On Low Treewidth Graphs and Supertrees

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Abstract

Compatibility of unrooted phylogenetic trees is a well studied problem in phylogenetics. It asks to determine whether for a set of $k$ input trees $T_1, \ldots, T_k$ there exists a larger tree (called a supertree) that contains the topologies of all $k$ input trees. When any such supertree exists we call the instance compatible and otherwise incompatible. It is known that the problem is NP-hard and FPT, although a constructive FPT algorithm is not known. It has been shown that whenever the treewidth of an auxiliary structure known as the display graph is strictly larger than the number of input trees, the instance is incompatible. Here we show that whenever the treewidth of the display graph is at most 2, the instance is compatible. Furthermore, we give a polynomial-time algorithm to construct a supertree in this case. Finally, we demonstrate both compatible and incompatible instances that have display graphs with treewidth 3, highlighting that the treewidth of the display graph is (on its own) not sufficient to determine compatibility.
1 Introduction

One of the central challenges within computational evolutionary biology is to infer the evolutionary history of a set of contemporary species (or more generally, taxa) $X$ using only the genotype of the contemporary species. This evolutionary history is usually modeled as a phylogenetic tree, essentially a tree in which the leaves are bijectively labeled by the elements of $X$ and the internal nodes of the tree represent (hypothetical) ancestors [14].

There is already an extensive literature available on the extent to which different optimization criteria on the space of phylogenetic trees (e.g. likelihood, parsimony) are able to identify the “true” evolutionary history. In any case it is well-known that most of these problems are NP-hard, and this intractability is a serious obstacle when constructing phylogenetic trees for large numbers of taxa. This has been one of the motivations behind supertree methods [3]. Here the goal is to first construct phylogenetic trees for small (overlapping) subsets of $X$ and then to puzzle the partial trees together into a single tree on $X$ that contains all the topologies of the partial trees, in which case we say the partial trees are compatible, or to conclude that no such tree exists.

The computational complexity landscape of the compatibility problem is uneven. In the case that all the partial trees are rooted (i.e. in which the flow of evolution is assumed to be away from a designated root, towards the taxa) the problem is polynomial-time solvable, using the algorithm of Aho [1]. However, in the case of unrooted trees the problem is NP-hard, even when all the partial trees have at most 4 taxa [15]. Nevertheless, due to the fact that many tree-building algorithms actually construct unrooted trees, and because of the risk of distorting the underlying phylogenetic signal through a poor choice of root location, it remains attractive to try and solve this NP-hard variant of the problem directly.

In this article we approach the unrooted compatibility problem from a graph-theoretical angle. There is a recent trend in this direction, which to a large extent can be traced back to a seminal paper of Bryant and Lagergren [6]. They observed that there is a relationship between the compatibility question and the treewidth of an auxiliary graph known as the display graph. The display graph is obtained by identifying the taxa of the input trees, and treewidth is an intensely well-studied parameter in the algorithmic graph theory literature (for a survey see e.g. [5]). Low (or bounded) treewidth often facilitates algorithmic tractability. A linear time algorithm for computing treewidth is due to Bodlaender [4]. Though the theoretic runtime of the Bodlaender’s algorithm is linear, the algorithm is impractical because of the huge constant hidden in the big-$O$. For small treewidth, e.g. $q = 2, 3$, there is a practical algorithm by Arnborg, Corneil and Proskurowski [2] running in time $O(n^{q+2})$, where $n$ is the number of vertices in the input graph.

Given that the treewidth is a measure of “distance from being a tree”, it is tempting to try and exploit this tractability in questions pertaining to phylogenetic compatibility and incongruence. Bryant and Lagergren observed that for $k$ unrooted trees to be compatible, it is necessary (but not sufficient) that
the display graph has treewidth at most $k$. The upper bound on the treewidth that this condition generates, subsequently makes it possible to formulate and answer the compatibility question in a computationally efficient way. However, this efficiency is purely theoretical in nature, obtained via the indirect route of monadic second order logic [7], and it remains a challenge to succinctly characterize phylogenetic compatibility. Since Bryant and Lagergren various other authors have picked up this thread (e.g. [11]), with particular attention for triangulation-based approaches (see e.g. [16] [12] [17]) although the question remains: what exactly is the role of treewidth in compatibility?

Here we take a step forward in understanding the link between treewidth and compatibility. We prove that if the display graph of a set of unrooted binary trees has treewidth at most 2, then the input trees are compatible, and this holds for any number of input trees. In other words, it is not necessary to look deeper into the structure of the display graph, compatibility is immediately guaranteed. The proof of this, based on graph separators and graph minors, is surprisingly involved. Moreover, we describe a simple polynomial-time algorithm to construct a supertree for the input trees, when this condition holds. We also show that in some sense this result is “best possible”: we show how to construct both compatible and incompatible instances that have display graphs of treewidth 3, for any number of trees. This confirms that the treewidth of the display graph cannot, on its own, fully capture phylogenetic compatibility, and that auxiliary information is indeed necessary if we are to obtain a complete characterization.

