

## THE LEAFAGE OF A CHORDAL GRAPH

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### Abstract

The *leafage*  $l(G)$  of a chordal graph  $G$  is the minimum number of leaves of a tree in which  $G$  has an intersection representation by subtrees. We obtain upper and lower bounds on  $l(G)$  and compute it on special classes. The maximum of  $l(G)$  on  $n$ -vertex graphs is  $n - \lg n - \frac{1}{2} \lg \lg n + O(1)$ . The *proper leafage*  $l^*(G)$  is the minimum number of leaves when no subtree may contain another; we obtain upper and lower bounds on  $l^*(G)$ . Leafage equals proper leafage on claw-free chordal graphs. We use asteroidal sets and structural properties of chordal graphs.

**Keywords:** chordal graph, subtree intersection representation, leafage.

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### 1. INTRODUCTION

A simple graph is *chordal* (or *triangulated*) if every cycle of length exceeding 3 has a chord. The *intersection graph* of a family of sets is the graph defined by assigning one vertex for each set and joining two vertices by an edge if and only if the corresponding sets intersect. A graph is *chordal* if and only if it is the intersection graph of a family of subtrees of a host tree [3, 8, 23];

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such a family is a *subtree representation* of the graph. The *interval graphs* are the chordal graphs having subtree representations in which the host tree is a path; this allows the subtrees to be viewed as intervals on the real line. Given the many applications of interval graphs and the ease of computation on interval graphs, it is natural to ask for measures of how far a chordal graph is from being an interval graph.

The *leafage*  $l(G)$  of a chordal graph  $G$  is the minimum number of leaves of the host tree in a subtree representation of  $G$ . Interval graphs are the chordal graphs with leafage at most two. We derive bounds on leafage and study classes in which equality holds, including  $k$ -trees, block graphs, and chordal graphs having a dominating clique. We prove that the maximum leafage of a chordal graph on  $n$  vertices is the maximum  $k$  such that  $k \leq \binom{n-k}{\lfloor (n-k)/2 \rfloor}$ ; this is  $n - \lg n - \frac{1}{2} \lg \lg n + O(1)$ . Our proofs provide algorithms for computing leafage in some special classes.

Among the interval graphs are the *proper interval graphs*, which are those representable using a family of intervals in which no interval properly contains another. As observed in [8], every chordal graph has a subtree representation in which no subtree properly contains another; call this a *proper subtree representation*. By analogy with leafage, the *proper leafage*  $l^*(G)$  of a chordal graph  $G$  is the minimum number of leaves in a proper subtree representation of  $G$ . We extend a characterization of proper interval graphs by Roberts [19] to obtain a lower bound on proper leafage:  $l^*(G)$  is at least the maximum number of “modified extreme points” occurring in an induced subgraph of  $G$ . We present examples where the bound is arbitrarily bad, but the bound is sharp for  $k$ -trees, where it equals the number of simplicial vertices.

A notion analogous to leafage has already been characterized for a representation model based on containment. Leclerc [14] proved that a graph is the comparability graph of a partial order of dimension at most  $d$  if and only if it is the containment poset of a family of subtrees of a tree with at most  $d$  leaves. Our notion of leafage has been applied in [17], and the analogue of leafage for directed graphs is studied in [16].

We use well-known properties of chordal graphs from [3, 6, 11, 20, 23]. A *simplicial vertex* in a graph is a vertex  $v$  whose neighborhood  $N(v)$  induces a clique. A *cutset* (also called *separating set* or *vertex cut*) is a set of vertices whose deletion leaves a disconnected subgraph. Every cutset of a chordal graph induces a clique, and thus by induction every non-clique chordal graph has a nonadjacent pair of simplicial vertices [6]. The neighborhood of a simplicial vertex is a *simplicial neighborhood*. The subgraph of  $G$  induced

by the set  $S(G)$  of simplicial vertices is a disjoint union of cliques. We use  $S(G)$  to denote this subgraph in the same way that  $Q$  may denote a clique or its set of vertices. The deletion of a simplicial vertex cannot affect the existence of chordless cycles. Hence another characterization of a chordal graph [7, 20] is the existence of a *perfect elimination ordering*, meaning a vertex ordering  $v_n, \dots, v_1$  in which the vertices can be deleted such that for each  $i$ ,  $N(v_i) \cap \{v_i, \dots, v_1\}$  induces a clique.

Given a chordal graph  $G$ , the *derived graph*  $G'$  is the induced subgraph obtained by deleting all the simplicial vertices of  $G$ . As an induced subgraph of a chordal graph,  $G'$  also is a chordal graph. We describe a subtree of a tree by the set of vertices inducing it, and with this understanding we write  $f(v)$  for the subtree representing  $v$  in a subtree representation  $f$ . We use  $m(T)$  for the number of leaves of a tree  $T$ .

Every pairwise intersecting family of subtrees of a tree has a common vertex [11, p. 92]. Hence if  $Q$  is a clique in  $G$ , any subtree representation  $f$  of  $G$  assigns some host vertex to all of  $Q$ . If distinct vertices  $q, q'$  are assigned to cliques  $Q, Q'$  with  $Q \subset Q'$ , then for  $v \in Q$  the entire  $q, q'$ -path in the host belongs to  $f(v)$ . The first edge on this path can be contracted to obtain a smaller representation without changing the number of leaves. Therefore, we may restrict our attention to *minimal representations*, which are those subtree representations having a bijection between the maximal cliques of  $G$  and the vertices of the host tree. This restriction is *not valid* for proper leafage. We use the term *optimal representation* to refer to a subtree representation having the minimum number of host leaves (subject to appropriate conditions).

Gavril [9] and Shibata [22] proved that minimal representations correspond to maximum weight spanning trees in the weighted clique graph of  $G$ , where the *weighted clique graph* has a vertex for each maximal clique of  $G$ , and the weight of the edge  $QQ'$  is  $|Q \cap Q'|$ . Thus  $l(G)$  equals the minimum number of leaves in a maximum weight spanning tree of the weighted clique graph of  $G$ . This observation does not seem to simplify the problem.

## 2. ASTEROIDAL SETS AND SPECIAL CLASSES

Our first lower bound for  $l(G)$  generalizes the notion of asteroidal triple. We prove constructively that this bound is exact for trees and more generally for  $k$ -trees.

An *asteroidal triple* in a graph is a triple of distinct vertices such that each pair is connected by some path avoiding the neighborhood of the third

vertex. Interval graphs are the chordal graphs without asteroidal triples ([10, 15]). A set  $S \subseteq V(G)$  is an *asteroidal set* if every triple of vertices in  $S$  is an asteroidal triple. This concept arises also in [18, 23]. Let  $a(G)$  denote the maximum size of an asteroidal set in  $G$ . This parameter has subsequently been named the *asteroidal number* in [1, 2, 12, 13]; these papers explore further properties of asteroidal sets, asteroidal number, and leafage.

We define a notion like asteroidal sets for subtrees. If  $T_i, T_j, T_k$  are subtrees of a tree, then  $T_k$  is *between*  $T_i$  and  $T_j$  if  $T_i$  and  $T_j$  are disjoint and the unique path connecting them intersects  $T_k$ . A collection of pairwise disjoint subtrees such that none is between two others is an *asteroidal collection* of subtrees.

**Lemma 1.** *If  $T_1, \dots, T_n$  is an asteroidal collection of subtrees of a tree  $T$ , then  $T$  has at least  $n$  leaves.*

**Proof.** For each leaf  $v$  of  $T$ , we assign to  $v$  the first subtree in  $\{T_i\}$  encountered on the path from  $v$  to the nearest vertex of degree at least 3. Such a subtree exists, else we could delete the edges of that path to reduce  $m(T)$  without affecting  $\{T_i\}$ . If  $m(T) < n$ , then some subtree  $T_k$  in our list is assigned to no leaf. Let  $x$  be a vertex of  $T_k$ , and let  $P$  be a maximal path in  $T$  containing  $x$ . The endpoints of  $P$  are leaves of the tree, and  $T_k$  is between the subtrees assigned to those leaves. The contradiction yields  $m(T) \geq n$ . ■

**Theorem 1.** *In a subtree representation of a chordal graph  $G$ , the subtrees corresponding to an asteroidal set of vertices form an asteroidal collection, and  $l(G) \geq a(G)$ .*

**Proof.** Let  $f$  be a subtree representation of  $G$  in  $T$ . Every asteroidal triple of vertices is an independent set, and thus every asteroidal set is an independent set. Hence the subtrees corresponding to an asteroidal set in a subtree representation of  $G$  are pairwise disjoint. If none is between two others, then the subtrees form an asteroidal collection in  $T$ , and Lemma 1 yields the bound.

