

On strongly chordal graphs that are not leaf powers

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Abstract. A common task in phylogenetics is to find an evolutionary tree representing proximity relationships between species. This motivates the notion of leaf powers: a graph $G = (V, E)$ is a leaf power if there exist a tree T on leafset V and a threshold k such that $uv \in E$ if and only if the distance between u and v in T is at most k . Characterizing leaf powers is a challenging open problem, along with determining the complexity of their recognition. Leaf powers are known to be strongly chordal, but few strongly chordal graphs are known to *not* be leaf powers, as such graphs are difficult to construct. Recently, Nevries and Rosenke asked if leaf powers could be characterized by strong chordality and a finite set of forbidden induced subgraphs.

In this paper, we provide a negative answer to this question, by exhibiting an infinite family \mathcal{G} of (minimal) strongly chordal graphs that are not leaf powers. During the process, we establish a connection between leaf powers, alternating cycles and quartet compatibility. We also show that deciding if a chordal graph is \mathcal{G} -free is NP-complete.

1 Introduction

In phylogenetics, a classical method for inferring an evolutionary tree of species is to construct the tree from a distance matrix, which depicts how close or far each species are to one and another. Roughly speaking, similar species should be closer to each other in the tree than more distant species. In some contexts, the actual distances are ignored (e.g. when they cannot be trusted due to errors), and only the notions of “close” and “distant” are preserved. This corresponds to a graph in which the vertices are the species, and two vertices share an edge if and only if they are “close”. This motivates the definition of *leaf powers*, which was proposed by Nishimura et al. in [16]: a graph $G = (V, E)$ is a leaf power if there exist a tree T on leafset $V(G)$ and a threshold k such that $uv \in E$ if and only if the distance between u and v in T is at most k . Hence the tree T , which we call a *leaf root*, is a potential evolutionary history for G , as it satisfies the notions of “close” and “distant” depicted by G . It is also worth noting that this type of similarity graph is also encountered in the context of gene *orthology* inference, which is a special type of relationship between genes (see e.g. [12,21]). A similarity graph G is used as a basis for the inference procedure, and being able to verify that G is a leaf power would provide a basic test as to whether G correctly depicts similarity, as such graphs are known to contain errors [11].

A considerable amount of work has been done on the topic of leaf powers (see [6] for a survey), but two important challenges remain open: to determine

the computational complexity of recognizing leaf powers, and to characterize the class of leaf powers from a graph theoretic point of view. Despite some interesting results on graph classes that are leaf powers [4,5,10], both problems are made especially difficult due to our limited knowledge on graphs that are *not* leaf powers. Such knowledge is obviously fundamental for the characterization of leaf powers, but also important from the algorithmic perspective: if recognizing leaf powers is in P , a polynomial time algorithm is likely to make usage of structures to avoid, and if it is NP-hard, a hardness reduction will require knowledge of many non-leaf powers in order to generate “no” instances.

It has been known for many years that leaf powers must be strongly chordal (i.e. chordal and sun-free). Brandstädt et. al exhibited one strongly chordal non-leaf power by establishing an equivalence between leaf powers and NeST graphs [3,5]. Recently [15], Nevries and Rosenke found seven such graphs, all identified by the notion of bad 2-cycles in *clique arrangements*, which are of special use in strongly chordal graphs [14]. These graphs have at most 12 vertices, and in [13], the authors conjecture that they are the only strongly chordal non-leaf powers. This was also posed as an open problem in [6]. A positive answer to this question would imply a polynomial time algorithm for recognizing leaf powers, as strong chordality can be checked in $O(\min\{m \log n, n^2\})$ time [17,19].

In this paper, we unfortunately give a negative answer to this question. We exhibit an infinite family \mathcal{G} of strongly chordal graphs that are not leaf powers, and each graph in this family is minimal for this property (i.e. removing any vertex makes the graph a leaf power). This is done by first establishing a new necessary condition for a graph G to be a leaf power, based on its *alternating cycles* (which are cyclic orderings of vertices that alternate between an edge and a non-edge). Namely, there must be a tree T that can satisfy the edges/non-edges of each alternating cycle C of G after (possibly) subdividing some of its edges (see Section 3 for a precise definition). This condition has two interesting properties. First, every graph currently known to not be a leaf power fails to satisfy this condition. And more importantly, this provides new tools for the construction of novel classes of non-leaf powers. In particular, alternating cycles on four vertices enforce the leaf root to contain a specific *quartet*, a binary tree on four leaves. This connection lets us borrow from the theory of *quartet compatibility*, which is well-studied in phylogenetics (see e.g. [1,2,18,20]). More precisely, we use results from [18] to create a family \mathcal{G} of strongly chordal graphs whose 4-alternating cycles enforce a minimal set of incompatible quartets. We then proceed to show that deciding if a chordal graph G contains a member of \mathcal{G} as an induced subgraph is NP-complete. Thus, \mathcal{G} -freeness is the first known property of non-leaf powers that we currently ignore how to check in polynomial time. This result also indicates that if the problem admits a polynomial time algorithm, it will have to make use of strong chordality (or some other structural property), since chordality alone is not enough to identify forbidden structures quickly.

The paper is organized as follows: in Section 2, we provide some basic notions and facts. In Section 3, we establish the connection between leaf powers, alter-

nating cycles and quartets, along with its implications. In Section 4, we exhibit the family \mathcal{G} of strongly chordal graphs that are not leaf powers. We then show in Section 5 that deciding if a chordal graph is \mathcal{G} -free is NP-complete.

2 Preliminary notions

All graphs in this paper are simple and finite. For $k \in \mathbb{N}^+$, we use the notation $[k] = \{1, \dots, k\}$. We denote the set of vertices of a graph G by $V(G)$, its set of edges by $E(G)$, and its set of non-edges by $\overline{E}(G)$. By $G[X]$ we mean the subgraph induced by $X \subseteq V(G)$. The set of neighbors of $v \in V(G)$ is $N(v)$. The P_4 is the path of length 3 and the $2K_2$ is the graph consisting of two vertex-disjoint edges. A k -sun, denoted S_k , is the graph obtained by starting from a clique of size $k \geq 3$ with vertices x_1, \dots, x_k , then adding vertices a_1, \dots, a_k such that $N(a_i) = \{x_i, x_{i+1}\}$ for each $i \in [k-1]$ and $N(a_k) = \{x_k, x_1\}$. A graph is a sun if it is a k -sun for some k , and G is *sun-free* if no induced subgraph of G is a sun.

