $c$ and $v$ and a $T$-distance of at least 4 to $a$, which is impossible to realise. □

Lemma 5 suggests that branching vertices are helpful when trying to deduce information about $T$. The following result highlights the consequence of two branching vertices being adjacent in $S$.

Lemma 6. Let $S$ be a basic tree with at least two vertices. Suppose that $S^2$ is a 5-leaf power, and let $T$ be a 3-Steiner root of $S^2$. Let $v$ and $w$ be two adjacent branching vertices of $S$, and let $a$, $b$, $c$, $d$, $x$ and $y$ be six further vertices, such that $a$ and $b$ are adjacent to $v$, $c$ and $d$ are adjacent to $w$, $x$ is adjacent to $a$, and $y$ is adjacent to $c$ in $S$. Let $B$ be the subtree of $S$ spanned by $a$, $b$, $c$, $d$, $v$ and $w$. Then the subtree $T[V_B]$ of $T$ spanned by the real vertices corresponding to the vertices of $B$ is obtained from $B$ by subdividing $vw$ exactly once.

Proof. By Lemma 4 and Lemma 5, $T[V_B]$ is obtained from $B$ by a subdivision of some of its edges by exactly one vertex. As $d_T(a, b) \leq 3$ and $d_T(c, d) \leq 3$, we must have $1 \in \{d_T(a, v), d_T(b, v)\}$ and $1 \in \{d_T(c, w), d_T(d, w)\}$. So if $d_T(v, w) = 1$, then at least one of $d_T(a, c), d_T(a, d), d_T(b, c)$ and $d_T(b, d)$ is equal to 3, a contradiction. Hence $d_T(v, w) = 2$, and thus $d_T(a, v) = d_T(b, v) = d_T(c, w) = d_T(d, w) = 1$. □

Lemma 6 suggests that adjacent pairs of branching vertices in $S$ have, roughly speaking, a significant impact on their neighbourhoods. It will be important to distinguish between two classes of degree-2 paths, those of lengths 1, 2 and 4 and those of lengths 3, 5 and larger. The following result is a simple consequence of Lemmas 4–6.

Corollary 4. Let $S$ be a basic tree satisfying (i) and (ii) of Theorem 2. Then $S^2$ is not a 5-leaf power.

Proof. Let $P_k$ (with vertices $v_0, \ldots, v_{k-1}$) be a shortest path in $S$ such that $|v_0, v_1|$ and $|v_{k-2}, v_{k-1}|$ are both distinct pairs of branching vertices of $S$. By (ii) of Theorem 2, such a $P_k$ exists. Clearly, $k \geq 3$. Suppose to the contrary that $S^2$ is a 5-leaf power. Since $S^2$ has no true twins, it has a 3-Steiner root $T$.

If $k = 3$, then, by Lemma 6 (with $v = v_0$ and $w = v_1$), we have $d_T(v_0, v_1) = 2$, and, by Lemma 6 (with $v = v_1$, $w = v_2$ and $a = v_0$), we have $d_T(v_0, v_1) = 1$, a contradiction. We cannot have $k = 4$, as that would contradict the minimality of $P_k$. So we may assume $k \geq 5$. Let $X$ be the set of vertices of $P_k$ and all the vertices that are adjacent to a branching vertex of $P_k$.

By Lemmas 4 and 5, the subtree of $T$ spanned by the real vertices corresponding to the vertices in $X$ is obtained from $S[X]$ by a subdivision of some of its edges by exactly one vertex.

By (i) of Theorem 2 and the minimality of $P_k$, the path between $v_1$ and $v_{k-2}$ consists of degree-2 paths of lengths 2 or 4. Suppose $uvw$ is one of the degree-2 paths of length 2 with $a$ being the second neighbour of $u$ in $P_k$ and $b$ being some third neighbour of $u$ in $S$. Suppose further that $d_T(a, u) = 2$. If $d_T(b, u) = 2$, then $d_T(a, b) = 4$, contradicting $d_T(a, b) \leq 3$. Hence $d_T(b, u) = 1$. If $d_T(u, v) = 2$, then $d_T(a, v) = 4$, contradicting $d_T(a, v) \leq 3$. Hence $d_T(u, v) = 1$. If $d_T(v, w) = 1$, then $d_T(b, w) = 3$, contradicting $d_T(b, w) \geq 4$. Thus, assuming $d_T(a, u) = 2$, we have $d_T(v, w) = 2$.