Suppose that  $f(w)$  is between  $f(u)$  and  $f(v)$ . Let  $P$  be a  $u, v$ -path in  $G$  containing no neighbor of  $w$ . Because every two successive vertices in  $P$  are adjacent, the corresponding subtrees in  $T$  have a common point, and hence the union  $\bigcup_{x \in P} f(x)$  of the subtrees representing these vertices is a connected subgraph  $T^-$  of  $T$ . Since  $P$  contains no neighbor of  $w$ ,  $T^-$  must be disjoint from  $f(w)$ , but this contradicts the assumption that the unique path between  $f(u)$  and  $f(v)$  in  $T$  contains a vertex of  $f(w)$ . ■

**Corollary 1.** *If  $G$  is a tree other than a star, then  $l(G)$  is the number of leaves in the derived tree  $G'$ .*

**Proof.** Suppose that  $G'$  has  $k$  leaves. For the lower bound, we obtain an asteroidal set. For each leaf of  $G'$ , select a leaf of  $G$  adjacent to it. This yields an asteroidal set  $S$  of size  $k$ , because for  $x, y \in S$ , the unique  $x, y$ -path in  $G$  consists of  $x, y$ , and a path between leaves of  $G'$  that are adjacent to  $x$  and  $y$ . This path contains no other leaf of  $G$  or  $G'$ , so it avoids the neighborhoods of other vertices in  $S$ .

For the upper bound, we construct a subtree representation. For the host tree  $T$ , begin with the tree obtained from  $G'$  by subdividing each edge once. Next, for each  $v' \in V(G')$ , choose one edge incident to  $v'$  in the current host and subdivide it  $k$  times, where  $k$  is the number of leaves of  $G$  incident to  $v'$ . Use each of these new vertices to represent one leaf of  $G$  incident to  $v'$ , and let  $f(v')$  consist of the vertex  $v'$  in  $T$  together with the vertices introduced by subdividing edges incident to  $v'$ . This yields a representation of  $G$ . Since  $G$  is not a star,  $G'$  has at least two leaves, and  $T$  and  $G'$  have the same number of leaves. ■

A  $k$ -tree is a chordal graph that can be constructed from  $K_k$  by a sequence of vertex additions in which the neighborhood of each new vertex is a  $k$ -clique of the current graph. With additional lemmas, we can generalize the construction of Corollary 1 to  $k$ -trees.

**Lemma 2.** *In a non-clique  $k$ -tree, the simplicial vertices are the vertices of degree  $k$  and form an independent set.*

**Proof.** The smallest non-clique  $k$ -tree has  $k + 2$  vertices and satisfies the claim. When a vertex receives a new neighbor, its degree exceeds  $k$ , and its old neighborhood cannot be contained among the other  $k - 1$  neighbors of the new simplicial vertex. Hence vertices of degree exceeding  $k$  (and neighbors of simplicial vertices) are not simplicial. ■

Every minimal cutset of a  $k$ -tree induces a  $k$ -clique (Rose [20]). Indeed, non-clique  $k$ -trees are precisely the connected graphs in which the largest clique has  $k + 1$  vertices and every minimal cutset induces a  $k$ -clique. Since deleting a simplicial vertex of a  $k$ -tree leaves a smaller  $k$ -tree, the construction procedure defining a  $k$ -tree can begin from any  $k$ -clique. These properties yields the following statement, which does not hold for general chordal graphs (it fails for the interval graph  $2P_4 \vee K_1$ ). (The *join*  $G \vee H$  of two graphs  $G$  and  $H$  is obtained from the disjoint union  $G + H$  by adding as edges  $\{uv : u \in V(G), v \in V(H)\}$ .)

**Lemma 3.** *If  $G$  is a non-clique  $k$ -tree having distinct simplicial neighborhoods, then  $G$  has distinct simplicial neighborhoods that are not cutsets of  $G'$ .*

**Proof.** By Lemma 2, every simplicial neighborhood in  $G$  is contained in  $V(G')$ . We call a simplicial vertex  $v$  *good* in  $G$  if  $G' - N(v)$  is connected.

If  $G$  is a non-clique  $k$ -tree, then  $G$  has only one simplicial neighborhood if and only if  $G' = K_k$ . If  $G' \neq K_k$ , then  $G$  has a simplicial vertex  $x$  such that  $G - x$  has distinct simplicial neighborhoods unless  $G$  has  $k + 3$  vertices and  $G' = K_{k+1}$ . There is one such  $k$ -tree, and its two simplicial vertices are good. This serves as the basis for induction.

For the induction step, choose  $x \in S(G)$ . The induction hypothesis implies that  $G - x$  has two good simplicial vertices  $u, v$  with distinct neighborhoods. If  $G' = (G - x)'$ , then every simplicial vertex of  $G - x$  is also simplicial in  $G$ . In this case,  $u, v$  are good for  $G$ .

Hence we may assume that  $G' \neq (G - x)'$ , which means that some simplicial vertex of  $G - x$  is not simplicial in  $G$ . Such a vertex  $y$  must be a neighbor of  $x$ . Applied to  $G - x$ , Lemma 2 implies both that  $y$  is unique and that  $(G - x)' = G' - y$ .

If  $y \notin N(v)$ , then  $(G - x)' - N(v) = [G' - N(v)] - y$ . Hence  $v$  remains good for  $G$  unless  $y$  is isolated in  $G' - N(v)$  (similarly for  $u$ ). Since  $y$  and  $v$  each have degree  $k$  in  $G - x$ , this requires  $N_{G-x}(y) = N_{G-x}(v)$ , so we may assume that  $y = v$  and that  $u$  is good in  $G$ . Also,  $u, x$  have distinct neighborhoods in  $G$ , since  $y \in N(x)$  and  $y = v$  is simplicial in  $G - x$ . Thus it suffices to prove that  $x$  is good in  $G$ .

Let  $z$  be the unique member of  $N(y) - N(x)$ . Since  $y$  is good in  $G - x$  and  $(G - x)' - N(y) = [G' - N(x)] - z$ , it suffices to show that  $z$  is not isolated in  $G' - N(x)$ . If so, then  $z$  has exactly  $k$  neighbors in  $G'$ . By Lemma 2,  $z \in S(G')$ , but  $G'$  cannot have adjacent simplicial vertices. ■

**Theorem 2.** *If  $G$  is a non-clique  $k$ -tree, then  $l(G) = \max\{2, r(G)\}$ , where  $r(G)$  is the number of distinct simplicial neighborhoods of  $G$  that are not cutsets in  $G'$ .*

**Proof.** When  $G$  is a non-clique  $k$ -tree,  $G$  has distinct simplicial neighborhoods unless  $G'$  is a nonempty clique, which occurs if and only if  $G$  is the join of a  $k$ -clique and an independent set. Such a  $k$ -tree is an interval graph.

When  $G$  has distinct simplicial neighborhoods, Lemma 3 implies that  $r(G) \geq 2$ . Let  $\mathbf{R}(G)$  be the set of simplicial neighborhoods of  $G$  that are not cutsets of  $G'$ . For the lower bound, we construct an asteroidal set of

size  $r(G)$  by selecting one simplicial neighbor of each  $R \in \mathbf{R}(G)$ . Given three such vertices  $x, y, z$ , there is a  $y, z$ -path in  $G$  avoiding  $N(x)$  because  $G' - N(x)$  is connected.

For the upper bound, we use induction to construct a subtree representation with the desired number of leaves, in which for each  $R \in \mathbf{R}(G)$ , the maximal cliques containing the simplicial vertices  $\{v \in S(G) : N(v) = R\}$  occur at a pendant path in the host tree  $T$ , in any specified order. We begin with the case where  $G' = K_k$ . Here  $G$  is the join of  $K_k$  and  $j$  simplicial vertices, and  $T = P_j$ , with each vertex of  $G'$  assigned all of  $T$  and each vertex of  $S(G)$  assigned one vertex of  $T$ .

For the induction step, we may assume that  $G'$  has more than one maximal clique and that  $r(G) \geq 2$ . By Lemma 3, we may choose  $x \in S(G)$  such that  $G' - N(x)$  is connected. The graph  $G - x$  is a smaller  $k$ -tree, and we apply the induction hypothesis. Let  $f$  be a subtree representation of  $G - x$  in a host tree  $T^-$  that has the specified properties. If  $N(x) = N(y)$  for some  $y \in S(G)$ , then  $r(G - x) = r(G)$ ; here we obtain  $T$  by inserting another vertex in the pendant path in  $T^-$  that corresponds to  $N(x)$ , assigning the new vertex to  $N(x) \cup \{x\}$ . If  $N(x) \neq N(y)$  for all  $y \in S(G) - \{x\}$ , and no neighbor of  $x$  is simplicial in  $G - x$ , then  $\mathbf{R}(G - x) = \mathbf{R}(G) - \{N(x)\}$ , and we are permitted to add a leaf in expanding  $f$  to a subtree representation of  $G$ . Since  $N(x)$  is a clique in  $G - x$ , its corresponding subtrees have a common vertex in  $T^-$ , and we can append a new leaf to that vertex, assigned to  $N(x) \cup \{x\}$ .