A graph G is *chordal* if it has no induced cycle with four vertices or more, and G is *strongly chordal* if it is chordal and sun-free. A vertex v is *simplicial* if $N(v)$ is a clique, and v is *simple* if it is simplicial and, in addition, for every $x, y \in N(v)$, one of $N(x) \subseteq N(y) \setminus \{x\}$ or $N(y) \subseteq N(x) \setminus \{y\}$ holds. An ordering (x_1, \dots, x_n) of $V(G)$ is a *perfect elimination ordering* if, for each $i \in [n]$, x_i is simplicial in $G[\{x_i, \dots, x_n\}]$. The ordering is *simple* if, for each $i \in [n]$, x_i is simple in $G[\{x_i, \dots, x_n\}]$. It is well-known that a graph is chordal if and only if it admits a perfect elimination ordering [9], and a graph is strongly chordal if and only if it admits a simple elimination ordering [8].

Denote by $L(T)$ the set of leaves of a tree T . We say a graph $G = (V, E)$ is a k -leaf power if there exists a tree T with $L(T) = V$ such that for any two distinct vertices $u, v \in V$, $uv \in E$ if and only if the distance between u and v in T is at most k . Such a tree T is called a k -leaf root of G . A graph G is a *leaf power* if there exists a positive integer k such that G is a k -leaf power.

A *quartet* is an unrooted binary tree on four leaves (an unrooted tree T is binary if all its internal vertices have degree exactly 3). For a set of four elements $X = \{a, b, c, d\}$, there exist 3 possible quartets on leafset X which we denote $ab|cd$, $ac|bd$ and $ad|bc$, depending on how internal edge separates the leaves. We say that T *contains* a quartet $ab|cd$ if $\{a, b, c, d\} \subseteq L(T)$ and the path between a and b does not intersect the path between c and d . We denote $\mathcal{Q}(T) = \{ab|cd : T \text{ contains } ab|cd\}$. We say that a set of quartets Q is *compatible* if there exists a tree T such that $Q \subseteq \mathcal{Q}(T)$, and otherwise Q is *incompatible*.

For a tree T and $x, y \in V(T)$, $p_T(x, y)$ denotes the set of edges on the unique path between x and y . We may write $p(x, y)$ when T is clear from the context. It will be convenient to extend the definition of leaf powers to weighted edges. A *weighted* tree (T, f) is a tree accompanied by a function $f : E(T) \rightarrow \mathbb{N}^+$ weighting its edges. If $F \subseteq E(T)$, we denote $f(F) = \sum_{e \in F} f(e)$. The distance $d_{T,f}(x, y)$ between two vertices of T is given by $f(p(x, y))$, i.e. the sum of the weights of the edges lying on the $x - y$ path in T . We may write $d_f(x, y)$ for short. We say that (T, f) is a *leaf root* of a graph G if there exists an integer k such that $xy \in E(G)$ iff $d_f(x, y) \leq k$. We will call k the *threshold* corresponding

to (T, f) . Note that in the usual setting, the edges of leaf roots are not weighted, though arbitrarily many degree 2 vertices are allowed. It is easy to see that this distinction is merely conceptual, since an edge e with weight $f(e)$ can be made unweighted by subdividing it $f(e) - 1$ times.

A tree T is *unweighted* if it is not equipped with a weighting function. We say an unweighted tree is an *unweighted leaf root* of a graph G if there is a weighting f of $E(T)$ such that (T, f) is a leaf root of G .

A first observation that will be of convenience later on is that, even though the usual definition of leaf powers does not allow edges of weight 0, they do not alter the class of leaf powers.

Lemma 1. *Let G be a graph, and let (T, f) be a weighted tree in which $L(T) = V(G)$ and $f(e) \geq 0$ for each $e \in E(T)$. If there exists an integer k such that $uv \in E(G) \Leftrightarrow d_f(u, v) \leq k$, then T is an unweighted leaf root of G .*

Proof. If no edge has weight 0, there is nothing to do. Otherwise, we devise a weighting function f' for T . Let $d = \max_{x, y \in V(T)} |p(x, y)|$. Set $f'(e) = (d+1) \cdot f(e)$ for each $e \in E(T)$ having $f(e) > 0$, and $f'(e) = 1$ for each $e \in E(T)$ having $f(e) = 0$. If $d_f(x, y) \leq k$, then $d_{f'}(x, y) \leq (d+1)k + d$, and if $d_f(x, y) \geq k+1$, then $d_{f'} \geq (d+1)k + (d+1)$. The threshold $(d+1)k + d$ shows that T is an unweighted leaf root of G . \square

A tree T' is a *refinement* of a tree T if T can be obtained from T' by contraction of edges. A consequence of the above follows.

Lemma 2. *Let T be an unweighted leaf root of a leaf power G . Then any refinement T' of T is also an unweighted leaf root of G .*

Proof. We may take a weighting f such that (T, f) is a leaf root of G , refine it in order to obtain T' , weight the newly created edges by 0 and apply Lemma 1. \square

The following was implicitly proved in [4]. We include the proof in the Appendix for the sake of completeness.

Lemma 3. *Suppose that G has a vertex v of degree 1. Then G is a leaf power if and only if $G - v$ is a leaf power.*

3 Alternating cycles and quartets in leaf powers

In this section, we restrict our attention to alternating cycles in leaf powers, which let us establish a new necessary condition on the topology of unweighted leaf roots. This will serve as a basis for the construction of our family of forbidden induced subgraphs. Although we will not use the full generality of the statements proved here, we believe they may be of interest for future studies.

Let (A, B) be a pair such that $A \subseteq E(G)$ and $B \subseteq \overline{E}(G)$. We say a weighted tree (T, f) *satisfies* (A, B) if there exists a threshold k such that for each edge $\{x, y\} \in A$, $d_f(x, y) \leq k$ and for each non-edge $\{x, y\} \in B$, $d_f(x, y) > k$. Thus (T, f) is a leaf root of G iff it satisfies $(E(G), \overline{E}(G))$. For an unweighted tree T ,

we say that T *can satisfy* (A, B) if there exists a weighting f of $E(T)$ such that (T, f) satisfies (A, B) .