2 Preliminaries

Let $X$ be a finite set. An unrooted phylogenetic $X$-tree is a tree whose leaves are bijectively labeled by the elements of set $X$. It is called binary when all its inner nodes (nonleaf nodes) are of degree 3. An unrooted binary phylogenetic tree on four leaves is called a quartet. In the remainder of the article we focus almost exclusively on unrooted binary trees, often writing simply trees or $X$-trees for short.

We call elements of $X$ taxa or leaves. For some $X$-tree $T$ and some subset $X' \subseteq X$ we denote by $T(X')$ the subtree of $T$ induced by $X'$ and by $T|X'$ the tree obtained from $T(X')$ by suppressing vertices of degree 2. Furthermore, we say a tree $S$ displays a tree $T$ if $T$ can be obtained from a subgraph of $S$ by suppressing vertices of degree two.

Given a set $X$ a split is defined as a bipartition of $X$. If we label the components of the partition by $A$ and $B$, then we can denote the split by $A|B$. Note that each edge of an $X$-tree naturally induces a split. If $A|B$ is a split induced by an edge of a tree $T$, then we say that $T$ contains split $A|B$. We use $ab|cd$ to denote the quartet in which taxa $a$ and $b$ are on one side of the internal edge and $c$ and $d$ are on the other. We write $ab|cd \in T$ if $T$ displays $ab|cd$.

Given a set $T$ of $k$ trees $T_1, ..., T_k$ we wish to know if there exists a single tree $S$ that displays $T_i$ for all $i \in \{1, ..., k\}$. A tree that displays all the input trees,
if such a tree exists, is called a supertree. When a supertree does exist we call the instance compatible, otherwise incompatible. A supertree is not necessarily unique. To see when such a tree is unique and many more details on this topic we refer the reader to [9] or [14].

The display graph $D(T)$ of a set of trees $T$ is the graph obtained from the disjoint union of trees in $T$ by identifying vertices with the same taxon labels. Note that $D(T)$ can be disconnected if and only if the trees in $T$ can be bipartitioned into two sets $T_1, T_2$ such that $X(T_1) \cap X(T_2) = \emptyset$, where $X(T)$ refers to the set of taxa of $T$. In such a case $T$ permits a supertree if and only if both $T_1$ and $T_2$ do. Hence for the remainder of the article we focus on the case when $D(T)$ is connected.

Before we can start discussing our result we need a few graph theoretic definitions. Let $G = (V, E)$ be an undirected graph. For any two subsets of vertices $A, B \subseteq V$ and any $Z \subseteq V$ we say $Z$ separates sets $A$ and $B$ in $G$ if every path in $G$ that starts at some vertex $u \in A$ and ends at some vertex $v \in B$ contains a vertex from $Z$. Such a set $Z$ is called an $(A, B)$-separator, or simply a separator. A graph $M$ is a minor of a graph $G$ if $M$ can be obtained from a subgraph of $G$ by contracting edges.

The treewidth of a graph $G$, denoted $tw(G)$, has a somewhat technical definition. We give it here for completeness although for the main result it is sufficient to note that trees have treewidth 1, and that graphs with treewidth at most 2 are exactly those graphs that do not have a $K_4$-minor (where $K_4$ is the complete graph on 4 vertices) [8]. We will also use the well-known fact that if $M$ is a minor of $G$, $tw(M) \leq tw(G)$ [8].

Let $G$ be a graph, $T$ a tree and $(B_t)_{t \in T}$ a family of subsets of $V(G)$, also called bags, indexed by vertices of $T$. We say $T$ is a tree-decomposition of $G$ if the following conditions are satisfied:

$\begin{enumerate} 
\item[(T_1)] V(G) = \cup_{t \in T} B_t; \\
\item[(T_2)] for every edge $e \in G$ there exists a bag $B_t$ in $T$ such that both endpoints of $e$ lie in $B_t$; \\
\item[(T_3)] $B_u \cap B_v \subseteq B_w$ whenever vertices $u, v, w$ of $T$ are such that $w$ is on a path from $u$ to $v$ in $T$. 
\end{enumerate}$

The width of a tree-decomposition is the size of its largest bag minus one. The treewidth of a graph $G$, also denoted $tw(G)$, is the minimum width over all possible tree-decompositions of $G$. For remaining graph theory terminology we refer to standard texts such as [8].

3 Main Results

We begin with some simple lemmas.

**Lemma 1** [10, Corollary 1]. Let $T_1$ and $T_2$ be two unrooted phylogenetic trees on the same set of taxa $X$. Then $T_1$ and $T_2$ are compatible if and only if there do not exist four taxa $a, b, c, d \subseteq X$ such that $ab|cd \in T_1$ and $ac|bd \in T_2$. 
Lemma 2 Let $D$ be the display graph of the two quartets $ab|cd$ and $ac|bd$. Then $D$ has $K_4$ as a minor. Hence, $\text{tw}(D) \geq 3$.