In the remaining case, some neighbor  $z$  of  $x$  is simplicial in  $G - x$ . By Lemma 2,  $z$  is unique. Let  $Q = N_{G-x}(z)$ , and let  $q$  be the vertex assigned by  $f$  to the maximal clique  $Q \cup \{z\}$ . If  $Q$  is not a cutset of  $(G - x)'$ , then by the induction hypothesis we may assume that  $q$  is a leaf of  $T^-$ . In this case  $Q$  is a cutset of  $G'$  (it isolates  $z$ ), so  $r(G) = r(G - x)$  even if  $Q$  is a simplicial neighborhood in  $G$ . On the other hand, if  $Q$  is a cutset of  $(G - x)'$ , then  $r(G) = r(G - x) + 1$ . In either case, we expand  $T^-$  by adding a leaf adjacent to  $q$  and assign it to  $N(x) \cup \{x\}$ . The resulting  $T$  has  $r(G)$  leaves. Furthermore, since  $N(x)$  is not the neighborhood of any simplicial vertex other than  $x$ , the claim about arbitrarily ordering the cliques involving a given simplicial neighborhood also holds. ■

We prove that  $l(G) = a(G)$  for one more class of chordal graphs. The *blocks* of a graph are its maximal subgraphs that have no cut-vertex. A *block graph* is a graph in which every block is a clique (equivalently, a graph is a block graph if and only if it is the intersection graph of the blocks in some graph).

Block graphs have no chordless cycles. A *leaf block* of  $G$  is a block containing only one cut-vertex of  $G$ .

**Theorem 3.** *If  $G$  is a block graph that is not a clique, then  $l(G) = \max\{2, r'(G)\}$ , where  $r'(G)$  is the number of cut vertices of  $G$  that are simplicial vertices in  $G'$ .*

**Proof.** In  $G$ , each maximal clique is a block, and a vertex belongs to  $G'$  if and only if it is a cut-vertex of  $G$ . Also, if a cut vertex of  $G$  is a simplicial vertex of  $G'$ , then it belongs to a leaf block of  $G$ . We form an asteroidal set by selecting, for each simplicial vertex  $v$  of  $G'$ , one simplicial vertex from one leaf block of  $G$  containing  $v$ . This set has size  $r'(G)$ . When  $r'(G) = 1$ ,  $G$  consists of two cliques sharing one vertex and is an interval graph.

For the upper bound, we build by induction on  $r'(G)$  a subtree representation such that the cliques that are leaf blocks containing a particular simplicial vertex of  $G'$  appear on a pendant path of the host tree. If  $r'(G) \leq 2$ , then  $G'$  is a path  $v_1, \dots, v_p$ . To form the subtree representation, first form a path  $u_0, \dots, u_{2p+2}$  with  $f(v_i) = \{u_{2i-2}, u_{2i-1}, u_{2i}, u_{2i+1}\}$ . This assigns an edge to each complete subgraph of  $G'$ . Now subdivide edges as needed to insert a vertex for each component of  $S(G)$  in the path assigned to its neighborhood in  $G'$ .

When  $r'(G) > 2$ , we choose a simplicial vertex  $v$  of  $G'$ . Letting  $U$  be the set of neighbors of  $v$  in leaf blocks of  $G$ , we have  $r'(G - U) < r'(G)$ . The induction hypothesis provides a representation for  $G - U$ ; to any vertex of the host assigned to clique containing  $v$ , we append a path having one vertex for each leaf block of  $G$  containing  $v$ . These cliques appear at those vertices, and the entire path is added to the subtree representing  $v$ . ■

Consider the chordal graph  $G$  in Figure 1 formed by adding one simplicial vertex adjacent to each edge of  $G' = 2K_2 \vee K_1$ . Here  $a(G) = 3$  but  $l(G) = 4$ , as we will see.

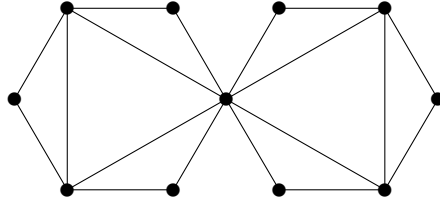


Figure 1. A graph with leafage 4 but no asteroidal 4-set



## 3. DOMINATORS AND A GENERAL UPPER BOUND

As observed in the introduction, when studying  $l(G)$  we may assume a bijection between the maximal cliques of  $G$  and the vertices of the host. There is a natural order on the maximal cliques. If  $v_n, \dots, v_1$  is a perfect elimination ordering of  $G$ , then the reverse ordering  $v_1, \dots, v_n$  constructs  $G$  by iteratively adding a vertex adjacent to a clique. With respect to (the reverse of) a given perfect elimination ordering, we say that a maximal clique is created whenever the vertex being added increases the number of maximal cliques in the graph that has been built. Each additional vertex enlarges one maximal clique or creates one new maximal clique. This defines a *creation ordering*  $Q_1, \dots, Q_m$  of the maximal cliques of  $G$  (with respect to a given perfect elimination ordering).

**Lemma 4.** *Let  $Q_1, \dots, Q_m$  be the creation ordering of the maximal cliques of a connected chordal graph  $G$  with respect to some perfect elimination ordering. For each  $i$  with  $2 \leq i \leq m$ , there is an index  $j < i$  such that  $Q_i \cap Q_k \subseteq Q_i \cap Q_j$  for all  $k < i$ . We call  $Q_j$  the dominator of  $Q_i$  and write  $j = \rho(i)$ .*

**Proof.** By induction on  $n$ , the order of  $G$ ; the claim is vacuous for  $n = 1$ . For  $n > 1$ , apply the induction hypothesis to  $G - v_n$ , where  $v_n$  is the first vertex of the perfect elimination ordering. When  $v_n$  is added, it belongs to only one maximal clique.

Either  $v_n$  enlarges a previous maximal clique, or it creates a new maximal clique. If  $v_n$  enlarges a maximal clique  $Q_i$ , then the intersection condition holds with the same choice of dominators as for  $G - v_n$ , because  $v_n$  belongs to no other maximal clique. If  $v_n$  creates a new maximal clique  $Q_m$ , then  $N(v_n)$  is a proper subset of some earlier clique  $Q_j$ ; set  $j = \rho(m)$  (this choice need not be unique). Since  $N(v_n)$  contains the intersection of  $Q_m$  with each other clique, the dominator condition holds. ■

**Lemma 5.** *Let  $Q_1, \dots, Q_m$  be the creation ordering of the maximal cliques of  $G$  associated with some perfect elimination ordering. Let  $T$  be the tree with vertices  $q_1, \dots, q_m$  and edges  $q_i q_j$  such that  $j = \rho(i)$ . Assigning  $q_i$  to all vertices of  $Q_i$  yields a subtree representation of  $G$  in  $T$ . Furthermore, each clique of  $G$  corresponding to a leaf of  $T$  contains a vertex appearing in no other maximal clique of  $G$ .*

**Proof.** By induction on  $n$ , the order of  $G$ ; the claim is trivial for  $n = 1$ . For  $n > 1$ , apply the induction hypothesis to  $G - v_n$ , where  $v_n$  is the first vertex

in the perfect elimination ordering. If adding  $v_n$  enlarges a maximal clique  $Q_i$ , then it suffices to enlarge the representation  $f$  by setting  $f(v_n) = q_i$ . If adding  $v_n$  creates a new maximal clique  $Q_m$  with dominator  $Q_j$ , then  $T$  gains the pendant edge  $q_m q_j$  and is still a tree. Leaves still contain unique representatives, since we let  $f(v_n) = q_m$ . Finally, since  $Q_j$  contains  $N(v_n)$ , the subtrees assigned to the vertices of  $N(v_n)$  can be extended from  $q_j$  to include  $q_m$ . Hence we obtain the desired subtree representation of  $G$ . ■

To obtain an upper bound on  $l(G)$ , we consider a partial order associated with  $G$ . An *antichain* in a partial order is a set of pairwise incomparable elements, and the *width*  $w(P)$  of a partial order  $P$  is the maximum size of its antichains. Dilworth's Theorem [4] states that the elements of a finite partial order of width  $k$  can be partitioned into  $k$  chains (totally ordered subsets). Such a set of chains is a *Dilworth decomposition*.

For each simplicial neighborhood  $R$  in a chordal graph  $G$ , we define the *modified simplicial neighborhood* to be  $R' = R - S(G)$ . Let  $\mathbf{R}'(G)$  denote the set of modified simplicial neighborhoods in  $G$ . For  $v \in S(G)$ , we also define  $N'(v) = N(v) - S(G)$ .