Suppose $uvwxy$ is one of the degree-2 paths of length 4 with $a$ being the second neighbour of $u$ in $P_k$ and $b$ being some third neighbour of $u$ in $S$. Suppose further that $c$ is the second neighbour of $y$ in $P_k$ and $e$ is some third neighbour of $y$ in $S$. Finally, suppose that $d_T(a, u) = 2$. By the above argument, we have $d_T(u, v) = 1$ and $d_T(v, w) = 2$. If $d_T(w, x) = 2$, then $d_T(v, x) = 4$, contradicting $d_T(v, x) \leq 3$. Hence $d_T(v, x) = 1$. Suppose $d_T(x, y) = 1$. If $d_T(y, c) = 1$, then $d_T(v, c) = 3$, contradicting $d_T(v, c) \geq 4$. Hence $d_T(y, c) = 2$. If $d_T(e, y) = 1$, then $d_T(w, e) = 3$, contradicting $d_T(w, e) \geq 4$. Hence $d_T(y, e) = 2$. But then $d_T(c, e) = 4$, contradicting $d_T(c, e) \leq 3$. Thus, assuming $d_T(a, u) = 2$, we have $d_T(x, y) = 2$.

By Lemma 6 (with $v = v_0$ and $w = v_1$), we have $d_T(v_0, v_1) = 2$. Hence, by the above argument, we can inductively deduce $d_T(v_{k-3}, v_{k-2}) = 1$. However, by Lemma 6 (with $v = v_{k-2}, w = v_{k-1}$ and $a = v_{k-3}$), we have $d_T(v_{k-3}, v_{k-2}) = 1$, a contradiction. □
Finally, suppose that $S$ is a basic tree with a subtree satisfying (i) and (ii) of Theorem 2. Then it is easy to see that $S$ also has a basic such subtree $S'$. By Corollary 4, $S'^2$ is not a 5-leaf power, which implies that $S^2$ is not a 5-leaf power, because $S'^2$ is a subgraph of $S^2$ and being a $k$-leaf power is a hereditary property.

4.2. Second part of the proof

**Lemma 7.** Let $S$ be a basic tree with at most one pair of adjacent branching vertices and whose degree-2 paths are exclusively of length 1, 2 or 4. Then there is a 3-Steiner root for $S^2$, which is obtained by subdividing some of the edges of $S$ exactly once, leaving edges between leaves and branching vertices unaltered.

**Proof.** Suppose there is no pair of adjacent branching vertices. Then root the tree at any of its leaves, say at $v$. Leave every degree-2 path of length 1 unaltered. For every degree-2 path $abc$ of length 2, with $d_5(a, v) < d_5(c, v)$, subdivide $bc$ exactly once. For every degree-2 path $abcde$ of length 4, with $d_5(a, v) < d_5(e, v)$, subdivide $bc$ and $de$ exactly once. It is a straightforward check to see that the obtained tree is an appropriate 3-Steiner root.

Suppose there is exactly one pair of adjacent branching vertices, say $(v, w)$. Leave every degree-2 path of length 1 other than $vw$ unaltered, and subdivide $vw$ exactly once. For every degree-2 path $abc$ of length 2, with $d_5(a, v) < d_5(c, v)$, subdivide $bc$ exactly once. For every degree-2 path $abcde$ of length 4, with $d_5(a, v) < d_5(e, v)$, subdivide $bc$ and $de$ exactly once. Again, it is a straightforward check to see that the obtained tree is an appropriate 3-Steiner root. □

The general case with some degree-2 paths of length 3, 5 or larger occurring can be treated by induction on the number of those paths.

**Theorem 4.** Let $S$ be a basic tree, for which every subtree with degree-2 paths of degree-2 paths of length 1, 2 or 4 only contains at most one pair of adjacent branching vertices. Then there is a 3-Steiner root for $S^2$, which is obtained by subdividing some of the edges of $S$ exactly once, leaving edges between leaves and branching vertices unaltered.

**Proof.** Let $n$ be the number of degree-2 paths of length 3, 5 or larger. If $n = 0$, then we are done by Lemma 7. Let us assume that $n = k \geq 1$ and that the hypothesis is true for all $n < k$. Then pick any degree-2 path $v_0v_1 \ldots v_{l-1}v_l$ of length 3, 5 or larger. By deleting $v_2$ in $S$, let $S_1$ be the remaining component containing $v_0$ and $v_1$, and, by deleting $v_{l-2}$ in $S$, let $S_2$ be the remaining component containing $v_{l-1}$ and $v_l$. By induction, there is a 3-Steiner root for $S_1^2$, respectively $S_2^2$, which is obtained by subdividing some of the edges of $S_1$, respectively $S_2$, exactly once, leaving edges between leaves and branching vertices unaltered. Thus, $v_0v_1$ and $v_{l-1}v_l$ are left unaltered in the two respective 3-Steiner roots. It is now straightforward to see that the two $3$-Steiner roots can be joined together, by subdividing some of the edges of $v_1 \ldots v_{l-2}$ exactly once, to form an appropriate 3-Steiner root for $S$. To be more precise, $v_0v_1$ and $v_{l-2}v_{l-1}$ get subdivided exactly once, and the remaining edges of the initially picked degree-2 path are subdivided in such a way that no consecutive edges get subdivided and no three consecutive edges are left unaltered. □

5. Proof of Theorem 1

5.1. Proof of part (i) of Theorem 1

We prove Theorem 1 (i) by constructing an explicit example that is in $L(k + l)$ but not in $L(k)$.