Proof: Both $Q_1$ and $Q_2$ have two inner nodes each. It is immediate to see that those four inner nodes form a $K_4$ minor in $D$. □

Theorem 1 Let $T_1$ and $T_2$ be two unrooted phylogenetic trees. Let $D$ be the display graph of $T_1$ and $T_2$. Then $T_1$ and $T_2$ are compatible if and only if $\text{tw}(D) \leq 2$.

Proof: Let $T_1$ and $T_2$ be two trees on taxa sets $X$ and $X'$ respectively. Let $X^* = X \cap X'$. Then $T_1$ and $T_2$ are compatible if and only if $T_1|X^*$ and $T_2|X^*$ are compatible [14]. Thus we only have to consider two trees $T_1$ and $T_2$ on the same set of taxa $X$. Let $D(T_1, T_2)$ be their display graph. Suppose for the sake of contradiction that $\text{tw}(D(T_1, T_2)) \leq 2$ while $T_1$ and $T_2$ are incompatible. From Lemma 1 $T_1$ and $T_2$ contain incompatible quartets $Q_1$ and $Q_2$ (w.l.o.g. let $T_i$ display $Q_i$) and since $Q_i$ is displayed in $T_i$, $D(Q_1, Q_2)$ is a minor of $D(T_1, T_2)$. Since $D(Q_1, Q_2)$ is a minor of $G$, and using Lemma 2 $\text{tw}(G) \geq \text{tw}(D(Q_1, Q_2)) \geq 3$, contradicting the fact that $\text{tw}(D(T_1, T_2)) \leq 2$. This completes our proof in one direction; for the other see [6]. □

In the following main theorem we emphasize that the trees in $T$ do not need to be on the same set of taxa, but that for this proof the input trees do need to be binary.

Theorem 2 Let $T$ be a set of $k$ binary unrooted phylogenetic trees $T_1, \ldots, T_k$ and let $D$ be their display graph. If $\text{tw}(D) \leq 2$, then $T_1, \ldots, T_k$ are compatible, in which case a supertree can be constructed in polynomial time.

Proof: We give a constructive proof in which we will build a supertree $S$ for $T$. The idea is to find an appropriate separator of $D$ and to reduce the problem into smaller instances of the same problem i.e. an induction proof. The induction will be on the cardinality of $X = \cup_{T_i \in T} X(T_i)$. For the base case observe that an instance with $|X| \leq 3$ is trivially compatible.

Before we start the construction we apply a number of operations on $D$ that are safe to do, in the sense that they preserve (in)compatibility of the instance and do not cause the treewidth of $D$ to rise. We remove any taxon that has degree 1 in $D$ and contract any inner vertex that has degree 2 in $D$. This clearly affects neither the compatibility nor the treewidth. Furthermore, for every tree $T_i$ with $i \in \{1, \ldots, k\}$ that has fewer than 4 leaves, we exclude it from the display graph. Such a tree carries no topological information and thus does not change the compatibility, while removing something from a graph cannot increase its treewidth. The cleaning up procedure means that we apply all these operations on $D$ repeatedly until we cannot apply them anymore (see figure 1). In other words, we can assume $D$ to have treewidth exactly 2, that all inner vertices of $D$ have degree 3, that all taxa have degree at least 2 and that no tree has fewer than 4 taxa.
Consider a planar embedding of the display graph \( D(T) \). This exists and can be found in polynomial time because \( D(T) \) has treewidth at most 2. The boundary of a face \( F \) of \( D(T) \), denoted \( B(F) \), is the set of edges and vertices that are incident to the interior of the face. We say that two distinct faces \( F_1, F_2 \) are minimally adjacent if the following three conditions hold: (1) \( F_1 \) and \( F_2 \) are adjacent; (2) \( B(F_1) \cap B(F_2) \) is isomorphic to a path containing at least one edge; (3) the internal vertices of the path \( B(F_1) \cap B(F_2) \) all have degree 2 in \( D(T) \), and the two endpoints of the path each have degree 3 or higher in \( D(T) \).

We now show that if the treewidth of \( D \) is 2 we can always find two such faces, neither equal to the outer face, in polynomial time.

**Observation 1** Let \( T \) be a non-empty set of unrooted binary trees on \( X \) such that \( \text{tw}(D(T)) = 2 \) and assume \( D(T) \) is cleaned up. Consider any planar embedding of \( D(T) \). Then there exist two distinct faces \( F_1, F_2 \) in \( D(T) \) such that \( F_1 \) and \( F_2 \) are adjacent and neither is equal to the outer face.