**Theorem 4.** *If  $P(G)$  is the inclusion order on the collection  $\mathbf{R}'(G)$  of modified simplicial neighborhoods in a chordal graph  $G$ , then  $l(G) \leq w(P(G))$ .*

**Proof.** Let  $C_1, \dots, C_k$  be a Dilworth decomposition of  $P(G)$ , with  $C_j$  consisting of  $R_{j1} \subseteq \dots \subseteq R_{jr_j}$ . For each chain  $C_j$  we create a path  $P_j$  to be part of the host tree in a subtree representation  $f$ . If  $u, v \in S(G)$  are adjacent, then  $N'(u) = N'(v)$ . For  $R \in \mathbf{R}'(G)$ , let  $m(R)$  be the number of components of  $S(G)$  for which  $R$  is the common modified simplicial neighborhood. We assign to  $R_{ji}$  exactly  $m(R_{ji})$  consecutive vertices on  $P_j$ , each of which will be the entire image for the vertices of one component of  $S(G)$ . We put the vertices for  $R_{j1}$  at one end of the path (the *small* end, pass through those for each  $R_{ji}$  as  $i$  increases, and reach the vertices for  $R_{jr_j}$  at the *big* end of the path. Each vertex of the subpath for  $R_{ji}$  is assigned to each vertex in  $R_{ji}$ . For each  $v' \in V(G')$ , we have assigned to  $v'$  a (possibly empty) subpath from the big end of each  $P_j$ .

The problem is now to add host vertices to hook together the big ends of these paths so that 1) the only leaves are the small ends of  $P_1, \dots, P_k$ , 2) the maximal cliques not containing simplicial vertices of  $G$  are represented, and 3) the vertices assigned to each vertex of  $G'$  form a subtree of the resulting tree.

The maximal cliques of  $G$  that do not contain simplicial vertices of  $G$  are maximal cliques of  $G'$ . Let  $f'$  be the subtree representation of  $G'$  generated

by Lemma 5 in a host tree  $T'$ . In  $T' \cup \{P_1, \dots, P_k\}$  all maximal cliques of  $G$  are represented. Each “big end”  $R_{jr_j}$  is contained in (possibly with equality) a maximal clique  $Q$  of  $G'$ ; add an edge from the big end of  $P_j$  to the vertex for  $Q$  in  $T'$ . (If  $R_{jr_j} = Q$ , then this edge can be contracted.) The result is a tree  $T$ . Each  $v' \in V(G')$  was assigned a subtree in  $T'$ ; if  $v'$  received additional vertices in  $P_j$ , then these have been attached to a vertex of  $f'(v')$ , so the image  $f(v')$  is still a tree.

Finally, we show that each leaf of  $T'$  receives an edge from some path  $P_j$ ; thus all leaves in the full tree  $T$  are small ends of  $P_1, \dots, P_k$ . Let  $q$  be a leaf of  $T'$ . By Lemma 5, the clique of  $G'$  corresponding to  $q$  contains a vertex in no other maximal clique of  $G'$ . Such a vertex  $v'$  is simplicial in  $G'$ . Since  $G'$  contains no simplicial vertices of  $G$ ,  $v'$  has a neighbor  $v \in S(G)$ . Let  $C_j$  be the chain in  $P(G)$  containing  $N(v)$ . The big end of  $P_j$  must be attached to  $q$ , because  $R_{jr_j}$  contains  $v'$  and  $q$  is the only vertex of  $T'$  assigned to  $v'$ . ■

#### 4. CHARACTERIZATION OF MAXIMUM ASTEROIDAL SETS

The sharpness of the upper bound in Theorem 4 depends on the structure of  $G'$ . When  $G'$  is a single clique, it has no cutset, and Lemma 6 below implies that  $a(G) = l(G) = w(P(G))$ . Among such graphs we find the  $n$ -vertex chordal graph with maximum leafage. Lemma 6 is a lower bound on  $a(G)$  in terms of a subposet of  $P(G)$ . Given a chordal graph  $G$ , the *restricted simplicial neighborhood poset*  $P'(G)$  is obtained from  $P(G)$  by deleting those modified simplicial neighborhoods that contain cutsets of the derived graph  $G'$ .

**Lemma 6.** *If  $P'(G)$  is the restricted simplicial neighborhood poset of a chordal graph  $G$ , then  $G$  has an asteroidal set consisting of  $w(P'(G))$  simplicial vertices.*

**Proof.** Let  $R_1, \dots, R_r$  be a maximum antichain in  $P'(G)$ . For each  $R_i$ , choose  $v_i \in S(G)$  with  $N'(v_i) = R_i$ . Given distinct vertices  $v_i, v_j, v_k$  in the resulting set, we may choose  $v'_j \in R_j - R_i$  and  $v'_k \in R_k - R_i$  because  $R_1, \dots, R_r$  is an antichain. By the definition of  $P'(G)$ ,  $G' - R_i$  is connected and contains a  $v'_j, v'_k$ -path  $P$ . Appending  $v_j$  and  $v_k$  yields a  $v_j, v_k$ -path avoiding  $N(v_i)$ . ■

**Theorem 5.** *The maximum leafage of a chordal graph with  $n$  vertices is the maximum  $k$  such that  $k \leq \binom{n-k}{\lfloor (n-k)/2 \rfloor}$ . In terms of  $n$ , the value is  $n - \lg n - \frac{1}{2} \lg \lg n + O(1)$ .*

**Proof.** When  $k$  satisfies the inequality, we construct a chordal  $n$ -vertex graph with an asteroidal set of size  $k$ . To a clique  $Q$  of order  $n - k$ , we add  $k$  simplicial vertices whose neighborhoods are distinct  $\lfloor (n - k)/2 \rfloor$ -subsets of  $G' = Q$ . By Lemma 6,  $S(G)$  is an asteroidal set of size  $k$ , and hence  $l(G) \geq k$  by Lemma 1.

Let  $G$  be an  $n$ -vertex chordal graph with maximum leafage. Theorem 4 implies that  $l(G) \leq w(P(G))$ . Let  $m = |S(G)|$ . Since the elements of  $P(G)$  are distinct modified simplicial neighborhoods,  $w(P(G)) \leq m$ . Since elements  $P(G)$  are subsets of an  $n - m$ -element set,  $w(P(G)) \leq \binom{n-m}{\lfloor (n-m)/2 \rfloor}$ . Thus  $w(P(G)) \leq \min\{m, \binom{n-m}{\lfloor (n-m)/2 \rfloor}\}$ . Since the second term decreases with  $m$ , the width cannot exceed the maximum  $k$  such that  $k \leq \binom{n-k}{\lfloor (n-k)/2 \rfloor}$ . This proves the upper bound. To obtain the asymptotic maximum, we apply Stirling's approximation to  $k = \binom{n-k}{\lfloor (n-k)/2 \rfloor}$ . ■

We can improve the lower bound resulting from Lemma 6 by applying Lemma 6 to every connected induced subgraph of  $G$ .

**Theorem 6.** *If  $G$  is a chordal graph, then the maximum size of an asteroidal set in  $G$  is the maximum of  $w(P'(H))$  over all connected induced subgraphs  $H$  of  $G$ .*

**Proof.** Every induced subgraph  $H$  of a chordal graph  $G$  is chordal. If  $H$  has an  $x, y$ -path  $P$  avoiding  $N(z)$  for some  $x, y, z \in V(H)$ , then  $P$  is also an  $x, y$ -path avoiding  $N(z)$  in  $G$ , since  $G$  has no additional edges among vertices of  $H$ . Thus every asteroidal set in  $H$  is an asteroidal set in  $G$ , and the lower bound follows from Lemma 6.

For the upper bound we construct, from a maximum asteroidal set  $A$  in  $G$ , a connected induced subgraph  $H$  of  $G$  such that  $|A| = w(P'(H))$ . For each triple  $x, y, z \in A$ , there is an  $x, y$ -path in  $G$  avoiding  $N(z)$ . We may assume that each such path is chordless, since shortening the path by using chords still avoids  $N(z)$ . Let  $H$  be the subgraph of  $G$  induced by the vertices in the union of all these chordless paths. It suffices to show that (1)  $S(H) = A$ , (2)  $P(H)$  is an antichain of size  $|A|$ , and (3)  $P'(H) = P(H)$ .

Since  $H$  is an induced subgraph of  $G$ ,  $N_H(x) \subseteq N_G(x)$ , so the vertices of  $A$  are simplicial in  $H$ . All members of  $V(H) - A$  are internal vertices of chordless paths between vertices of  $A$ . Such a vertex cannot be simplicial in

$H$ , because its neighbors on such a path are not adjacent; this proves (1). If  $N_H(x) \subseteq N_H(y)$  for some  $x, y \in A$ , then every  $x, z$ -path intersects  $N(y)$ ; since  $A$  is asteroidal, this proves (2).