**Theorem 5.** For every $k \geq 3$, $P_{2k-2}^2$ is a $k$-leaf power which is not a $k'$-leaf power, for any $2 \leq k' < k$.

**Proof.** Let $k = 3$, the path $P_3 = P_3^1$ with two edges is an appropriate example. For $k \geq 4$, let $P$ be the path $P_{2k-3}$. Note that $P_{2k-2}$ is a $k$-leaf power without true twins. Suppose that $P_{k-2}$ is a $k'$-leaf power, for some $2 \leq k' < k$. Clearly, $k' = 2$ cannot hold, so that we may assume $3 \leq k' < k$. Then there must be a $(k' - 2)$-Steiner root $T$ for $P_{k-2}$, that is, $P_{k-2} \leq T_{k-2}$. By Lemma 2 (with $m = 1$), we must have $d_T(v_{k-3}, v_{k-2}) \leq (k' - 2) - (k - 2) + 1 \leq 0$, a contradiction. □

5.2. Proof of part (ii) of Theorem 1 — the easy direction

In [5], we introduce the following notion: Let $k \geq 2$ and $\ell > k$ be integers and $G = (V, E)$ be a finite simple graph. A tree $T$ is a $(k, \ell)$-leaf root of $G$, if $V$ is the set of leaves of $T$ and, for any two distinct $x, y \in V$, we have $xy \in E \implies d_T(x, y) \leq k$ and $xy \not\in E \implies d_T(x, y) \geq \ell$. We say that $G$ is a $(k, \ell)$-leaf power if and only if there is a $(k, \ell)$-leaf root of $G$.

**Lemma 8.** Let $k \geq 2$, and let $l$ be a positive integer which is even or satisfies $l \geq k - 2$. Then $L(k) \subset L(k + l)$. In particular, we have:

(i) If $l$ is even, then every $k$-leaf root can be transformed into a $(k + l)$-leaf root of the same graph by subdividing all external edges precisely $l/2$ times.

(ii) If $l \geq k - 2$, then every $k$-leaf root can be transformed into a $(k + l)$-leaf root of the same graph by first subdividing all internal edges precisely once and then subdividing all external edges precisely $\lfloor (l - k + 2)/2 \rfloor$ times.

**Proof.** Let $G = (V, E)$ be an arbitrary $k$-leaf power, and let $S$ be an arbitrary $k$-leaf root of $G$.

To show (i), suppose that $l$ is even. Let $T$ be the tree obtained from $S$ by subdividing all external edges precisely $l/2$ times, keeping the identification of $V$ and the leaves. Then, for any two distinct vertices $x, y \in V$, we have $d_T(x, y) = d_S(x, y) + l$ and, hence, $xy \in E \iff d_S(x, y) \leq k \iff d_T(x, y) \leq k + l$. Thus, $T$ is a $(k + l)$-leaf root of $G$.  


To show (ii), suppose that \( l \geq k - 2 \). Let \( T \) be the tree obtained from \( S \) by first subdividing all internal edges precisely once and then subdividing all external edges precisely \( \lfloor (l - k + 2)/2 \rfloor \) times, keeping the identification of \( V \) and the leaves. Then, for any two distinct vertices \( x, y \in V \), we have \( d_T(x, y) = 2d_S(x, y) - 2 + 2\lfloor (l - k + 2)/2 \rfloor \). If \( xy \in E \), then \( d_S(x, y) \leq k \) and, hence, \( d_T(x, y) \leq 2k - 2 + 2\lfloor (l - k + 2)/2 \rfloor \). If \( xy \notin E \), then \( d_S(x, y) \geq k + 1 \) and, hence, \( d_T(x, y) \geq 2k + 2\lfloor (l - k + 2)/2 \rfloor \).

So, \( T \) is a \( (2k - 2 + 2\lfloor (l - k + 2)/2 \rfloor, 2k + 2\lfloor (l - k + 2)/2 \rfloor) \)-leaf root of \( G \) and, hence, both a \( (2k - 2 + 2\lfloor (l - k + 2)/2 \rfloor) \)-leaf root and a \( (2k - 2 + 2\lfloor (l - k + 2)/2 \rfloor) \)-leaf root of \( G \). In particular, whether or not \( l - k + 2 \) is even, \( T \) is a \((k + l)\)-leaf root of \( G \). \( \square \)

5.3. Proof of part (ii) of Theorem 1 — the hard direction

Here we need to show that, if \( k \geq 2 \) and \( l \) is an odd integer satisfying \( 1 \leq l \leq k - 3 \), then \( L(k) \nsubseteq L(k + l) \).

There is nothing to prove for \( k = 2 \) and \( k = 3 \). For \( k = 4 \), only \( l = 1 \) needs attention, and, by Theorem 2 and its detailed discussion above, the implication holds (see, for example, Fig. 2).