A sequence of $2c$ distinct vertices $C = (x_0, y_0, x_1, y_1, \dots, x_{c-1}, y_{c-1})$ is an *alternating cycle* of a graph G if for each $i \in \{0, \dots, c-1\}$, $x_i y_i \in E(G)$ and $y_i x_{i+1} \notin E(G)$ (indices are modulo c in all notions related to alternating cycles). In other words, the vertices of C alternate between an edge and a non-edge. We write $V(C) = \{x_0, y_0, \dots, x_{c-1}, y_{c-1}\}$, $E(C) = \{x_i y_i : 0 \leq i \leq c-1\}$ and $\overline{E}(C) = \{y_i x_{i+1} : 0 \leq i \leq c-1\}$. A weighted tree *satisfies* C if it satisfies $(E(C), \overline{E}(C))$, and an unweighted tree *can satisfy* C if it can satisfy $(E(C), \overline{E}(C))$. The next necessary condition for leaf powers is quite an obvious one, but will be of importance throughout the paper.

Proposition 1. *If G is a leaf power, then there exists an unweighted tree T that can satisfy every alternating cycle of G .*

As it turns out, every graph that is currently known to not be a leaf power fails to satisfy the above condition (actually, we may even restrict our attention to cycles of length 4 and 6, as we will see). This suggests that it is also sufficient, and we conjecture that if there exists a tree that can satisfy every alternating cycle of G , then G is a leaf power. As a basic sanity check towards this statement, we show that in the absence of alternating cycles, a graph is indeed a leaf power.

Proposition 2. *If a graph G has no alternating cycle, then G is a leaf power.*

Proof. Since a chordless cycle of length at least 4 contains an alternating cycle, G must be chordal. By the same argument, G cannot contain an induced gem (the gem is obtained by taking a P_4 , and adding a vertex adjacent to each vertex of the P_4). In [4], it is shown that chordal gem-free graphs are leaf powers. \square

We will go a bit more in depth with alternating cycles, by first providing a characterization of the unweighted trees that can satisfy an alternating cycle C . Let T be an unweighted tree with $V(C) \subseteq V(T)$. For each $i \in \{0, \dots, c-1\}$, we say the path in T between x_i and y_i is *positive*, and the path between y_i and x_{i+1} is *negative* (with respect to C).

Lemma 4. *An unweighted tree T can satisfy an alternating cycle $C = (x_0, y_0, \dots, x_{c-1}, y_{c-1})$ if and only if there exists an edge e of T that belongs to strictly more negative paths than positive paths w.r.t. C .*

Proof. Due to space constraints, we only prove the (\Rightarrow) direction. The proof of sufficiency is relegated to the Appendix.

(\Rightarrow) : suppose that no edge is on more negative paths than positive paths, and yet T can satisfy C . Let f be a weighting such that (T, f) satisfies C with some threshold k . For each $i \in \{0, \dots, c-1\}$, let $A_i = p(y_i, x_{i+1}) \setminus p(x_{i+1}, y_{i+1})$ and $B_i = p(x_{i+1}, y_{i+1}) \setminus p(y_i, x_{i+1})$. Moreover, let $R_i = p(y_i, x_{i+1}) \cap p(x_{i+1}, y_{i+1})$. Observe that $f(p(y_i, x_{i+1})) = f(A_i) + f(R_i) = f(p(x_{i+1}, y_{i+1})) + f(A_i) - f(B_i)$. We claim that for any integer $j \geq 1$,

$$f(p(x_0, y_0)) < f(p(x_j, y_j)) + \sum_{i=0}^{j-1} (f(A_i) - f(B_i))$$

(where the indices of the x_j, y_j, A_i and B_i are taken modulo c). This is easily proved by induction. For $j = 1$, we have $f(p(x_0, y_0)) \leq k < f(p(y_0, x_1)) = f(p(x_1, y_1)) + f(A_0) - f(B_0)$ since x_0y_0 is an edge of C but y_0x_1 is not. For higher values of j , the same argument can be applied inductively: suppose $f(p(x_0, y_0)) < f(p(x_{j-1}, y_{j-1})) + \sum_{i=0}^{j-2} (f(A_i) - f(B_i))$. The claim follows from the fact that $f(p(x_{j-1}, y_{j-1})) \leq k < f(p(y_{j-1}, x_j)) = f(p(y_j, x_j)) + f(A_{j-1}) - f(B_{j-1})$.

Using the above claim, by setting $j = c$, we obtain $f(p(x_0, y_0)) < f(p(x_0, y_0)) + \sum_{i=0}^{c-1} (f(A_i) - f(B_i))$, i.e. $\sum_{i=0}^{c-1} f(B_i) < \sum_{i=0}^{c-1} f(A_i)$. Then $\sum_{i=0}^{c-1} (f(B_i) + f(R_i)) < \sum_{i=0}^{c-1} (f(A_i) + f(R_i))$. But since $p(y_i, x_{i+1})$ is the disjoint union of A_i and R_i , and $p(x_{i+1}, y_{i+1})$ the disjoint union of B_i and R_i , this implies $\sum_{i=0}^{c-1} f(p(x_{i+1}, y_{i+1})) < \sum_{i=0}^{c-1} f(p(y_i, x_{i+1}))$. For any given edge e , $f(e)$ is summed as many times as it appears on a positive path on the left-hand side, and as many times as it appears on a negative path on the right-hand side. Since, by assumption, no edge appears on more negative than positive paths, we have reached a contradiction since this inequality is impossible. \square

Lemma 4 lets us relate quartets and 4-alternating cycles easily. If $C = (x_0, y_0, x_1, y_1)$, the edges of the quartets $x_0x_1|y_0y_1$ and $x_0y_1|y_0x_1$ do not meet the condition of Lemma 4, and therefore no unweighted leaf root can contain these quartets. This was already noticed in [15], although this was presented in another form and not stated in the language of quartets.