It remains only to show that  $P'(H) = P(H)$ . First note that  $N'_H(x) = N_H(x)$  for  $x \in S(H)$  since  $S(H) = A$  is an independent set. Thus it suffices to show that  $N_H(x)$  does not contain a cutset of  $H'$  for  $x \in A$ . Suppose that  $Q$  is a minimal cutset of  $H'$  contained in  $N_H(x)$ . Since  $Q$  is a minimal cutset of a chordal graph  $H'$ ,  $Q$  induces a clique, and every component of  $H' - Q$  contains a simplicial vertex of  $H'$ . Each such vertex is a neighbor of a simplicial vertex of  $H$ . This yields vertices  $y, z \in A$  such that every  $y, z$ -path in  $H$  intersects  $Q$ , which contradicts  $A$  being an asteroidal set. ■

For the graph  $G$  in Figure 2, the four simplicial vertices of degree 2 establish  $a(G) \geq 4$ . Equality holds; these vertices and their neighborhoods together induce the only connected induced subgraph  $H$  such that  $w(P'(H)) = 4$ . Although  $w(P'(H))$  is computable from  $H$  in polynomial time, the difficulty of finding  $H$  makes the complexity of computing  $a(G)$  unclear. For example, if  $F$  is formed by adding a pendant edge to each leaf of the graph in Figure 2, then  $w(P'(F)) = 2$  and  $a(F) = 4$ , but  $F$  has no simplicial vertex  $x$  such that  $w(P'(F - x)) > 2$ . Thus  $H$  cannot be found greedily.

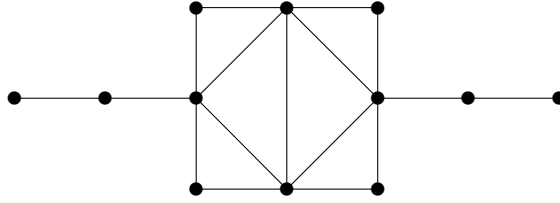


Figure 2. A graph with  $a(G) > w(P'(G))$

In the computation of  $a(G)$ , it may be useful to confine the maximum asteroidal set to the set  $S(G)$  of simplicial vertices.

**Lemma 7.** *If  $G$  is a chordal graph, then  $S(G)$  contains a maximum asteroidal set of  $G$ .*

**Proof.** Let  $A$  be a maximum asteroidal set of  $G$ . If  $x \in A$  is not simplicial in  $G$ , then  $x$  has nonadjacent neighbors. Hence  $x$  belongs to a minimal cutset of  $G$ . Since  $G$  is chordal, this cutset induces a clique  $Q$ . As in the proof of Theorem 6,  $A - x$  is confined to one component of  $G - Q$ . Any

other component of  $G - Q$  contains a simplicial vertex of  $G$  that is not in  $Q$ . Choose such a vertex  $w$  to replace  $x$  in  $A$ . To verify that  $A - x + w$  is an asteroidal set, it suffices to note that if  $y, z \in A$  and  $P$  is a  $y, x$ -path avoiding  $N(z)$ , then  $P$  can be extended from  $x$  to  $w$  to obtain a  $y, w$ -path avoiding  $N(z)$ . ■

## 5. LEAFAGE WHEN $G'$ HAS (AT MOST) TWO CLIQUES

We have observed that  $l(G) = a(G) = w(P(G))$  when  $G'$  is a clique. Computing leafage in general means determining the savings  $w(P(G)) - l(G)$  in constructing an optimal subtree representation. By studying antichains in more detail, we will be able to compute leafage when  $G'$  is the union of two maximal cliques.

An *ideal* of a poset  $P$  is a subposet  $Q$  such that all elements below elements of  $Q$  also belong to  $Q$ . The inclusion order on the set of ideals of  $P$  is a lattice, because the union and intersection of two ideals is an ideal. Every antichain in  $P$  is associated naturally with the ideal for which it forms the set of maximal elements. The ordering of the antichains that corresponds to the inclusion ordering on the ideals has  $A \leq B$  when for every  $x \in A$  there exists  $y \in B$  such that  $x \leq y$ .

Dilworth [5] proved that the set of maximum-sized antichains also forms a lattice under this ordering. When  $P$  is finite, the lattice of maximum-sized antichains is finite and has a unique minimal element, which we denote by  $A_P$ . In an arbitrary poset, a maximum antichain can be found quickly using network flow methods or bipartite matching. It is well-known that in the bipartite graph  $\Gamma(P)$  with partite sets  $\{x^- : x \in P\}$  and  $\{x^+ : x \in P\}$  and edge set  $\{x^-y^+ : x < y \text{ in } P\}$ , the maximum size of a matching is  $|P| - w(P)$ . Using this, we can find  $A_P$ .

**Lemma 8.** *In a finite poset  $P$ , the unique minimal maximum antichain  $A_P$  can be found in polynomial time.*

**Proof.** Using a bipartite matching algorithm, we find a maximum matching of  $\Gamma(P)$ . These edges link the elements of  $P$  into chains that form a Dilworth decomposition  $C_1, \dots, C_{w(P)}$  of  $P$ . Every maximum antichain uses one element from each  $C_i$ . If the minimal elements of the chains form an antichain, then this is  $A_P$ . Otherwise, there is some relation  $x > y$  among these elements. Since  $y$  is below every element of the chain containing  $x$ , no maximum antichain contains  $y$ . Since  $y$  belongs to no maximum antichain in  $P$ , we have  $w(P - y) = w(P)$ , and thus the same chain partition

with  $y$  deleted forms a Dilworth decomposition of  $P - y$ . Iterating this procedure with the minimal remaining elements eventually produces an antichain of size  $w(P)$ . Since no maximum antichains of  $P$  were destroyed, this set is  $A_P$ . ■

**Lemma 9.** *Let  $\mathbf{C}$  be a Dilworth decomposition of  $P$ . If  $x \in A_P$  and  $C'$  is the chain consisting of  $x$  and the elements above  $x$  on its chain in  $\mathbf{C}$ , then  $w(P - C') = w(P) - 1$ . Equivalently,  $P$  has a Dilworth decomposition using  $C'$  as one chain.*

**Proof.** Let  $k = w(P)$ . Since  $A_P - x$  is an antichain in  $P - C'$ , it suffices to show that  $P - C'$  has no antichain of size  $k$ . Let  $C$  be the chain containing  $x$  in  $\mathbf{C}$ . If  $P - C'$  has an antichain  $A$  of size  $k$ , then  $A$  must contain an element  $y$  below  $x$  on  $C$ , since  $w(P - C) < k$ . Also  $A$  is an antichain of size  $k$  in  $P$ , and hence  $A_P < A$ . In particular,  $x$  is less than some member of  $A$ , which creates a forbidden relation between  $y$  and another member of  $A$ . ■

**Lemma 10.** *Let  $Q_1, Q_2$  be distinct maximal cliques of the derived graph  $G'$  of a chordal graph  $G$ . Let  $P = P(G)$ , and define induced subposets  $P_1 = \{x \in P : Q_1 \cap Q_2 \subset x \subseteq Q_1\}$ ,  $P_2 = \{x \in P : Q_1 \cap Q_2 \subset x \subseteq Q_2\}$ , and  $\bar{P} = P_1 \cup P_2$ . Suppose that  $A_P$  has elements  $a_1 \in P_1$  and  $a_2 \in P_2$ . If  $w(P) \geq w(P - \bar{P}) + 2$ , then  $P(G)$  has a Dilworth decomposition in which  $a_1, a_2$  occur as minimal elements of chains.*

**Proof.** With these hypotheses, Lemma 9 implies that  $P$  has a Dilworth decomposition containing a chain  $C_1$  with  $a_1$  as its minimal element. Let  $P^* = P - C_1$ , and let  $A^* = A_P - \{a_1\}$ . Since  $A^*$  is a maximum antichain of  $P^*$ , we have  $A_{P^*} \leq A^*$  in the lattice of maximum antichains of  $P^*$ .

Let  $\Gamma$  be the bipartite graph with partite sets  $A_{P^*}$  and  $A^*$  (each of size  $w(P) - 1$ ) defined by putting  $x \in A_{P^*}$  adjacent to  $y \in A^*$  if  $x \leq y$  in  $P$ . If  $\Gamma$  has a vertex cover with fewer than  $w(P^*)$  vertices, then the vertices not in the cover form an independent set, and this independent set forms an antichain of size exceeding  $w(P^*)$  in  $P^*$ . Hence there is no such cover, and by the König-Egerváry Theorem  $\Gamma$  has a complete matching  $M$ .

Let  $B = A_P \cap P_2$ ; note that  $B \subseteq A^*$ . For  $b \in B$ , let  $b'$  be the element matched to  $b$  in  $M$ , and let  $B' = \{b' : b \in B\}$ . We claim that  $B' \subseteq P_2$ . For  $b \in B$ , we have  $b' \leq b$  in  $P$ , so  $b' \subseteq b \in B \subseteq P_2$ . Thus  $b' \subseteq Q_2$ . If  $b' \subseteq Q_1 \cap Q_2$ , then  $b'$  is properly contained in every element of  $\bar{P}$ . Since  $b' \in A_{P^*}$ , this implies that  $A_{P^*}$  is disjoint from  $\bar{P}$ , and we have  $w(P - \bar{P}) \geq |A^*| = w(P) - 1$ . We assumed that  $w(P) \geq w(P - \bar{P}) + 2$ , so  $b'$  must intersect  $Q_2 - Q_1$ . This implies that  $b' \in P_2$ .