**Proof:** Without loss of generality we prove this for the case when \( D(T) \) is connected. Recall that all vertices in \( D(T) \) have degree at least 2, and at least one vertex has at least degree 3 (due to the existence of internal nodes). Hence, by the handshaking lemma, the number of edges in \( D(T) \) is strictly larger than the number of vertices, and thus we can use Euler’s formula to conclude that \( D(T) \) has at least 3 faces. One of these is the outer face, so \( D(T) \) has at least two faces not equal to the outer face. Hence, \( D(T) \) contains at least two simple cycles. If any two simple cycles have a common edge, then we are done, so let us assume that all simple cycles in \( D(T) \) are edge disjoint (and chordless). However, this is not possible due to the fact that in every simple cycle of a display graph at least two vertices have degree 3 or higher and the fact that all vertices in the graph have degree at least 2. (In particular, a simple cycle can never act as a “sink” to absorb excess degree, and there are also no leaves to fulfill this function.)
Observation 2 Let \( \mathcal{T} \) be a non-empty set of unrooted binary trees on \( X \). Assume \( D(\mathcal{T}) \) is cleaned up and \( tw(D(\mathcal{T})) = 2 \). Consider any planar embedding of \( D(\mathcal{T}) \). Let \( e \) be a cut-edge of \( D(\mathcal{T}) \), and let \( D_1, D_2 \) be the two components obtained by deleting \( e \). Then both \( D_1 \) and \( D_2 \) have their own pair of adjacent faces, neither equal to the outer face.

Proof: This is a simple adaptation of the previous proof. Deleting \( e \) reduces the degree of two vertices by exactly one, and all other degrees are unchanged. So \( D_1 \) and \( D_2 \) both contain at most one vertex of degree 1. From the previous “sink” observation we see that both \( D_1 \) and \( D_2 \) must contain two simple cycles with intersecting edges, and we are done. \( \square \)

Lemma 3 Let \( \mathcal{T} \) be a non-empty set of unrooted binary trees on \( X \). Assume \( D(\mathcal{T}) \) is cleaned up and \( tw(D(\mathcal{T})) = 2 \). Consider any planar embedding of \( D(\mathcal{T}) \). Then there exist two distinct faces \( F_1, F_2 \) in \( D(\mathcal{T}) \) such that \( F_1 \) and \( F_2 \) are minimally adjacent and neither is equal to the outer face. Also, these can be found in polynomial time.

Proof: Fix any planar embedding of \( D(\mathcal{T}) \). Let \( G \) be the dual graph of \( D(\mathcal{T}) \) (i.e. a graph whose vertices are the faces of \( D(\mathcal{T}) \), including the outer face, and whose edges are the adjacency relation on those faces). We label each face \( F \) of \( G \) with the length of a shortest path in \( G \) from \( F \) to the outer face. Clearly, the outer face has label 0. Let \( k \) be the maximum label ranging over all faces. We select a pair of distinct faces \( (F_1, F_2) \) such that (1) \( F_1 \) has label \( k \); (2) \( F_2 \) is adjacent to \( F_1 \); (3) \( F_2 \) has the largest label ranging over all faces that are adjacent to a face with label \( k \). By Observation 2, \( F_1 \) and \( F_2 \) both have label at least 1. Note also that the label of \( F_2 \) is either \( k - 1 \) or \( k \). Clearly, \( F_1 \) and \( F_2 \) both satisfy property (1) of minimal adjacency.

Consider now the sequence of vertices and edges \( v_1, e_1, v_2, e_2, \ldots, v_n = v_1 \) that define the boundary of face \( F_1 \). Observe that with the exception of \( v_1 = v_n \), all vertices on the boundary are distinct. This is because, if the boundary of the face intersects with itself, it creates a new face \( F_3 \) “inside” \( F_1 \) whose shortest path to the outer face is strictly larger than \( k \), contradicting the minimality of \( k \). Hence, \( B(F_1) \) is a simple cycle. From this it follows that \( B(F_1) \cap B(F_2) \) is a subgraph of a simple cycle. In particular, it can be (a) a simple cycle or (b) a set of one or more paths (where some of the paths might have length 0). We show that (a) cannot happen. To see this, observe that (a) can only happen if \( B(F_1) \subseteq B(F_2) \). From the degree constraints mentioned earlier the simple cycle defining \( F_1 \) contains at least 2 vertices of degree 3 or higher, in \( D(\mathcal{T}) \). These two vertices \( u_1, u_2 \) generate paths that cannot enter the interior of \( F_1 \), because they would then necessarily slice \( F_1 \) up into smaller faces. Moreover, there cannot exist a path from \( u_1 \) to \( u_2 \) that avoids \( B(F_1) \), because this would imply the existence of a third face \( F_3 \) adjacent to \( F_1 \), such that \( B(F_1) \cap B(F_3) \) contains an edge not in \( B(F_2) \). In particular, this would contradict \( B(F_1) \subseteq B(F_2) \). For a similar reason, the generated paths cannot re-intersect with \( B(F_1) \). Careful analysis shows that the only remaining possibility is that \( F_2 \) is the outer face,
contradicting the fact that the label of \( F_2 \) is at least 1. Hence we conclude that (a) is not possible, and that (b) must hold.