Corollary 1. *Let $C = (x_0, y_0, x_1, y_1)$ be a 4-alternating cycle of a graph G . Then a tree T can display C if and only if T contains the $x_0y_0|x_1y_1$ quartet.*

We will denote by $RQ'(G)$ the set of *required quartets* of G , that is $RQ'(G) = \{x_0y_0|x_1y_1 : (x_0, y_0, x_1, y_1) \text{ is an alternating cycle of } G\}$. The only graphs on 4 vertices that contain an alternating cycle are the P_4 , the $2K_2$ and the C_4 . However, the C_4 contains two distinct alternating cycles: if four vertices $abcd$ in cyclic order form a C_4 , then (a, b, d, c) and (d, a, c, b) are two alternating cycles. The first implies the $ab|cd$ quartet, whereas the second implies the $ad|cb$ quartet. This shows that no leaf power can contain a C_4 . Thus $RQ'(G)$ can be constructed by enumerating the $O(n^4)$ induced P_4 and $2K_2$ of G . It is worth mentioning that deciding if a given set of quartets is compatible is NP-complete [20]. However, $RQ'(G)$ is not *any* set of quartets since it is generated from P_4 's and $2K_2$'s of a strongly chordal graph, and the hardness does not immediately transfer.

Now, denote by $RQ(G)$ the set of quartets that any unweighted leaf root of G must contain, if it exists. Then $RQ'(G) \subseteq RQ(G)$, and equality does not hold in general. Below we show how to find some of the quartets from $RQ(G) \setminus RQ'(G)$ (Lemma 5, which is a generalization of [15, Lemma 2]).

Lemma 5. *Let $P_1 = x_0x_1 \dots x_p$ and $P_2 = y_0y_1 \dots y_q$ be disjoint paths of G (with possible chords) such that for any $0 \leq i < p$ and $0 \leq j < q$, $\{x_i, x_{i+1}, y_j, y_{j+1}\}$ are the vertices of an alternating cycle. Then $x_0x_p|y_0y_q \in RQ(G)$.*

Proof. First note that in general, if a tree T contains the quartets $ab|c_ic_{i+1}$ for $0 \leq i < l$, then T must contain $ab|c_0c_l$ (this is easy to see by trying to construct such a T : start with the $ab|c_0c_1$ quartet, and insert c_2, \dots, c_l in order - at each insertion, c_i cannot have its neighbor on the $a - b$ path). For any $0 \leq i < p$, we may apply this observation on $\{a, b\} = \{x_i, x_{i+1}\}$. This yields $x_ix_{i+1}|y_0y_q \in RQ(G)$, since $x_ix_{i+1}|y_jy_{j+1} \in RQ'(G)$ for every j . Since this is true for every $0 \leq i < p$, we can apply this observation again, this time on $\{a, b\} = \{y_0, y_q\}$ (and the c_i 's being the x_i 's) and deduce that $y_0y_q|x_0x_p \in RQ(G)$. \square

In particular, suppose that G has two disjoint pairs of vertices $\{x_0, x_1\}$ and $\{y_0, y_1\}$ such that x_0 and x_1 (resp. y_0 and y_1) share a common neighbor z (resp. z'), and $z \notin N(y_0) \cup N(y_1)$ (resp. $z' \notin N(x_0) \cup N(x_1)$). Then $x_0x_1|y_0y_1 \in RQ(G)$.

In the rest of this section, we briefly explain how all known non-leaf powers fail to satisfy Proposition 2. We have already argued that a leaf power cannot contain a C_4 . As for a cycle C_n with $n > 4$ and vertices x_0, \dots, x_{n-1} in cyclic order, observe that $x_ix_{i+1}|x_{i+2}x_{i+3} \in RQ(C_n)$ since they form a P_4 , for each $i \in \{0, \dots, n-1\}$ (indices are modulo n). In this case it is not difficult to show that $RQ(C_n)$ is incompatible, providing an alternative explanation as to why leaf powers must be chordal.

A similar argument can be used for S_n , the n -sun, when $n \geq 4$. If we let x_0, \dots, x_{n-1} be the clique vertices of S_n arranged in cyclic order, again $x_ix_{i+1}|x_{i+2}x_{i+3} \in RQ(S_n)$ for $i \in \{0, \dots, n-1\}$, here because of Lemma 5 and the degree 2 vertices of S_n . Only S_3 , the 3-sun, requires an ad-hoc argument, and it is currently the only known non-leaf power for which the set of required quartets are compatible. Figure 1 illustrates how alternating cycles show that S_3 is not a leaf power. There are only two trees that contain $RQ'(S_3) = \{ay|cz, by|cx, bz|ax\}$, and for both, there is an alternating cycle such that each edge is on the same number of positive and negative paths. We do not know if there are other examples for which quartets are not enough to discard the graph as a leaf power. Moreover, an open question is whether for each even integer n , there exists a non-leaf power and a tree that can satisfy every alternating cycle of length $< n$, but not every alternating cycle of length n .

As for the seven strongly chordal graphs presented in [15], they were shown to be non-leaf powers by arguing that $RQ(G)$ was not compatible (although the proof did not use the language of quartet compatibility).

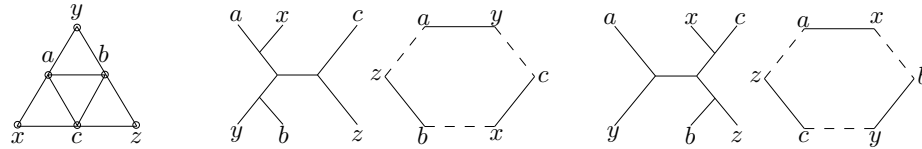


Fig. 1. The 3-sun S_3 , and the two trees that contain $RQ'(S_3) = \{ay|cz, by|cx, bz|ax\}$, with each tree accompanied by the alternating cycle of S_3 that it cannot satisfy.

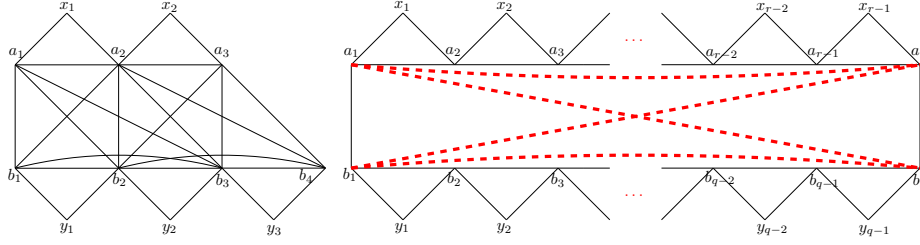


Fig. 2. The graph $G_{3,4}$ on the left, followed by its generalization $G_{r,q}$ on the right. In the latter, all edges between the a_i 's and b_i 's are present, except the non-edges depicted by red dashed lines.