For \( k = 5 \), only \( l = 1 \) needs to be treated. This is done in Lemma 9, showing \( L(5) \nsubseteq L(6) \).

For \( k = 6 \), the two cases \( l = 1 \) and \( l = 3 \) need to be covered. For \( k = 7 \), the two cases \( l = 1 \) and \( l = 3 \) need to be dealt with. In general, for \( k \geq 6 \), in order to show \( L(k) \nsubseteq L(k + l) \) for all odd \( l \) with \( 1 \leq l \leq k - 3 \), it is enough to show this for the largest odd \( l \) with \( 1 \leq l \leq k - 3 \), denoted \( l' \), say. Just recall that, by Lemma 8, for any odd \( l \) with \( 1 \leq l \leq k - 3 \), we have \( L(k + l) \subseteq L(k + l') \). It is straightforward that \( l' = 2\lfloor (k - 4)/2 \rfloor + 1 \). This is done in Lemma 10, proving the existence of an element of \( L(k) \setminus L(k + l) \) for \( k \geq 6 \), which is by far the hardest part of the paper.

**Lemma 9.** There is a 5-leaf power, which is not a 6-leaf power.

**Proof.** Let \( S \) be the tree in Fig. 4. Of course, \( S^3 \) is a 5-leaf power. It is straightforward that \( S^3 \) has no true twins. Suppose that \( S^3 \) is also a 6-leaf power, and let \( T \) be a 4-Steiner root of \( S^3 \). Now consider the subtree \( S^{(2)} = S[\{a, b, c, d\}] \). By Lemma 4, \( T[\{a, b, c, d\}] \) is obtained from subdividing some of its edges exactly once.

Suppose \( d_T(u, v) = 2 \). Then, since \( d_S(u, b) = 3 \) implies \( d_T(u, b) \leq 4 \), we have \( 2 \leq d_T(v, b) = d_T(u, b) - d_T(u, v) \leq 2 \).

Then \( d_T(v, b) = 2 \) and, by symmetry, \( d_T(v, x) = 2 \). But then \( d_T(b, x) = d_T(b, v) + d_T(v, x) = 4 \), implying \( d_S(b, x) \leq 3 \), a contradiction. Hence \( d_T(u, v) = 1 \). By symmetry, we may also assume \( d_T(v, w) = 1 \), \( d_T(w, x) = 1 \) and \( d_T(y, x) = 1 \).

But then \( d_T(u, y) = d_T(u, v) + d_T(v, w) + d_T(w, x) + d_T(y, x) = 4 \), implying \( d_S(u, y) \leq 3 \), a contradiction. \( \square \)

**Definition 2.** Let \( C_i \) be a claw; that is, a star with three leaves. For \( i > 1 \), let \( C_i \) be the tree obtained from \( C_{i-1} \) by adding precisely two leaves at every leaf of \( C_{i-1} \). For every \( j \geq 1 \), let \( C_{ij} \) be the tree obtained from \( C_j \) by subdividing every external edge of \( C_j \) exactly \( j \) times.

Note that, for all \( i \geq 1 \), every non-leaf of \( C_i \) has degree 3. Note further that, for all \( 1 \leq i' \leq i \) and \( 1 \leq j' \leq j \), the tree \( C_{i'j'} \) is a subtree of \( C_{ij} \).

**Lemma 10.** For all \( k \geq 6 \), we have \( (C_{k^2-k-3})^{k^2-2} \in L(k) \setminus L(k+l) \), where \( l = 2\lfloor (k - 4)/2 \rfloor + 1 \).

5.3.1. Proof of Lemma 10

**Proof.** Let \( k \geq 6 \) be an arbitrary integer, and let \( l = 2\lfloor (k - 4)/2 \rfloor + 1 \). Let \( C = (V, E) \) be the graph \( C_{k^2-k-3} \). Clearly, \( C^{k^2-2} \) is a \( k \)-leaf power. Suppose that \( C^{k^2-2} \) is also a \((k + l)\)-leaf power, and let \( S \) be a \((k + l)\)-leaf root of \( C^{k^2-2} \). It remains to contradict this assumption.

Let \( \lambda \) be a bijection from \( V \) to the leaf set of \( S \), such that, for any two distinct \( x, y \in V \), we have \( d_C(x, y) \leq k - 2 \iff d_S(\lambda(x), \lambda(y)) \leq k + l \). Note that any two distinct vertices of \( C \) are contained in a path with at most \( 2k - 4 \) edges, such that \( C^{k^2-2} \) has no pair of true twins. Hence, for any two distinct \( x, y \in V \), we have \( d_C(\lambda(x), \lambda(y)) \neq 2 \) for all \( x \in V \), let \( \rho(x) \) be the neighbour of \( \lambda(x) \) in \( S \), and let \( T \) be the subtree of \( S \) spanned by \( \{\rho(x), x \in V \} \). Then \( \rho \) is an injection and, for any two distinct \( x, y \in V \), we have \( d_C(x, y) \leq k - 2 \iff d_T(\rho(x), \rho(y)) \leq k + l - 2 \). So \( C^{k^2-2} \) is a subgraph of \( T^{k^2-2} \), where the isomorphic copy of \( C^{k^2-2} \) is given by \( \rho \). So \( T \) is a \((k + l - 2)\)-Steiner root of \( C^{k^2-2} \), and we call \( \{\rho(x), x \in V \} \) the set of real vertices and the remaining vertices the Steiner vertices of \( T \).