We now establish property (2) of minimal adjacency. In particular we show that \( B(F_1) \cap B(F_2) \) has a single component. By the definition of adjacency, and the fact that (b) holds, at least one component in \( B(F_1) \cap B(F_2) \) is a path \( P \) on one or more edges. Clearly, the two endpoints of \( P \) must (in \( D(T) \)) have degree 3 or higher, otherwise \( P \) could be extended further. Without loss of generality consider the lower endpoint \( u \). Let \( e \) be an edge incident to \( u \) (in \( D(T) \)) that is not in \( B(F_1) \cap B(F_2) \) but which is incident to \( F_1 \) (such an edge must exist). The second face incident to \( e \) cannot be \( F_2 \), because otherwise \( e \) would be in \( P \), so it must be some other face \( F_3 \neq F_2 \). Suppose there exists a path \( P' \neq P \) in \( B(F_1) \cap B(F_2) \). (Possibly, \( P' \) is a single vertex). In this case it is possible to draw a closed curve that passes through \( P \) and \( P' \) and such that the only face interiors that it intersects with, are those of \( F_1 \) and \( F_2 \) (see Figure 2). Informally this means that face \( F_3 \) is entirely “enclosed” by \( F_1 \) and \( F_2 \).

More precisely, it means that any (shortest) path in \( G \) from \( F_3 \) to the outer face must pass through \( F_1 \) or \( F_2 \). If such a shortest path travels via \( F_1 \), then the label of \( F_3 \) is at least \( k + 1 \), contradicting the maximality of \( k \). If it travels via \( F_2 \), then it has label \( k \) or \( k + 1 \). The latter is clearly a contradiction, but also the former because this contradicts our earlier choice of \( F_2 \) (i.e. we should have chosen \( F_3 \) instead of \( F_2 \)). Hence, \( B(F_1) \cap B(F_2) \) indeed consists of a single path \( P \) (containing at least one edge).

It remains to prove property (3). We have already established that the endpoints of \( P \) have degree 3 or more in \( D(T) \). If \( P \) has no interior vertices, or all interior vertices of \( P \) have degree 2 in \( D(T) \), we are done. So suppose \( P \) contains an interior vertex \( u \) of degree 3 or more in \( D(T) \). Let \( e \) be an edge incident to \( u \) (in \( D(T) \)) that is not in \( B(F_1) \cap B(F_2) \). Clearly, \( e \) starts a path that extends into the interior of \( F_1 \) or \( F_2 \). If \( e \) is not a cut-edge then the path it starts must re-intersect with the boundary of \( F_1 \) or \( F_2 \), but this causes a face to be partitioned into smaller pieces, which is not possible. Hence, \( e \) must be a cut-edge. From Observation 2 deleting \( e \) yields two or more adjacent faces that
are entirely “enclosed” by $F_1$ or $F_2$. If they are enclosed by $F_1$ then they both have label $k + 1$, which is a contradiction. If they are enclosed by $F_2$, and $F_2$ has label $k$, the same contradiction is obtained. If they are enclosed by $F_2$, and $F_2$ has label $k - 1$, then they both have label $k$, contradicting the fact that we chose $F_2$ in the first place.

Polynomial time is assured since recognition of treewidth 2, planar embeddings and determination of the labels can all be computed in linear time.

So let $F_1$ and $F_2$ be two minimally adjacent faces of $D$, neither equal to the outer face. Denote by $p(u, v)$ the path $B(F_1) \cap B(F_2)$ they share. By definition $u$ and $v$ must have degree at least 3 in $D$. Also, by minimal adjacency of $F_1$ and $F_2$ and due to cleaning up, none of the interior nodes of $p(u, v)$ can be internal tree nodes. Moreover, since we removed all trees on fewer than four taxa, at most one leaf can appear as an interior node of some trees. Now, $u$ and $v$ can either be both leaves, both inner nodes or one of them a leaf another an inner node. These are the three cases we have to consider.

Case(i) is when both $u$ and $v$ are leaves. We claim this cannot happen. In this case, path $p(u, v)$ must be an edge. But if it is an edge it is connecting two leaves and will have already been removed during cleaning up.

Case(ii) is when $u$ is a leaf and $v$ is an inner node. Again we have that path $p(u, v)$ must be an edge $(u, v)$ which both faces share. Let $x$, respectively $y$, be any vertex other than $u$ or $v$ on the boundary of $F_1$, respectively $F_2$. See Figure 3(a). We claim that any path between $x$ and $y$ must contain either $u$ or $v$. In particular, suppose there exists a path $p(x, y)$ such that $u, v \notin p(x, y)$. Let $x'$ and $y'$ be vertices on $p(x, y)$ such that the subpath $p(x', y')$ is the shortest subpath of $p(x, y)$ with the property that both of its endpoints are on the boundaries of $F_1$ and $F_2$, respectively. See Figure 3(a). Then $D$ contains a $K_4$ minor formed by vertices $u, v, x', y'$. This is a contradiction on $D$ having treewidth 2. So we have that any path between $x$ and $y$ passes through either $u$ or $v$. Thus $\{u, v\}$ is a separator of $D$.