4 Strongly chordal graphs that are not leaf powers

We will use a known set of (minimally) incompatible quartets as a basis for constructing our graph family.

Theorem 1 ([18]). *For every integers $r, q \geq 3$, the quartets $Q = \{a_i a_{i+1} | b_j b_{j+1} : i \in [r-1], j \in [q-1]\} \cup \{a_1 b_1 | a_r b_q\}$ are incompatible. Moreover, any proper subset of Q is compatible.*

We now construct the family $\{G_{r,q} : r, q \geq 3\}$ of minimal strongly chordal graphs that are not leaf powers. The idea is to simply enforce that $RQ(G_{r,q})$ contains all the quartets of Q in Theorem 1. Figure 2 illustrate the graph $G_{3,4}$ and a general representation of $G_{r,q}$. For integers $r, q \geq 3$, $G_{r,q}$ is as follows: start with a clique of size $r + q$, partition its vertices into two disjoint sets $A = \{a_1, \dots, a_r\}$ and $B = \{b_1, \dots, b_q\}$, and remove the edges $a_1 a_r, a_1 b_q, b_1 b_q$ and $b_1 a_r$. Then for each $i \in [r-1]$ insert a node x_i that is a neighbor of a_i and a_{i+1} , and for each $i \in [q-1]$, insert another node y_i that is a neighbor of b_i and b_{i+1} .

We note that in [15], the graph $G_{3,3}$ was one of the seven graphs shown to be a strongly chordal non-leaf power. Hence $G_{r,q}$ can be seen as a generalization of this example. It is possible that the other examples of [15] can also be generalized.

Theorem 2. *For any integers $r, q \geq 3$, the graph $G_{r,q}$ is strongly chordal, is not a leaf power and for any $v \in V(G_{r,q})$, $G_{r,q} - v$ is a leaf power.*

Proof. One can check that $G_{r,q}$ is strongly chordal by the simple elimination ordering: $x_1, x_2, \dots, x_{r-1}, y_1, \dots, y_{q-1}, a_1, b_1, a_r, b_q, a_2, \dots, a_{r-1}, b_2, \dots, b_{q-1}$.

To see that $G_{r,q}$ is not a leaf power, we note that the incompatible set of quartets of Theorem 1 is a subset of $RQ(G_{r,q})$: $a_i a_{i+1} | b_j b_{j+1} \in R(G_{r,q})$ by Lemma 5 and the paths $a_i x_i a_{i+1}$ and $b_j y_j b_{j+1}$, and $a_1 b_1 | a_r b_q \in RQ(G_{r,q})$ since they induce a $2K_2$.

We now show that for any $v \in V(G_{r,q})$, $G_{r,q} - v$ is a leaf power. First suppose that $v \in A \cup B$, say $v = a_i$ without loss of generality. Then in $G_{r,q} - a_i$, x_i (or take x_{i-1} if $i = r$) has degree one, and so by Lemma 3, $G_{r,q} - a_i$ is a leaf power if and only if $G_{r,q} - a_i - x_i$ is a leaf power. Therefore, it suffices to show that

$G_{r,q} - x_i$ is a leaf power. We may thus assume that $v = x_i$ for some i (the $v = y_i$ case is the same by symmetry).

$$\begin{array}{ll} p := 2(2i-1)(2r-2i-1)(2q-3) & p_1 := p/(2i-1) \\ p_2 := p/(2q-3) & p_3 := p/(2r-2i-1) \end{array}$$

Now for the x_j 's and y_j 's. For each $j \in [r-1] \setminus \{i\}$, the edge e incident to x_j has $f(e) = 2p - 2p_1$ if $j < i$ and $f(e) = 2p - 2p_3$ if $j > i$. For $j \in [q-1]$, the edge e incident to y_j has $f(e) = 2p - 2p_2$ if $j \leq q-3$, $f(e) = 2p - 2p_2 - 1$ if $j = q-2$ and $f(e) = p - 2$ if $j = q-1$. Each x_j is easily seen to be satisfied, as the only vertices of T within distance $2p$ of x_j are a_j and a_{j+1} . This is equally easy to see for the y_j vertices, with the exception of y_{q-1} . In (T, f) , y_{q-1} can reach b_q and b_{q-1} within distance $2p$ as required, but we must argue that it cannot reach a_i nor a_{i+1} (which is enough, since all the other leaves are farther from y_{q-1}). But this follows from that fact that $p_1, p_3 > 2$. This shows that (T, f) is a leaf root of $G_{r,q} - x_i$, and concludes the proof. \square

Interestingly, the $G_{r,q}$ graphs might be subject to various alterations in order to obtain different families of strongly chordal non-leaf powers. One example of such an alteration of $G_{r,q}$ is to pick some $j \in \{2, \dots, r-2\}$ and remove the edges $\{a_i b_q : 2 \leq i \leq j\}$. One can verify that the resulting graph is still strongly chordal, but requires the same set of incompatible quartets as $G_{r,q}$.

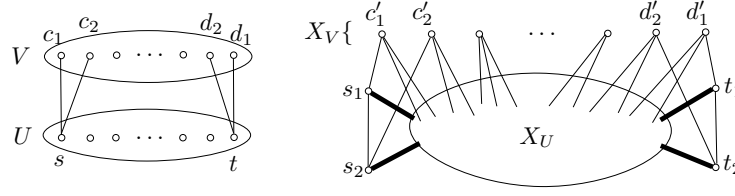


Fig. 4. An illustration of the reduction: G is on the left (only edges incident to s and t are drawn), H is on the right (thick edges mean that every possible edge is present).