With  $B' \subseteq P_2$ , we next claim that  $B' = B$ . A set not in  $P_2$  that contains an element of  $P_2$  contains  $Q_2$ . Since  $a_2 \in A_P \cap P_2$ , no such element is in the antichain  $A_P$ . Thus  $b'$  is not below any element of  $A_P - B$ . Also  $b'$  is not above any element of  $A_P - B$ , because  $b' \subseteq b$  and  $A_P$  is an antichain. Hence  $A' = (A_P - B) \cup B'$  is an antichain in  $P$ , with size  $w(P)$  since  $|B| = |B'|$ . Since  $B' \leq B$ , we have  $A' \leq A_P$  in the lattice. Since  $A_P$  is the minimal element of the lattice, this yields  $A' = A_P$  and  $B' = B$ .

Since  $B' = B$ , we have proved that all the elements of  $A_P$  belonging to  $P_2$  also belong to  $A_{P^*}$ . In particular,  $a_2 \in A_{P^*}$ . Applying Lemma 9 again, we obtain a Dilworth decomposition of  $P^*$  containing a chain  $C_2$  with  $a_2$  as its minimal element. Together with  $C_1$ , this is the desired Dilworth decomposition of  $P$ .  $\blacksquare$

Recall that  $P'(G)$  is the subposet of  $P(G)$  obtained by discarding the modified simplicial neighborhoods that contain cutsets of  $G'$ . When the modified simplicial neighborhoods contained in a particular maximal clique  $Q_i$  of  $G'$  form a chain under inclusion, we say that  $Q_i$  is *degenerate*.

**Theorem 7.** *Let  $G$  be a chordal graph such that  $G'$  is the union of two maximal cliques  $Q_1, Q_2$ . With  $P = P(G)$ ,  $P' = P'(G)$ , and  $Q = Q_1 \cap Q_2$ ,  $l(G)$  has the following value:*

- 1)  $l(G) = w(P) - \alpha$  if  $w(P') \leq w(P) - 2$  and  $\alpha$  of the cliques  $Q_1, Q_2$  are nondegenerate and contain distinct elements of  $A_P - P'$ .
- 2)  $l(G) = w(P)$  if  $w(P') = w(P) - 1$  and every element of  $A_P - P'$  belongs to a degenerate  $Q_i$ .
- 3)  $l(G) = w(P')$  otherwise.

**Proof.** Lemma 6 and Theorem 4 imply that  $w(P') \leq l(G) \leq w(P)$ , so we may assume that  $w(P') < w(P)$ . The only minimal cutset of  $G'$  is  $Q$ , so the elements of  $P$  discarded to form  $P'$  are those containing  $Q$ . Also, every element of  $P$  is contained in  $Q_1$  or in  $Q_2$ .

We first consider improvements to the upper bound. If  $w(P') \leq w(P) - 1$ , then  $A_P$  has an element  $x$  outside  $P'$ , which means  $Q \subseteq x$ . We may assume that  $x \subseteq Q_1$ ; we can improve the upper bound if  $Q_1$  is nondegenerate. By Lemma 9, we can find a Dilworth decomposition of  $P$  such that one chain has  $x$  as its bottom element. Each chain consists of subsets of  $Q_1$  or consists of subsets of  $Q_2$ . Using the construction in the proof of Theorem 4, we produce two host subtrees, with a total of  $w(P)$  leaves together (if  $Q_2$  is also nondegenerate), one of which has vertices for simplicial neighborhoods contained in  $Q_1$ , the other for  $Q_2$ . Furthermore,



$x$  appears at a leaf in the tree for  $Q_1$ . Since  $x$  contains  $Q$ , we can add an edge between the vertex for  $x$  and the vertex representing  $Q_2$  in the other tree. This yields a subtree representation of  $G$  with  $w(P) - 1$  leaves. (If  $Q_2$  is degenerate, then the initial pair of subtrees has a total of  $w(P) + 1$  leaves, but the tree for subsets of  $Q_2$  is a path with the vertex for  $Q_2$  as a leaf, and the added edge eliminates two leaves.)

If  $w(P') \leq w(P) - 2$  and  $Q_1, Q_2$  contain distinct elements of  $A_P - P'$ , then we may be able to save another leaf. The hypotheses of Lemma 10 hold (with  $P' = P - \bar{P}$ ), and Lemma 10 guarantees a Dilworth decomposition of  $P$  having chains with bottom elements  $x, y$  such that  $x, y \in P'$ ,  $Q \subseteq x \subseteq Q_1$ , and  $Q \subseteq y \subseteq Q_2$ . As above, we use the construction in the proof of Theorem 4 to produce representations in two host subtrees, one having  $x$  at a leaf and the other having  $y$  at a leaf. The two subtrees have a total of  $w(P) + 2 - \alpha$  leaves (each of  $Q_1, Q_2$  that is degenerate increases the number of leaves in the initial pair of trees by one). By adding the edge  $xy$ , we produce a subtree representation of  $G$  with  $w(P) - \alpha$  leaves.

We next prove that  $w(P) - \alpha$  is a lower bound when  $w(P') \leq w(P) - 2$ . The latter inequality implies that no element of  $A_P$  is contained in  $Q$ . Hence  $m_1 + m_2 = w(P)$ , where  $A_P$  consists of  $m_1$  subsets of  $Q_1$  and  $m_2$  subsets of  $Q_2$ . Suppose first that  $m_1, m_2 > 0$ . By the argument in Lemma 6, the simplicial vertices of  $G$  corresponding to the elements of  $A_P$  contained in  $Q_i$  yield an asteroidal set  $U_i$  of size  $m_i$ . Consider an optimal representation of  $G$ . Since the host has a vertex for each maximal clique of  $G$  and simplicial vertices of  $G$  appear in exactly one maximal clique, each vertex of  $U_i$  is assigned one host vertex. Let  $T_i$  be the subtree of the host consisting of all paths between vertices representing  $U_i$ . Since  $U_i$  is an asteroidal set, Theorem 1 implies that the corresponding subtrees form an asteroidal collection. Since these trees are single vertices, the leaves of  $T_i$  are precisely the  $m_i$  vertices assigned to elements of  $U_i$ .

If the vertex assigned to  $u \in U_i$  lies between the vertices assigned to  $v, w \in U_{3-i}$ , then every  $v, w$ -path in  $G$  contains a neighbor of  $u$ . On the other hand, the vertices  $v, w$  have neighbors  $v', w' \in Q_{3-i} - Q_i$ , and the path  $v, v', w', w$  avoids  $N(u)$ . This contradiction implies that the trees  $T_1, T_2$  are disjoint. We now have a total of  $w(P)$  leaves in two disjoint subtrees, except that this total increases by one for each  $Q_i$  that is degenerate or contains no element of  $A_P - P'$ . The host contains a unique path between these subtrees, which reduces the number of leaves by at most two. Hence the host has a subtree with  $w(P) - \alpha$  leaves, and  $l(G) \geq w(P) - \alpha$ .

When  $w(P') = w(P) - 1$  and every element of  $A_P - P'$  belongs to a

degenerate  $Q_i$ , a similar argument shows that  $l(G) = w(P) - 1$ . ■

Perhaps these ideas can be combined with the “dominator tree” to obtain a polynomial-time algorithm in general. The condition that  $G'$  has at most two cliques is recognizable, since the algorithm of Rose, Tarjan, and Leuker [21] finds a perfect elimination ordering (if one exists) in time linear in the number of vertices plus edges, and from this the maximal cliques and simplicial vertices are available. An algorithm for recognizing chordal graphs with leafage at most 3 can be obtained from the material in [18].

## 6. PROPER LEAFAGE AND EXTREME POINTS

We now consider proper leafage. The graphs with proper leafage 2 are the proper interval graphs, which Roberts [19] proved are precisely the unit interval graphs. Less well-known is a structural characterization proved by Roberts; we generalize this to obtain bounds on proper leafage.

The *closed neighborhood* of a vertex  $a$  is the set  $N[a] = N(a) \cup \{a\}$ . Vertices with the same closed neighborhood are *equivalent* in  $G$ ; this defines an equivalence relation on  $V(G)$ . Each equivalence class induces a clique, and vertices  $x, y$  from distinct classes are adjacent if and only if every vertex equivalent to  $x$  is adjacent to every vertex equivalent to  $y$ . The *reduction*  $G^*$  of a graph  $G$  is the subgraph induced by selecting one vertex from each equivalence class. A graph is *reduced* if it has no pair of distinct equivalent vertices.

A vertex  $a \in V(G)$  is an *extreme point* (EP) in  $G$  if (1)  $a$  is simplicial and (2) every pair of vertices in  $N(a)$  that are not equivalent to  $a$  have a common neighbor outside  $N[a]$ . The simplicial vertices in  $K_4 - e$  are extreme points, but  $K_4 - e$  is not reduced since the three-valent vertices have the same closed neighborhood. Roberts used extreme points and reduced subgraphs to characterize proper interval graphs.