**Definition 3.** For any two distinct vertices \( v \) and \( w \) of \( T \), let \( T(v, w) \) denote the component obtained from \( T \) by deleting \( v \) that contains \( w \).
**Property 1.** Let \( x \in V \) be any vertex of degree 3 in \( C \), and let \( a, b \) and \( c \) be its three neighbours. Then the subtree \( T' \) of \( T \) spanned by \( \{ \rho(a), \rho(b), \rho(c) \} \) has a unique vertex \( \tau(x) \) of degree 3 in \( T' \), and, for all \( y \in \{ a, b, c \} \), the inequality \( d_{T'}(\tau(x), \rho(x)) < d_T(\tau(x), \rho(y)) \) holds.

**Proof.** As \( T' \) is spanned by \( \{ \rho(a), \rho(b), \rho(c) \} \), it is either a path or a tree with leaf set \( \{ \rho(a), \rho(b), \rho(c) \} \) and a unique vertex \( \tau(x) \) of degree 3. Suppose that \( T' \) is a path and that, without loss of generality, its endvertices are \( \rho(a) \) and \( \rho(c) \). Note that \( axb \) and \( bxc \) are paths with two edges in \( C^{k-3} \), so that, by Lemma 1 (with \( p = k - 2 \) and \( l = 2 \) in the lemma), we have \( d_T(\rho(a), \rho(c)) < d_T(\rho(a), \rho(b)) \) and \( d_T(\rho(a), \rho(c)) < d_T(\rho(b), \rho(c)) \). Then \( d_T(\rho(a), \rho(c)) = d_T(\rho(a), \rho(b)) + d_T(\rho(b), \rho(c)) > d_T(\rho(a), \rho(x)) + d_T(\rho(x), \rho(c)) \geq d_T(\rho(a), \rho(c)) \), a contradiction. Pick \( y \in \{ a, b, c \} \). Now there is a \( z \in \{ a, b, c \} \setminus \{ y \} \), such that \( \rho(x) \not\in T(x, z) \). By the above argument, \( d_T(\rho(z), \rho(x)) < d_T(\rho(z), \rho(y)) \), and then, by subtracting \( d_T(\rho(z), \tau(x)) \) from both sides, \( d_T(\tau(x), \rho(y)) < d_T(\tau(x), \rho(y)) \). □

**Definition 4.** For any two not necessarily distinct vertices \( v \) and \( w \) of \( T \), let \( \Pi(v, w) \) denote the subpath of \( T \) connecting \( v \) and \( w \).

**Property 2.** Let \( x, y \in V \) be any two adjacent vertices of degree 3 in \( C \). Then \( \tau(y) \in T(x, \rho(y)) \). Furthermore, \( \tau(y) \not\in \Pi(\tau(x), \rho(y)) \).

**Proof.** Let \( a, b \) and \( x \) be the three neighbours of \( y \) in \( C \). Suppose that, for some \( z \in \{ a, b \} \), we have \( \rho(z) \not\in T(x, \rho(y)) \). Note that \( axb \) is a path with two edges in \( C^{k-3} \), so that, by Lemma 1 (with \( p = k - 2 \) and \( l = 2 \) in the lemma), we have \( d_T(\rho(y), \rho(z)) < d_T(\rho(x), \rho(z)) \). Hence \( d_T(\rho(y), \rho(z)) < d_T(\rho(x), \tau(z)) + d_T(\tau(x), \rho(z)) \), and, by subtracting \( d_T(\tau(x), \rho(z)) \) and since \( \rho(z) \not\in T(x, \rho(y)) \), we have \( d_T(\tau(x), \rho(y)) < d_T(\tau(x), \rho(y)) \), contradicting Property 1. Thus \( \rho(a) \) and \( \rho(b) \) are of smallest distance to \( \rho(y) \). By Property 1, we have \( d_T(\tau(x), \rho(y)) < d_T(\tau(x), \rho(y)) \). Hence \( d_T(\tau(x), \rho(y)) \not< \tau(y) \not\in \Pi(\tau(x), \rho(y)) \). Then \( d_T(\tau(y), \rho(y)) = d_T(\tau(x), \tau(y)) - d_T(\tau(x), \rho(y)) - d_T(\tau(x), \rho(y)) = d_T(\tau(x), \rho(y)) \), contradicting Property 1. Finally, suppose that \( \tau(y) \not\in \Pi(\pi(\tau(x), \rho(y)) \). Then \( d_T(\tau(y), \rho(y)) \not< d_T(\tau(x), \rho(y)) \) \( d_T(\tau(y), \rho(y)) \leq d_T(\tau(y), \rho(y)) \), contradicting Property 1 and completing the proof. □

The next property follows immediately from Property 2.