Removing $u$ and $v$ from the vertex set of $D$ disconnects it and divides the set of taxa into two sets $X_1$ and $X_2$, such that $X = X_1 \cup X_2 \cup \{u\}$. We claim that supertree $S$ as shown in Figure 3(b), where $S'$ is a supertree of $T_1, ..., T_k$ restricted to taxa set $X \setminus \{u\}$, displays all $k$ input trees $T_1, ..., T_k$. To prove this we have to show two things. One, that the supertree $S'$ exists (and that it has an edge corresponding to split $X_1 | X_2$) and two, that all quartets in $T_1, ..., T_k$ are also in $S$. The latter is sufficient because of a well known result in phylogenetics that a set of unrooted trees is compatible if and only if the set of quartets.

\footnote{We chose this less formal and more intuitive proof of Lemma 3 in order to keep the notation and presentation simple. An alternative approach was to use the Jordan Curve Theorem, see for e.g. [13].}
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Figure 3: (a) Two minimally adjacent faces $F_1$ and $F_2$ in $D$. The vertices $u, v, x', y'$ induce a $K_4$ minor. (b) A supertree as constructed in case (ii).

displayed by the trees is compatible [14].

To prove the first claim let $X' := X \setminus \{u\}$ and notice that by induction the instance $T_1, ..., T_k|X'$ is compatible and thus has a supertree. We now claim that there exists some supertree of $T_1, ..., T_k|X'$, call it $S'$, which contains split $X_1|X_2$. First of all notice that (a restriction of) $X_1|X_2$ must be a split in every input tree restricted to $X'$. To see this we show that there does not exist a quartet $ab|cd$ with $a, c \in X_1$ and $b, d \in X_2$ in any of the input trees (prior to removal of $u$ and $v$). Suppose such a quartet did exist in some tree. Then there would exist edge-disjoint paths $p(a, b)$ and $p(c, d)$ in $D$, where the interior nodes of these paths are internal tree nodes. Since removing $u$ and $v$ from $D$ disconnects it (such that $X_1$ and $X_2$ are subsequently in separate components), it must be that those paths had to use either $u$ or $v$. Since $u$ is a taxon it cannot be used for this purpose. So both paths had to use inner vertex $v$. However, this contradicts the edge-disjointness of the two paths. Hence quartet $ab|cd$ cannot be displayed by any tree.

We conclude from this that in each $T_i|X'$ there exists an edge $e$ that induces a split $A|B$, such that $A \subseteq X_1$ and $B \subseteq X_2$. Furthermore both $X_1$ and $X_2$ must contain at least one taxon each. (This follows because edge $(u, v)$ belongs to some input tree $T$, and walking from $u$ to $v$ along the boundary of $F_1$ whilst avoiding edge $(u, v)$ necessitates entering and leaving $T$ via its taxa, which in turn means that some taxon not equal to $u$ must exist on the part of the boundary of $F_1$ not shared by $F_2$. The same argument holds for $F_2$.) As such, in each $T_i|X'$ it is possible to contract (the subtree induced by) $X_1$ and/or $X_2$ into a single “meta-taxon”.

Let $T^*$ (respectively, $T^{**}$) be the set of trees obtained by taking the trees on $X'$ and contracting all the $X_2$ (respectively, $X_1$) taxa into a single meta-taxon $W_2$ (respectively, $W_1$). Note that contracting in this way cannot increase the treewidth of $D$ and that $1 \leq |X_i| < |X|$ for $i \in \{1, 2\}$. Hence, by induction supertrees of $T^*$ and $T^{**}$ exist. Finally, construct supertree $S'$ with split $X_1|X_2$ from two supertrees for $T^*$ and $T^{**}$ by adding an edge between $W_1$ and $W_2$ and afterwards suppressing $W_1$ and $W_2$. (The function of $W_1$ and $W_2$ was pre-
cisely to ensure that we would know how to glue the two separately constructed supertrees together).

To see the second claim note that since $S'$ is a supertree of $T_1, ..., T_k$ restricted to $X \setminus \{u\}$ we only have to show that quartets of $T_1, ..., T_k$ that contain taxon $u$ are displayed by $S$. So w.l.o.g. let $a \in X_1, b, c \in X_2$. Then if quartet $au|bc$ is displayed by some input tree $T$ it is also clearly displayed by the supertree $S$. We claim quartets $ub|ac$ or $uc|ab$ cannot exist in any of the input trees. These two quartets are the same up to relabeling so let’s consider quartet $ub|ac$ induced by some tree $T$ sitting inside $D$. Then $p(u, b)$ and $p(a, c)$ are edge-disjoint and contain no taxa. As argued before $p(a, c)$ must pass through $v$. But since $(u, v)$ is an edge it follows that it must belong to the same tree $T$, and therefore $v$ also lies on the path $p(u, b)$. But then it is not possible that $T$ displays $ub|ac$, contradiction.

**Case (iii)** is when both $u$ and $v$ are inner nodes. We could have that $p(u, v)$ is an edge, in which case $u$ and $v$ are inner nodes of the same tree, or we could have that $p(u, v)$ contains a single taxon $t$. Note that in the latter case $u$ and $v$ are inner nodes of two different trees and taxon $t$ must have degree 2 in $D$ due to the minimal adjacency of $F_1$ and $F_2$. The argument for $\{u, v\}$ being a separator of $D$ goes through in this case as well regardless of $p(u, v)$ being an edge or a path containing a single taxon $t$. We again denote by $X_1$ and $X_2$ the two sets of taxa that emerge from splitting $D$ by removing $u$ and $v$ (and $t$ if it exists on $(u, v)$).