**Theorem 8** (Roberts [19]). *A graph  $G$  is a proper interval graph if and only if every connected reduced induced subgraph of  $G$  has at most two extreme points.* ■

Roberts also proved that this statement holds when “extreme points” is replaced by “modified extreme points”. If  $H$  is a component of  $G - N[a]$ , let  $\partial H = \{x \in N[a] : x \text{ has a neighbor in } H\}$ . We say that a simplicial vertex  $a$  is a *modified extreme point* (MEP) if  $\partial H_1 = \partial H_2$  for every pair of components  $H_1, H_2$  of  $G - N[a]$ .

**Lemma 11.** *If  $a$  is an MEP in a connected chordal graph  $G$  that is not a clique, and  $S$  is the set vertices of  $N[a]$  not equivalent to  $a$ , then  $S$  is a minimal cutset of  $G$ .*

**Proof.** Every vertex of  $S$  has a neighbor in some component of  $G - N[a]$ . If  $a$  is an MEP, then the vertices of  $S$  with neighbors in each component of  $G - N[a]$  are the same. Hence deleting any proper subset of  $S$  does not separate  $G$ . ■

As observed by Gavril [8], every chordal graph has a subtree representation by a proper family of subtrees in a host tree, meaning that no subtree properly contains another. Roberts' characterization works because modified extreme points force leaves in a proper subtree representation much as asteroidal sets force leaves in a subtree representation. This does not hold for extreme points. Roberts observed that the concepts of EP and MEP are equivalent on claw-free connected chordal graphs. The following structural lemma implies that MEP's in chordal graphs are EP's, but we will see that the converse need not hold.

**Lemma 12.** *If  $G$  is a chordal graph, and  $S$  is a minimal cutset of  $G$ , then every component of  $G - S$  contains a vertex adjacent to every vertex of  $S$ .*

**Proof.** Let  $H$  be a component of  $G - S$ , and let  $x$  be a vertex of  $H$  having the maximum number of neighbors in  $S$ . If there exists  $v \in S - N(x)$ , then  $v$  must have a neighbor in  $V(H)$ , since  $S$  is a minimal cutset of  $G$ . Choose  $y \in N(v) \cap V(H)$  with minimal distance from  $x$  in  $H$ , and let  $P$  be a shortest  $x, y$ -path in  $H$ . Since  $G$  is chordal,  $S$  induces a clique, and hence every vertex of  $S \cap N(x)$  completes a cycle with  $P$  and  $v$ . This leads to a chordless cycle unless  $S \cap N(x) \subset N(y)$ , which contradicts the choice of  $x$ . ■

**Corollary 2.** *If  $G$  is a connected chordal graph other than a clique, then every MEP in  $G$  is an EP in  $G$ .*

**Proof.** Suppose  $a$  is an MEP of a  $G$ ; note that both MEP's and EP's must be simplicial. By Lemma 11, the set  $S$  of vertices of  $N[a]$  not equivalent to  $a$  is a minimal cutset. By Lemma 12, every component of  $G - S$  has a vertex adjacent to all of  $S$ . Hence any two vertices of  $S$  have a common neighbor outside  $S$ , and  $a$  is an EP. ■

We next explore the role of MEP's in proper subtree representations.

**Lemma 13.** *Let  $G$  be a non-clique chordal graph with a proper subtree representation  $f$  in a host tree  $T$ . If  $v$  is an MEP of  $G$  and  $f(v)$  does not contain a leaf of  $T$ , then  $T - f(v)$  has a component disjoint from all subtrees representing vertices outside  $N[v]$ .*

**Proof.** Let  $H$  be a component of  $G - N[v]$ . The subtrees for  $V(H)$  are confined to a single component of  $T - f(v)$ , since their union is connected and shares no vertex with  $f(v)$ . If  $w$  is a neighbor of  $v$  not equivalent to  $v$ , then  $w$  has a neighbor in  $H$ , by Lemma 12. Hence  $f(w)$  contains the edge between  $f(v)$  and the component of  $T - f(v)$  containing the subtrees for  $V(H)$ . If each component of  $T - f(v)$  contains a subtree for some vertex outside  $N[v]$ , then  $f(w)$  properly contains  $f(v)$ . ■

**Theorem 9.** *If  $G$  is a connected non-clique chordal, and  $H$  is a connected reduced induced subgraph of  $G$ , then  $l^*(G)$  is at least the number of MEP's in  $H$ .*

**Proof.** A proper subtree representation of  $G$  must contain a proper subtree representation of  $H$ . It suffices to show that every proper subtree representation  $f$  of  $H$  has a distinct leaf for each MEP of  $H$ . Let  $v$  be an MEP of  $H$ . If  $f(v)$  contains a leaf of  $T$ , associate this leaf with  $v$ . For example, if  $T - f(v)$  is connected, then there is only one edge from  $f(v)$  to the rest of  $T$ , and  $f(v)$  contains a leaf of  $T$ . If  $T - f(v)$  has more than one component and  $f(v)$  contains no leaf, then Lemma 13 yields a component  $T(v)$  of  $T - f(v)$  that is disjoint from the trees associated with the vertices of  $G - N[v]$ . In this case, assign a leaf of  $T(v)$  to  $v$ .

It suffices to show that the leaves associated with distinct MEP's are distinct. In a reduced graph, the simplicial vertices form an independent set. Hence MEP's  $u, v$  are non-adjacent, which implies that  $f(u), f(v)$  are disjoint. Furthermore,  $f(u)$  also cannot intersect a component  $T(v)$  of  $T - f(v)$  whose vertices belong to subtrees in  $f$  only for neighbors of  $v$ . These two statements imply that no leaf of  $T$  belonging to  $f(u)$  is associated with  $v$ . Finally, suppose that neither  $f(u)$  nor  $f(v)$  contains a leaf of  $T$ . In addition to  $f(u) \cap f(v) = \emptyset$ , we have observed that  $f(u) \cap T(v) = \emptyset$  and  $f(v) \cap T(u) = \emptyset$ . Since the subtrees  $T(u)$  and  $T(v)$  are obtained from  $T$  by deleting an edge incident to  $f(u)$  and to  $f(v)$ , respectively, we conclude that they cannot have a common leaf. ■

**Lemma 14.** *Every connected reduced chordal graph  $G$  has an optimal proper subtree representation in which each MEP is assigned a leaf of the host tree that is assigned to no other vertex.*

**Proof.** Let  $v$  be an MEP in  $G$ . If  $f(v)$  contains a leaf, we may extend  $f(v)$  by adding a new neighbor of the leaf and the leaf has the desired property. If  $f(v)$  does not contain a leaf, then there is a component  $T(v)$  of  $T - f(v)$  whose vertices are assigned only to neighbors of  $v$ . Since  $G$  is reduced, each neighbor of  $v$  has neighbors outside  $N[v]$ ; hence its subtree extends to another component of  $T - f(v)$ . We may therefore extend  $f(v)$  to a leaf of  $T(v)$  and to one added vertex beyond it while maintaining a proper subtree representation. ■

To obtain the best lower bound from Lemma 14, we may need to consider proper induced subgraphs. The graph  $P_5 \vee K_1$  has two simplicial vertices, two MEP's, and two EP's, but it has an induced  $K_{1,3}$  (which has three MEP's) and hence is not a proper interval graph. Nevertheless, MEP's provide the right answer for block graphs (compare this result with Theorem 3 and Corollary 1). Note the contrast between this result and the fact that the leafage of a tree  $G$  is the number of leaves in  $G'$ .

**Theorem 10.** *The proper leafage of a block graph that is not a clique is the number of leaf blocks. In particular, the proper leafage of a tree is the number of leaves. (The proper leafage of a clique is 2.)*

**Proof.** In the reduction  $G^*$  of a block graph  $G$ , each leaf block becomes an edge containing a simplicial vertex  $v$ . This vertex  $v$  is an MEP in  $G^*$ , because  $N(v)$  is a single vertex, and hence each component obtained by deleting  $N[v]$  has that vertex as its neighborhood in  $N[v]$ . This proves the lower bound; for the upper bound, we construct a representation.

If  $G$  is a clique, we form a proper subtree representation for  $G$  by using a collection of pairwise intersecting subpaths of a path, with the initial vertices appearing before all the terminal vertices and in the same order as the terminal vertices. We may choose the two vertices represented at the leaves arbitrarily.

Let  $m(G)$  denote the number of leaf blocks in  $G$ . By induction on the number of blocks in  $G$ , we build a proper subtree representation with  $\max\{m(G), 2\}$  leaves, having an arbitrary simplicial vertex from each leaf block appearing at the leaf corresponding to that block (two such vertices if  $G$  is a clique). We have verified this when  $G$  is a clique.

If  $G$  is choose a leaf block  $B$ , and let  $v$  be the cut-vertex of  $G$  in  $B$ . Let  $f'$  be the proper representation of  $B$  in a path that has  $v$  at one leaf and the arbitrarily specified simplicial vertex in  $B$  and the other leaf. If  $v$  belongs to at least two blocks other than  $B$ , then  $m(G - (B - v)) = m(G) - 1$ .