**Property 3.** Let \( x, y, z, \alpha \in V \) be four vertices of degree 3 in \( C \), such that \( y, z \) and \( \alpha \) are the three neighbours of \( x \) in \( C \). Then the subtree \( T' \) of \( T \) spanned by \( \{ \tau(x), \tau(y), \tau(z), \tau(\alpha) \} \) has the three leaves \( \tau(y), \tau(z) \) and \( \tau(\alpha) \) and \( \tau(x) \) as a vertex of degree 3. Furthermore, for any \( \beta \in \{ y, z, \alpha \} \), we have \( \tau(\beta) \not\in \Pi(\tau(x), \rho(x)) \) and \( \tau(\alpha) \not\in \Pi(\tau(\beta), \rho(\beta)) \).

The next property follows by induction and Property 3.

**Definition 5.** Let \( \Gamma' \) denote the set of all vertices of degree 3 in \( C \), and let \( C' \) be the subtree of \( C \) spanned by \( \Gamma' \).

Note that \( C' \) is isomorphic to \( C_{2^{k-1}} \).

**Property 4.** The function \( \tau \) from \( \Gamma' \) to the vertex set of \( T \) is injective. The subtree \( T' \) of \( T \) spanned by \( \{ \tau(x), x \in \Gamma' \} \) can be obtained by first dividing each \( C \) into \( C' \) and then renaming each original vertex \( x \in \Gamma' \) into \( \tau(x) \). For any distinct \( x, y \in \Gamma' \), the path \( \Pi(\tau(x), \rho(y)) \) does not contain \( \tau(y) \).

Roughly speaking, Property 4 describes the fact that \( T' \) in \( T \) is a topological copy of \( C' \) in \( C \). For any \( x \in \Gamma' \), the topological vertex \( \tau(x) \) could be far away from the real vertex \( \rho(x) \), where \( \rho(x) \) is the important vertex as far as distances in \( T \) are concerned, but the structural information in Property 4 provides enough control over \( T \) to derive a contradiction.

**Definition 6.** Let \( \Gamma^* \) denote the set of all vertices of \( C^* \) that have a neighbour in \( \Gamma' \).

Note that the subtree \( C^* \) of \( C \) spanned by \( \Gamma^* \) is isomorphic to \( C_{2^k} \).

**Property 5.** Let \( x \) and \( y \) be any two distinct elements of \( \Gamma^* \). Then \( 1 \leq d_C(x, y) \leq k - 2 \) implies \( d_T(\rho(x), \rho(y)) \leq l + d_C(x, y) \), and if \( d_C(x, y) \leq k - 1 \), then \( d_T(\rho(x), \rho(y)) \leq k + l - 1 \).

**Proof.** The first part follows from Lemma 2 with the variables \( p, k \) and \( m \) in the lemma being \( k - 2, k + l - 2 \) and \( d_C(x, y) \), respectively, and noting that there is always a subpath \( P_{2p+1} \) of \( C \) with \( (p_{2p-1}, p_{2p-1+m}) \) \( \in \{ (y, x), (x, y) \} \). The second part straightforwardly holds, since \( \rho \) homomorphically injects \( C^{k-2} \) into \( T^{k+l-2} \). □

The next property bounds the distance between corresponding topological and real vertices in \( T \) from above.

**Property 6.** For any \( x \in \Gamma' \), we have \( d_T(\tau(x), \rho(x)) \leq \lfloor k/2 \rfloor - 2 \).

**Proof.** Pick \( x \in \Gamma' \), and let \( a \) and \( b \) be two of its neighbours in \( C \). By Property 1, we have \( d_T(\tau(x), \rho(x)) < d_T(\tau(x), \rho(a)) \) and \( d_T(\tau(x), \rho(x)) < d_T(\tau(x), \rho(b)) \). Hence \( 2d_T(\tau(x), \rho(x)) \leq d_T(\tau(x), \rho(a)) + d_T(\tau(x), \rho(b)) = 2d_T(\rho(a), \rho(b)) - 2 \). By Property 5, as \( a, b \in \Gamma^* \), we have \( d_T(\rho(a), \rho(b)) \leq l + d_T(a, b) \). Hence \( 2d_T(\tau(x), \rho(x)) \leq l + d_T(a, b) \). We can thus deduce \( d_T(\tau(x), \rho(x)) \leq \lfloor (k - 4)/2 \rfloor = \lfloor k/2 \rfloor - 2 \). □
Before we begin with the final argument, another definition is needed.

**Definition 7.** Let \( I' \) denote the set of all vertices \( w \) of \( C \) with the property that, for every vertex \( w \) of \( C \) with \( d_C(v, w) \leq \left\lceil (k - 3)/2 \right\rceil \), we have \( w \in I' \). Let \( C'' \) be the subtree of \( C \) spanned by \( I'' \).