![Figure 4](image-url)

Figure 4: (a) A supertree constructed in case (iii) when there exists a taxon $t$ on the common boundary of the two faces. (b) Construction of a supertree in case (iii) when the common boundary of the two faces is a single edge.

**Subcase 1.** Consider first the subcase when some taxon $t \in p(u, v)$. As before we have to show that there exists some $S'$, a supertree of $T_1, ..., T_k$ restricted to $X' := X \setminus \{t\}$ with split $X_1|X_2$, and that the supertree $S$ as shown in Figure 3(a) displays all quartets induced by $T_1, ..., T_k$. The proof for this case is almost identical to that of case (ii). There we used the fact that $u$ was a leaf. We now show that all the statements made in case (ii) also hold when $u$ is an inner node and $t$ is a taxon on path $p(u, v)$. 
We saw that in case (ii) both $X_1$ and $X_2$ were nonempty and of strictly smaller cardinality than $X$. In this subcase, the fact that the cardinalities of $X_1$ and $X_2$ are strictly smaller than of $X$ follows from $t \in X$ but $t \notin X_1$ and $t \notin X_2$. The fact that the sets are nonempty also holds. Consider face $F_1$. Let $u$ be a node of some tree $T_1$ and $v$ a node of some other tree $T_2$. Then the path from $u$ to $v$ that follows the part of the boundary $F_1$ not shared by $F_2$, is a path between two vertices of different trees and so must contain some taxon $a \neq t$ (which is also in $X_1$). The same argument holds for $F_2$ and $X_2$.

Another thing we have to show here is that all input trees $T_u \in \mathcal{T}$ have to contain either $u$ or $v$. W.l.o.g. let $u \in p(a,c)$ and $v \in p(b,d)$. Furthermore paths $p(a,b)$ and $p(c,d)$ are edge-disjoint in $D$ and belong to the same tree $T$. But this is impossible since $u$ and $v$ belong to different trees in this case. Contradiction. So we conclude in this case too that every input tree restricted to $X'$ respects split $X_1 \mid X_2$, and hence the contraction of $X_1$ and $X_2$ into meta-taxa works exactly as described in case (ii). Hence, $S'$ indeed exists, can be constructed and has split $X_1 \mid X_2$.

Next, we claim that $S$ as shown in Figure 4(a) displays all quartets induced by $T_1, ..., T_k$. As before, since $S'$ is a supertree of $T_1, ..., T_k \mid X'$ we only need to check the quartets induced by $T_1, ..., T_k$ that contain taxon $t$. W.l.o.g. let $a \in X_1$ and $b, c \in X_2$. There are three possible topologies $a \mid \{b,c\}, b \mid \{a,c\}, c \mid \{a,b\}$. As before, $a \mid \{b,c\}$ is an easy case since if it appears in some $T \in D$ it clearly also appears in $S$, while topologies $b \mid \{a,c\}$ and $c \mid \{a,b\}$ are the same up to relabeling. So consider $b \mid \{a,c\}$ and suppose it is displayed by some tree $T$. Paths $p(b,t)$ and $p(a,c)$ are edge-disjoint and since the degree of $t$ is 2 in $D$ we have that $p(b,t)$ has to contain either $u$ or $v$. W.l.o.g. let $u \in p(b,t)$. Now, since $\{u,v\}$ is a separator of $D$ and $a \in X_1$ while $c \in X_2$, we have that either $u \in p(a,c)$ or $v \in p(a,c)$. If $u \in p(a,c)$ we have that paths $p(b,t)$ and $p(a,c)$ both contain node $u$, a contradiction on $b \mid \{a,c\}$ being displayed by $T$. If $v \in p(a,c)$ then edge $(v,t)$ and $(u,t)$ must both belong to the same tree $T$, which contradicts our earlier observation that $u$ and $v$ are necessarily in different trees.

**Subcase 2.** The last thing to consider is the subcase when $(u,v)$ is an edge while both $u$ and $v$ are inner nodes (necessarily of the same tree $T$). Let $X_1$ and $X_2$ be two disjoint sets of taxa that result from splitting $D$ after removing $u$ and $v$. We claim that $|X_1| \geq 2$ and $|X_2| \geq 2$. This follows directly from $u,v \in T$; any cycle that links them together must leave the tree $T$ via some taxon $a$ and re-enter it via a (necessarily different) taxon $b$. Since $u$ and $v$ belong to both faces $F_1$ and $F_2$ it follows that the boundaries of these two faces must each contain (at least) two taxa. The two taxa on the boundary of $(w.l.o.g.) F_1$ are still in the same connected component after deletion of $\{u,v\}$, but are not in the same connected component as the taxa from the boundary of $F_2$, so $|X_1| \geq 2$ and $|X_2| \geq 2$. 
Now we claim that the tree shown in Figure 4(b) is a supertree of $T_1, \ldots, T_k$. Let’s first explain what that image means. Note that apart from the tree $T$ in which the internal edge $e = (u, v)$ can be found, all other trees have taxa sets either completely contained inside $X_1$ or completely contained inside $X_2$. This is the case because otherwise there would be a path from some element in $X_1$ to some element in $X_2$, contradicting the fact that $\{u, v\}$ is a separator. The idea is to cut $T$ into two parts, one on $X_1$, one on $X_2$, recursively build supertrees of $T_1, \ldots, T_k|X_1$ and $T_1, \ldots, T_k|X_2$ and join them as indicated in the figure.