The induction hypothesis provides a representation  $f$  of  $G - (B - v)$ ; we complete this by adding an edge from the leaf assigned to  $v$  in  $f'$  to a vertex assigned to  $v$  in  $f$ . If  $v$  belongs to only one block other than  $B$ , then this is a leaf block in  $G - (B - v)$ , and  $m(G - (B - v)) = m(G)$ . In this case the representation  $f$  of  $G - (B - v)$  assigns a leaf to  $v$ , and we can add an edge from it to the leaf assigned to  $v$  in  $f'$  without increasing the number of leaves. ■

If  $v$  is a simplicial vertex of a  $k$ -tree, then  $N(v)$  is a minimal cutset, and Lemma 12 then implies that  $v$  is an MEP. Hence the proper leafage of a  $k$ -tree is at least the number of simplicial vertices. The 2-tree  $P_5 \vee K_1$  shows that this bound need not be sharp.

**Lemma 15.** *Let  $v$  be a cut vertex of a connected chordal graph  $G$  such that  $G - v$  has two components. If  $G_1, G_2$  are the subgraphs obtained by deleting the vertices of one of these components, then  $l^*(G) \geq l^*(G_1) + l^*(G_2) - 2$ . If  $G_1$  or  $G_2$  has proper leafage 2 and is not a clique, then  $l^*(G) \geq l^*(G_1) + l^*(G_2) - 1$ .*

**Proof.** Let  $f$  be an optimal proper subtree representation of  $G$ . Since each  $G_i$  is a connected subgraph, the union of the subtrees assigned to vertices of  $G_i$  is a subtree of the host; call these  $T_1, T_2$ . Furthermore, vertices of  $T_1 \cap T_2$  can only be assigned to  $v$ . If  $v$  appears alone at a leaf, then we could delete that leaf without losing the property of proper representation. Thus we may assume that each leaf of  $T$  is a leaf of exactly one of  $T_1$  or  $T_2$ . If we delete vertices assigned to any vertex outside  $G_i$ , we still have a subtree representation of  $G_i$ ; we can guarantee that it is a proper representation by growing a leaf from a vertex assigned to  $v$ . Hence we have proved that  $l^*(G_1) + l^*(G_2) \leq l^*(G) + 2$ .

If  $l^*(G_2) = 2$  and  $G_2$  is not a clique, then we can obtain a proper subtree representation of  $G_2$  with two leaves instead of growing an extra leaf from  $T_2$  in the construction above. Hence in this case we can improve the bound to  $l^*(G_1) + l^*(G_2) \leq l^*(G) + 1$ . ■

We can now present a class of examples where the gap between the proper leafage and the maximum number of MEP's in induced subgraphs becomes arbitrarily large. The  $n$ -kite  $G_n$  is the graph with  $3n + 1$  vertices consisting of a path  $P$  on successive vertices  $v_0, \dots, v_n$ , plus vertices  $\{u_1, \dots, u_n\}$  and  $\{w_1, \dots, w_n\}$  such that  $N(u_i) = N(w_i) = \{v_{i-1}, v_i\}$ . Although no induced subgraph has more than four MEP's,  $l^*(G_n) = n + 2$  for  $n \geq 2$ . Note first that  $l^*(G_1) = 2$ . For  $n = 2$ , the vertices  $\{u_1, w_1, v_1, u_2, w_2\}$  induce  $K_{1,4}$ , a

subgraph in which the four leaves are MEP's. Hence  $l^*(G_2) \geq 4$ . For  $n > 2$ , we form  $G_n$  by identifying  $v_{n-1}$  from  $G_{n-1}$  with  $v_0$  from  $G_1$ . By the second part of Lemma 15, we thus have  $l^*(G_n) \geq l^*(G_{n-1}) + 1$ , so  $l^*(G_n) \geq n + 2$  by induction. Figure 3 illustrates a construction that achieves equality. Note that all  $2n$  simplicial vertices are EP's, but we have leaves in the proper subtree representation for only half of them.

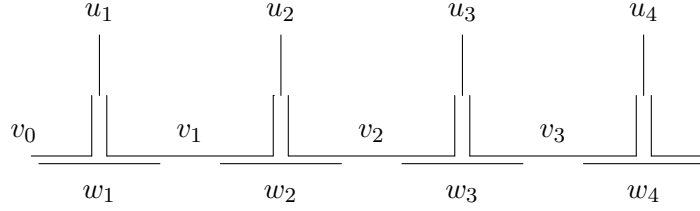


Figure 3. Optimal proper subtree representation of  $G_4$

Finally, we show that proper leafage equals leafage for  $K_{1,3}$ -free chordal graphs.

**Theorem 11.** *If  $G$  is a  $K_{1,3}$ -free non-clique chordal graph, then  $l(G)$ ,  $l^*(G)$ ,  $a(G)$ , and the number of inequivalent MEP's in  $G$  are equal.*

**Proof.** Recall that  $a(G)$  denotes the maximum size of an asteroidal set in  $G$ , and let  $m(G)$  be the number of inequivalent MEP's in  $G$ . If any of  $a(G), m(G), l(G)$  is 2, then  $G$  is an interval graph. Being  $K_{1,3}$ -free, such a graph  $G$  is also a unit-interval graph, and hence all the parameters equal 2. Hence we may assume the values exceed 2. We prove that  $m(G) = a(G) \leq l(G) \leq l^*(G) \leq a(G)$ . By Theorem 1 and the definition of proper leafage, we need only prove the first equality and the last inequality.

In proving that  $m(G) = a(G)$ , we may assume that  $G$  is reduced. Let  $X$  be the set of MEP's in  $G$ . To prove that  $m(G) \leq a(G)$ , we prove that  $X$  is an asteroidal set. It suffices to show that  $G - N[x]$  is connected for each  $x \in X$ . If not, then by the definition of MEP,  $G - N[x]$  has two components  $H_1, H_2$  such that  $U_1 = U_2$ , where  $U_i = \{y \in N(x) : N(y) \cap V(H_i) \neq \emptyset\}$ . Choose  $w \in U_1$ ,  $y \in N(w) \cap V(H_1)$ , and  $z \in N(y) \cap V(H_2)$ ; now  $w, x, y, z$  induce the forbidden  $K_{1,3}$ .

We next prove that  $a(G) \leq m(G)$ . Among all maximum-sized asteroidal sets, let  $X$  be one that maximizes the sum  $\sigma(X)$  of the pairwise distances between the elements. By the argument in Lemma 7, we may assume that

$X \subseteq S(G)$ . Consider  $x \in X$ . In order to prove that  $x$  is an MEP, it suffices to prove that  $G - N[x]$  has only one component. Since vertices of  $X - x$  are linked by paths avoiding  $N[x]$ , all of  $X - x$  belongs to the same component  $H_1$  of  $G - N[x]$ . If there is another component  $H_2$  of  $G - N[x]$ , a common neighbor of  $H_1$  and  $H_2$  in  $N(x)$  would create an induced  $K_{1,3}$ . Hence we could replace  $x$  in  $X$  by a vertex of  $H_2$  to obtain a maximum asteroidal set with greater distance sum.

For the last inequality, we build a proper subtree representation of  $G$  with  $a(G)$  leaves, by induction on  $n(G)$ , in which the vertices of a maximum asteroidal set  $X$  maximizing  $\sigma(X)$  appear at the leaves of the host tree. Again we may assume that  $G$  is reduced. As proved above, each  $x \in X$  is an MEP. Since  $G$  is  $K_{1,3}$ -free, distinct components of  $G - N[x]$  cannot have common neighbors in  $N(x)$ . By Lemma 11, the vertices of  $N(x)$  form a minimal cutset. Hence  $G - N[x]$  is connected. Thus  $G - N[x]$  cannot have an asteroidal set of size  $a(G)$ , since  $x$  would augment it to a larger asteroidal set in  $G$ .

Now the induction hypothesis guarantees a proper subtree representation of  $G - x$  with  $a(G - x)$  leaves. If  $a(G - x) = a(G)$ , then every maximum asteroidal set in  $G - x$  has a vertex  $y \in N(x)$ , including sets that maximize  $\sigma$  and have all elements simplicial. In such a representation, we have  $y$  at a leaf  $q$  of the host. We add a leaf adjacent to  $q$ , and to  $x$  we assign the minimal subtree containing  $q$  and at least one vertex of the subtree representing each vertex of  $N(x)$ . Since  $x$  is simplicial,  $N_G(x) \subseteq N_{G-x}[y]$ . Since the representation of  $G - x$  is proper, the result is a proper subtree representation of  $G$ .

Finally, if  $a(G - x) < a(G)$ , then we take the proper subtree representation of  $G - x$  guaranteed by induction for  $X - x$ , find a vertex of the host at which all of  $N(x)$  appear, extend those subtrees from that vertex to a new leaf  $q$ , and add another edge from  $q$  to another new vertex  $q'$ , assigning  $f(x) = \{q, q'\}$ . ■

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