Note that \( C'' \) is isomorphic to \( C_{2-(k-3)/2} \). It will be important to distinguish between the two cases of \( k \) being even or odd. In both cases, however, the final argument consists of two similar parts. First, we show a property about the \( r \)-distance between \( \tau(x) \) and \( \tau(y) \) for vertices \( x \) and \( y \) that are close in \( I'' \). To be more precise about the first part, for even \( k \), we show that \( d_I(\tau(x), \tau(y)) \geq 2 \) whenever \( x, y \in I'' \) are adjacent, and, for odd \( k \), we show that \( d_I(\tau(x), \tau(z)) \geq 3 \) whenever \( x, z \in I'' \) satisfy \( d_C(x, z) = 2 \). Second, we construct a long enough sequence of vertices \( x \) in \( I'' \) with a strictly increasing value of \( d_I(\tau(x), \rho(x)) \) to finally contradict Property 6. In fact, for even \( k \), we obtain a sequence increasing by at least 1, whereas, for odd \( k \), we obtain a sequence that increases by at least 2.

So suppose first that \( k = 2k' \), where \( k' \geq 3 \). Then we have \( l = 2\left\lceil (k - 4)/2 \right\rceil + 1 = 2k' - 3 \) and \( \left\lceil (k - 3)/2 \right\rceil = k' - 1 \). Suppose that there are two adjacent vertices \( x, y \in I'' \) with \( d_I(\tau(x), \tau(y)) = 1 \). Let \( a, b, c \) be the three neighbours of \( x \) in \( C \), and \( c \) and \( d \) be the three neighbours of \( y \) in \( C \). Then \( d_C(x, a') = k' - 1 \) and \( d_C(x, b') = k' - 1 \). Hence \( a', b' \in I'' \). Then, by Property 4, we have \( \rho(a') \in T(\tau(x), \rho(a)) \) and \( \rho(b') \in T(\tau(x), \rho(b)) \). Since \( d_C(a', b') = 2k' - 2 = k - 2 \), by Property 4, \( d_I(\tau(x), \rho(a')) \leq k + 1 = 2k' - 4 \). So, without loss of generality, we may assume that \( d_I(\tau(x), \rho(a')) \leq 2k' - 3 \). Similarly, let \( c' \in C(y, c) \) and \( d' \in C(y, d) \) satisfy \( d_C(y, c') = k' - 1 \) and \( d_C(y, d') = k' - 1 \). Without loss of generality, here we may assume that \( d_I(\tau(y), \rho(c')) \leq 2k' - 3 \). Then, however, we have \( d_C(a', c') = 2k' - 1 = k - 1 = 2k' - 3 \) and \( d_I(\tau(a'), \rho(c')) = d_I(\rho(a'), \tau(x)) + d_I(\tau(x), \tau(y)) + d_I(\tau(y), \rho(c')) \leq 4k' - 5 = k + 1 = 2k' - 3 \), contradicting Property 5. Thus, for any two adjacent vertices \( x, y \in I'' \), we must have \( d_I(\tau(x), \tau(y)) \geq 2 \).

Let \( v, w \in I'' \) be such that \( d_C(v, w) = 2k' - 2 \) and \( \rho(v) \notin T(\tau(x), \rho(a)) \). Then \( d_I(\tau(x), \tau(w)) \geq 4k' - 4 \). By Property 5, we have \( d_I(\tau(x), \rho(w)) \leq 4k' - 5 \), and hence \( \rho(w) \in T(\tau(x), \rho(a)) \). Thus, \( d_I(\tau(x), \rho(w)) \geq 4k' - 5 \). By Property 4, \( d_I(\tau(x), \rho(w)) \leq k + 1 = 3 = 4k' - 5 \). Without loss of generality, we may assume that \( d_I(\tau(x), \rho(w)) \leq 2k' - 3 \). Similarly, let \( c' \in C(z, c) \) and \( d' \in C(z, d) \) satisfy \( d_C(z, c') = k' - 1 = 2k' - 4 \) and \( d_C(z, d') = k' - 1 \). Without loss of generality, here we may assume that \( d_I(\tau(z), \rho(c')) \leq 2k' - 3 \). Then, however, we have \( d_C(a', c') = 2k' - 1 = k - 1 = 2k' - 3 \) and \( d_I(\tau(a'), \rho(c')) = d_I(\rho(a'), \tau(x)) + d_I(\tau(x), \tau(y)) + d_I(\tau(y), \rho(c')) \leq 4k' - 4 = k + 1 = 2k' - 3 \), contradicting Property 5. Thus, there is no triple of three distinct vertices \( x, y, z \in I'' \) with \( x, z \) being neighbours of \( y \) in \( C \) and \( d_I(\tau(x), \tau(y)) = 1 \) and \( d_I(\tau(x), \tau(z)) = 1 \). As such, \( I'' \) is an even number.