5 Hardness of finding $G_{r,q}$ in chordal graphs

We show that deciding if a chordal graph contains an induced subgraph isomorphic to $G_{r,q}$ for some $r, q \geq 3$ is NP-complete. We reduce from the following:

The Restricted Chordless Cycle (RCC) problem:

Input: a bipartite graph $G = (U \cup V, E)$, and two vertices $s, t \in V(G)$ such that $s, t \in U$, both s and t are of degree 2 and they share no common neighbor.

Question: does there exist a chordless cycle in G containing both s and t ?

The RCC problem is shown to be NP-hard in [7, Theorem 2.2]¹. We first need some notation. If P is a path between vertices u and v , we call u and v its *endpoints*, and the other vertices are *internal*. Two paths P_1 and P_2 of a graph G are said *independent* if P_1 and P_2 are chordless, do not share any vertex except perhaps their endpoints, and for any internal vertices x in P_1 and y in P_2 , $xy \notin E(G)$. Observe that there is a chordless cycle containing s and t if and only if there exist two independent paths P_1 and P_2 between s and t .

From a RCC instance (G, s, t) we construct a graph H for the problem of deciding if H contains an induced copy of $G_{r,q}$. Figure 4 illustrates the construction.

Let $V(H) = \{s_1, t_1, s_2, t_2\} \cup X_U \cup X_V$, where $X_U = \{u' : u \in U \setminus \{s, t\}\}$ and $X_V = \{v' : v \in V\}$. Denote $X_U^* = X_U \cup \{s_1, t_1, s_2, t_2\}$. For $E(H)$, add an edge between every two vertices of X_U^* *except* the edges $s_1t_1, s_1t_2, s_2t_1, s_2t_2$. Moreover, we add an edge between $u' \in X_U$ and $v' \in X_V$ if and only if $uv \in E(G)$. Let $\{c_1, c_2\} = N(s)$ and $\{d_1, d_2\} = N(t)$. Then add edges $s_1c'_1$ and $s_2c'_2$, and add the edges $t_1d'_1$ and $t_2d'_2$. Notice that X_V forms an independent set.

We claim that H is chordal. Note that each vertex v of X_V is simplicial, since $N(v)$ consists of vertices from X_U and at most one of $\{s_1, t_1, s_2, t_2\}$ (since s and t have no common neighbor). Moreover, $H - X_V$ is easily seen to be chordal, and it follows that H admits a perfect elimination ordering.

Theorem 3. *Deciding if a graph H contains a copy of $G_{r,q}$ for some $r, q \geq 3$ is NP-complete, even if H is restricted to the class of chordal graphs.*

¹ Strictly speaking, the problem asks if there exists a chordless cycle with both s and t of size at least k . However, in the graph constructed for the reduction, any chordless cycle containing s and t has size at least k if it exists - therefore the question of existence is hard. Also, s and t are not required to be in the same part of the bipartition, but again, this is allowable by subdividing an edge incident to s or t .

Proof. The problem is in NP, since a subset $I \subseteq V(H)$, along with the labeling of I by the a_i, b_i, x_i and y_i 's of a $G_{r,q}$ can serve as a certificate. As for hardness, let G be a graph and H the corresponding graph constructed as above. We claim that G contains two independent paths P_1 and P_2 between s and t if and only if H contains a copy of $G_{r,q}$ for some $r, q \geq 3$. The idea is that s_1, s_2 (resp. t_1, t_2) correspond to the a_1, b_1 (resp. a_r, b_q) vertices of $G_{r,q}$, while the P_1 and P_2 paths give the other vertices. The x_i and y_i 's are in X_V , and the a_i and b_i 's in X_U^* .

(\Rightarrow) Let P_1 and P_2 be two independent paths between s and t . Note that both paths alternate between U and V . Let $P_1 = (s = u_1, v_1, u_2, v_2, \dots, v_{r-1}, u_r = t)$ and $P_2 = (s = w_1, z_1, w_2, z_2, \dots, z_{q-1}, w_q = t)$. Note that since P_1 and P_2 are independent, every vertex of $G[V(P_1) \cup V(P_2)]$ has degree exactly 2.

We show that the set of vertices $I = \{s_1, t_1, s_2, t_2\} \cup \{x' : x \in V(P_1) \cup V(P_2) \setminus \{s, t\}\}$ forms a $G_{r,q}$. Denote $I_U = I \cap X_U$ and $I_V = I \cap X_V$. First observe that $\{s_1, t_1, s_2, t_2\} \cup I_U$ forms a clique, but minus the edges $\{s_1 t_1, s_1 t_2, s_2 t_1, s_2 t_2\}$. Hence $\{s_1, s_2\}$ will correspond to the vertices $\{a_1, b_1\}$ of $G_{r,q}$, and $\{t_1, t_2\}$ to $\{a_r, b_q\}$, and it remains to find the degree two vertices around this “almost-clique”. Observe that $\{v_1, z_1\} = \{c_1, c_2\}$ and $\{v_{r-1}, z_{q-1}\} = \{d_1, d_2\}$. Let $c_{i_1} = v_1, c_{i_2} = z_1$ and $d_{j_1} = v_{r-1}, d_{j_2} = z_{q-1}$, with $\{i_1, i_2\} = \{j_1, j_2\} = \{1, 2\}$. In H , the vertex sequence $(s_{i_1}, u'_2, \dots, u'_{r-1}, t_{j_1})$ forms a path in $G[I]$ in which every two consecutive vertices share a common neighbor, which lies in I_V . Namely, s_{i_1} and u'_2 share $v'_1 = c'_{i_1}$, u'_i, u'_{i+1} share v'_i , and u'_{r-1}, t_{j_1} share $v'_{r-1} = d'_{j_1}$. The same property holds for the consecutive vertices of the path $(s_{i_2}, w'_2, \dots, w'_{q-1}, t_{i_2})$. Note that these two paths are disjoint in H and partition I_U . Moreover, by construction each $x' \in I_V$ is a shared vertex for some pair of consecutive vertices, i.e. x' has at least two neighbors in I .

Therefore, it only remains to show that if $x' \in I_V$, then x' has only two neighbors in I . Suppose instead that x' has at least 3 neighbors in I , say y'_1, y'_2, y'_3 . Note that all three lie in X_U^* . We must have $|\{s_1, s_2\} \cap \{y'_1, y'_2, y'_3\}| \leq 1$, since s_1 and s_2 share no neighbor in X_V . Likewise, $|\{t_1, t_2\} \cap \{y'_1, y'_2, y'_3\}| \leq 1$. This implies that y'_1, y'_2, y'_3 are vertices corresponding to three distinct vertices of G , say y_1, y_2 and y_3 . Then x is a neighbor of y_1, y_2, y_3 and since, by construction, $x, y_1, y_2, y_3 \in V(P_1) \cup V(P_2)$, this contradicts that $G[V(P_1) \cup V(P_2)]$ has maximum degree 2.

(\Leftarrow) Suppose there is $I \subseteq V(H)$ such that $H[I]$ is isomorphic to $G_{r,q}$ for some $r, q \geq 3$. Add a label to the vertices of I as in Figure 2 (i.e. we assume that we know where the a_i 's, b_i 's, x_i 's and y_i 's are in I). We first show that a_1, b_1, a_r, b_q , which we will call the *corner* vertices, are s_1, s_2, t_1, t_2 . If one of a_1 or b_1 is in X_U , then both a_r and b_q must be in X_V , as otherwise there would be an edge between $\{a_1, b_1\}$ and $\{a_r, b_q\}$. But a_r and b_q must share an edge, whereas X_V is an independent set. Thus we may assume $\{a_1, b_1\} \cap X_U = \emptyset$. Suppose that a_1 or b_1 is in X_V , say a_1 . Because $b_1 \notin X_U$ as argued above, we must have $b_1 \in \{s_1, s_2, t_1, t_2\}$. Suppose w.l.o.g. that $b_1 = s_1$. Hence $a_1 = c'_1$. Now consider the location of the x_1 vertex of $G_{r,q}$. Then x_1 must be in X_U , in which case x_1 is a neighbor of $s_1 = b_1$, contradicting that I is a copy of $G_{r,q}$. Therefore, we may assume that $\{a_1, b_1\} \cap X_V = \emptyset$. By applying the same argument on a_r and b_q , we deduce that $\{a_1, b_1, a_r, b_q\} = \{s_1, s_2, t_1, t_2\}$. We will suppose, without loss

of generality, that $a_1 = s_1, b_1 = s_2$ and $\{a_r, b_q\} = \{t_1, t_2\}$ (otherwise we may relabel the vertices of the $G_{r,q}$ copy, though note that in doing so we cannot make assumptions on which t_i corresponds to which of $\{a_r, b_q\}$).

Now let $(s_1 = a_1, a_2, \dots, a_r = t_j)$, $j \in \{1, 2\}$ be the path between the “top” corners of the $G_{r,q}$ copy in H , such that $a_i a_{i+1}$ share a common neighbor x_i of degree 2 in $G[I]$, $i \in [r-1]$. Similarly, let $(s_2 = b_1, b_2, \dots, b_q = t_l)$, $(l \in \{1, 2\}$ and $l \neq j)$ be the path between the “bottom” corners of $G_{r,q}$, such that $b_i b_{i+1}$ share a common neighbor y_i of degree 2 for $i \in [q-1]$. We claim that $a_i \in X_U$ for each $2 \leq i \leq r-1$. Suppose instead that some a_i is not in X_U . Since $s_1 = a_1$ is a neighbor of a_i , we must have $a_i = c'_1$ (the only other possibility is $a_i = s_2$, but $s_2 = b_1$). The common neighbor x_{i-1} of a_{i-1} and a_i therefore lies in X_U . But then, x_{i-1} is a neighbor of $s_2 = b_1$, which is not possible. Therefore, each a_i belongs to X_U . By symmetry, each b_i also belongs to X_U . This implies that every x_i and y_i belong to X_V , with $x_1 = c'_1, x_{r-1} = d'_j, y_1 = c'_2$ and $y_{q-1} = d'_l$.

We can finally find our independent paths P_1 and P_2 . It is straightforward to check that $\{s, t, c_1\} \cup \{u : u' \in \{x_i, a_i\} \text{ for } 2 \leq i \leq r-1\}$ induces a path P_1 from s to t in G . Similarly, $\{s, t, c_2\} \cup \{u : u' \in \{y_i, b_i\} \text{ for } 2 \leq i \leq q-1\}$ also induces a path P_2 from s to t . Moreover, P_1 and P_2 share no internal vertex.

It only remains to show that P_1 and P_2 are independent, i.e. form an induced cycle. We prove that $G[V(P_1) \cup V(P_2)]$ has maximum degree 2. Suppose there is a vertex v of degree at least 3 in $G[V(P_1) \cup V(P_2)]$. Then $v \notin \{s, t\}$ since they have degree 2 in G . Moreover, $v \notin V$, as otherwise, $v' \in I_V$ which implies that v' is an x_i or a y_i and, by construction, v' has at least 3 neighbors in I , a contradiction. Thus $v \in U$, and its 3 neighbors lie in V . Hence, v' is either an a_i or a b_i and has three neighbors in I_V , which is again a contradiction. This concludes the proof. \square

6 Conclusion

In this paper, we have shown that leaf powers cannot be characterized by strong chordality and a finite set of forbidden subgraphs. However, many questions asked here may provide more insight on leaf powers. For one, is the condition of Proposition 1 sufficient? And if so, can it be exploited for some algorithmic or graph theoretic purpose? Also, we do not know if large alternating cycles are important, since so far, every non-leaf power could be explained by checking its alternating cycles of length 4 or 6. A constant bound on the length of “important” alternating cycles would allow enumerating them in polynomial time.

Also, we have exhibited an infinite family of strongly chordal non-leaf powers (along with some variations of it), but it is likely that there are others. One potential direction is to try to generalize all of the seven graphs found in [15]. The clique arrangement of $G_{r,q}$ may be informative towards this goal. Finally on the hardness of recognizing leaf powers, the hardness of finding $G_{r,q}$ in strongly chordal graphs is of special interest. A NP-hardness proof would now be significant evidence towards the difficulty of deciding leaf power membership. And in the other direction, a polynomial time recognition algorithm may provide important insight on how to find forbidden structures in leaf powers.