Let \( v, w \in I'' \) be such that \( d_C(v, w) = 2k' - 1 \) and \( d_I(\tau(x), \tau(v)) \geq 4k' - 4 \) and \( \rho(w) \notin T(\tau(x), \rho(a)) \). By Property 5, we have \( d_I(\tau(x), \rho(w)) \leq 4k' - 4 \), and hence \( \rho(w) \in T(\tau(x), \rho(a)) \). Similarly, \( d_I(\tau(x), \rho(w)) \geq 4k' - 5 \). Compared to the even case, settled above, there might be adjacent topological vertices around, but note that, for any four distinct vertices \( x, y, z, \alpha \in I'' \) with \( y, z \) and \( \alpha \) being the three neighbours of \( x \) in \( C \), crucially at most one of the pairs \( \tau(x), \tau(y) \tau(x), \tau(z) \text{ and } \tau(x), \tau(\alpha) \) contains two adjacent vertices in \( T \). Starting at the centre \( v_0 \) of \( C \), we can thus find a vertex \( v_1 \in I'' \) with \( d_C(v_0, v_1) = 2k' - 1 \) and \( d_I(\tau(v_1), \rho(v_1)) \geq 2 \), a vertex \( v_2 \in I'' \) with \( d_C(v_0, v_2) = 2k' - 2 \) and \( d_I(\tau(v_2), \rho(v_2)) \geq 4 \) and so forth. The existence of the vertex \( v_1 \) finally contradicts Property 6. Note that \( \left\lceil (k - 1)/2 \right\rceil (2k' - 1) \leq 4k' + 3k' + 1 = k' - 1 = \left\lceil (k - 1)/2 \right\rceil \).

Having derived a contradiction for the case of \( k \) being even and for the case of \( k \) being odd, we are now done. \( \square \)

5.4. Proof of Corollary 1

**Proof.** It follows from Theorem 1 that the following conditions are equivalent:

(i) \( L(k) \subseteq L(k') \).

(ii) \( k' - k \) is an even number or \( k' \geq 2k - 2 \).

We prove Corollary 1 by showing that

(iii) Every \( k \)-leaf root of every element \( G \) of \( L(k) \cap L(k') \) can be transformed into a \( k' \)-leaf root of \( G \) by the two simple operations of first possibly subdividing all internal edges exactly once and then possibly subdividing all external edges a fixed number of times.

is another equivalent condition.

By Lemma 8, we have \( (ii) \implies (iii) \).

In order to show \( (iii) \implies (ii) \), we suppose that \( (ii) \) does not hold and show that then \( (iii) \) does not hold. Indeed, suppose that \( k' - k \) is odd and \( k' \leq 2k - 3 \). Note that \( 1 \leq k' - k \leq k - 3 \) implies \( k \geq 4 \). Consider \( P_3 \), the path with vertex set \( \{a, b, c\} \).
and edge set \{ab, bc\}. Clearly, \(P_2 \in L(k) \cap L(k')\). Let \(T\) be the tree obtained from a path of \(k+1\) edges with endvertices \(a\) and \(c\) by adding a leaf \(b\) to the path, such that the distance between \(a\) and \(b\) is \(k\). Note that \(d_T(b, c) = 3\). So \(T\) is a \(k\)-leaf root of \(P_2\).

We will show that \(T\) cannot be transformed into a \(k'-\)leaf root of \(P_3\) by the two simple operations of first possibly subdividing all internal edges exactly once and then possibly subdividing all external edges a fixed number of times.

Consider \(T'\), which is obtained from \(T\) by subdividing all internal edges of \(T\) exactly once and possibly subdividing all external edges of \(T\) a fixed number of times. Then \(d_{T'}(a, b) \geq 2(k-2) + 2 = 2k - 2 > k'\), and hence \(T'\) is not a \(k'\)-leaf root of \(P_3\). Now consider \(T\), which is obtained from \(T\) by subdividing all external edges of \(T\) a fixed number \(l\) of times, and suppose that \(T'\) is a \(k'\)-leaf root of \(P_3\). Then \(k' \geq d_{T'}(a, b) = k + 2l\). As \(k' - k\) is an odd number, equality cannot hold, and we have \(k' > k + 2l\). Hence \(d_{T'}(a, c) = k + 1 + 2l \leq k'\), a contradiction. Clearly, \(T\) itself is not a \(k'\)-leaf root of \(P_3\), which finishes the proof. \(\Box\)

6. Conclusion

In this paper the question about the inclusion structure of the graph classes of leaf powers has been completely solved. As a by-product we obtain some information about the relationship of \(k\)-leaf roots for different \(k\) of the same graph.

In addition, a partial characterisation for \(L(4) \cap L(5)\) was given. A complete characterisation seems possible, but tedious. Characterisations for other interesting intersections, such as the intersection of the 5- and 6-leaf power classes, are still open problems.

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