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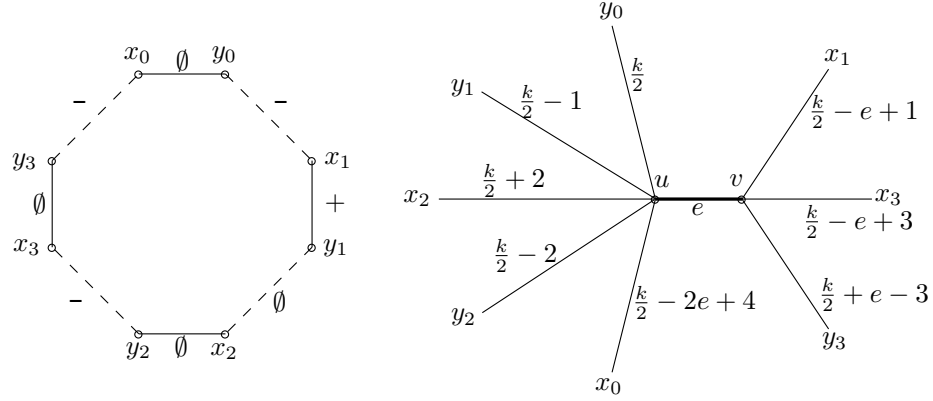


Fig. 5. An example alternating cycle C and tree T with a single internal edge uv . Edges and non-edges corresponding to a positive and negative path containing uv are labeled with a “+” and “-”, respectively, while the “ \emptyset ” label is for edges/non-edges corresponding to a path that is not negative nor positive. Here y_0 , y_2 and y_3 are negative, whereas y_1 is positive. The tree is labeled with the weights that would be given by the greedy procedure of the proof, starting at y_0 .

Appendix

6.1 Proof of Lemma 3

Proof. For the non-obvious direction, suppose that (T, f) is a leaf root of $G - v$ with threshold k . Let w be the neighbor of v in G . Then in (T, f) we can do the following modification: subdivide the edge wz incident to w into two edges wz' and $z'z$, set $f(wz') = 0$, $f(z'z) = f(wz)$, and insert v by making it adjacent to z' and setting $f(vz') = k$. As $f(z'z) > 0$, (T, f) satisfies the distance constraints on v , and we can apply Lemma 1 for the 0 edge. \square

Proof of Lemma 4, sufficiency

(\Leftarrow): let uv be an edge that appears on strictly more negative paths than positive paths. We prove that if u and v are the only two internal vertices of T (i.e. every leaf is adjacent to either u or v , as in Figure 5), then the statement holds. By Lemma 2, this is sufficient, since we can refine T into the desired tree afterwards.

Some more notation is required. For $z \in V(C)$, denote by $a(z)$ the single neighbor of z in T (with $a(z) \in \{u, v\}$). For a weighting function f , we may write $f(z)$ instead of $f(z, a(z))$. Let $X_0 = N(u) \setminus \{v\}$ and $X_1 = N(v) \setminus \{u\}$. Call two vertices x, y *separated* if $x \in X_i$ and $y \in X_{1-i}$ for some $i \in \{0, 1\}$. Call a vertex $y_i \in V(C)$ *positive* if y_i and x_{i-1} are not separated, but y_i and x_i are (i.e. y_i gives a “positive charge” to uv). Likewise, y_i is *negative* if y_i and x_{i-1} are separated but y_i and x_i are not. Otherwise, y_i is *neutral*.

Let P, N and Z denote, respectively, the number of positive, negative and neutral vertices among the y_i ’s. Then we must have $N \geq P + 2$. To see this, first

note that the number of paths, positive or negative, that go through uv must be even (since for each path that starts in X_0 and goes to X_1 , there must be a corresponding path from X_1 to X_0). Thus uv is on at least two more negative paths than positive paths. Then $N \geq P + 2$ follows, since negative vertices correspond to a negative path that cannot be matched with a positive path.

We now construct a weighting f of T so that it satisfies C . Put $e := f(uv) = c^2$ and set $k := 2c^{10}$ to be the threshold for T .² Suppose that y_0 is negative (otherwise relabel vertices), and set $f(y_0) = k/2$. Then traverse C in cyclic order starting from x_1 towards y_1 until x_0 is reached, weighting each vertex z encountered in a greedy manner, as follows:

- if $z = x_i$ and x_i is separated from y_{i-1} , set $f(x_i) = k + 1 - e - f(y_{i-1})$;
- if $z = x_i$ and x_i is not separated from y_{i-1} , set $f(x_i) = k + 1 - f(y_{i-1})$;
- if $z = y_i$ and y_i is separated from x_i , set $f(y_i) = k - e - f(x_i)$;
- if $z = y_i$ and y_i is not separated from x_i , set $f(y_i) = k - f(x_i)$.

At the end of this process, every edge of T will be weighted. Refer to Figure 5 for an example application of this procedure. One can check that all edge weights are positive integers since $f(z) \geq k/2 - ce$ for all $z \in V(C)$. When the process stops at x_0 , by construction f satisfies every edge and non-edge of C , except possibly the x_0y_0 edge of C . Hence it suffices to show that the above weighting satisfies $d_f(x_0, y_0) \leq k$. Since y_0 is negative, it is not separated from x_0 , and hence we must show that $f(x_0) \leq k/2$.

We have $f(x_1) = k/2 + 1 - e$. Now for $i \in \{1, \dots, c-1\}$, consider $\Delta_i := f(x_{i+1}) - f(x_i)$ (recall that indices are modulo c). If y_i is positive, then $f(y_i) = k - f(x_i) - e$ and $f(x_{i+1}) = k + 1 - f(y_i) = f(x_i) + e + 1$, implying $\Delta_i = e + 1$. Using the same logic on the other cases, we obtain that if y_i is negative, $\Delta_i = -e + 1$ and if y_i is neutral, $\Delta_i = 1$. Since $f(x_0) = f(x_1) + \sum_{i=1}^{c-1} \Delta_i$, we have $f(x_0) = f(x_1) + P \cdot (e + 1) + (N - 1) \cdot (-e + 1) + Z$ (we must use $N - 1$ instead of N because y_0 is negative, but is not between x_1 and x_0 in the visited cyclic order). This yields $f(x_0) \leq k/2 + 1 - e + e(P - N + 1) + c$. Since $N \geq P + 2$ and $e = c^2$, we obtain $f(x_0) \leq k/2$ as desired.

² We multiply k by 2 to ensure it is even