Now, consider the display graph $D$. Suppose we delete the edge $e = (u, v) \in T$, and replace it with two edges $e_1 = (u_1, v_1)$ and $e_2 = (u_2, v_2)$ (where $u_i$ and $v_i$ are $u$ and $v$ duplicated). Because $\{u, v\}$ is a separator, this creates two disjoint display graphs, one on $X_1$ and one on $X_2$. These are minors of the original display graph so have treewidth at most 2, and they are smaller instances of the problem. So by induction supertrees of these smaller instances exist. Let $S(X_1)$ be a supertree on $X_1$ and $S(X_2)$ be a supertree on $X_2$. All trees except $T$ will be displayed by the disjoint union of $S(X_1)$ and $S(X_2)$, because only $T$ has taxa from both $X_1$ and $X_2$. What is left to explain is how to glue $S(X_1)$ and $S(X_2)$ into a supertree $S$ such that $S$ displays $T$ as well.

Note that $S(X_i)$ contains an image of edge $e_i$. The image need not be an edge in $S(X_i)$, it could also be a path, whose endpoint we denote by $u_i$ and $v_i$ in Figure 4(b). Take any edge on path $p(u_i, v_i)$, call it $e_i′$, and subdivide it twice to create two adjacent degree-2 vertices; let $e_i″$ be the edge between them. Now, by identifying $e_i′$ and $e_i″$ we ensure that we get a supertree that displays (all the quartets in) $T$, as well as all the other trees.

This completes the case analysis. Polynomial time is achieved because all relevant operations (recognizing whether a graph has treewidth at most 2, finding a planar embedding, finding two minimally adjacent faces, finding the separator $\{u, v\}$, and all the various tree manipulation operations) can easily be performed in linear time.

We now give a summary of the algorithm that has already been implicitly described in the above proof. As input we are given $k$ phylogenetic trees on $|X|$ taxa. We construct the display graph $D$ of the $k$ trees and clean it up. The size of the display graph is at most $|X| + k(|X| - 1)$ vertices. We start by verifying (in time time linear in number of vertices of $D$) that the treewidth of $D$ is at most 2. Next we construct a planar embedding of $D$ and find its dual $G$. This step also only takes linear time.

We label the faces of $G$ (there are as many of them as vertices of $D$) by computing shortest paths from the outer face to each face of $G$. Since this is a single source shortest path problem, it too can be computed in time linear in $|V(D)|$. We select the largest label (and the face adjacent to the face with the largest label); these are our minimally adjacent faces $F_1$ and $F_2$. If two such faces do not exist, then the instance is trivially compatible.

By definition of minimal adjacency we know that the intersection of borders of the two faces must be isomorphic to a path $p(u, v)$ containing at least one edge. Denote by $X_1$ and $X_2$ are two sets of taxa obtained from separating $D$
by removing \{u, v\}.

We saw that we can w.l.o.g. assume \(v\) to be an inner node. If \(u\) is a leaf, then we construct a supertree \(S\) as shown in figure 3(b) and recursively solve two smaller instances with input trees \(T_i|X_1\) and \(T_i|X_2\) for \(i \in \{1, \ldots, k\}\). (Note that in the actual algorithm we also add an extra “meta-taxon” into each of the two smaller instances which tells us where to graft the two solutions back together). Otherwise, \(u\) is an inner node. In this case, path \(p(u, v)\) can either contain a taxon \(t\) or be an edge. When it contains a taxon \(t\) a supertree \(S\) is given in figure 4(a) and we recursively solve two smaller instances with input trees \(T_i|X_1\) and \(T_i|X_2\) for \(i \in \{1, \ldots, k\}\) (note that in this case the two taxa sets \(X_1\) and \(X_2\) are obtained after removing \{u, v, t\} from \(D\)). When \(u\) is an inner node and \(p(u, v)\) is an edge, then we construct a supertree as in figure 4(b) and recursively solve two smaller instances \(T_i|X_1\) and \(T_i|X_2\) for \(i \in \{1, \ldots, k\}\). We continue until the instance is trivially compatible.

Finally, we discuss the time complexity of the algorithm. One side of each recursively found split contains only one taxon in worst case, while the number of trees does not decrease. Therefore, in the worst case the number of iterations is \(|X|\), and as we just argued each iteration takes time that is linear in \(|X|\) and \(k\). Thus, the runtime of our algorithm is quadratic in the input size.

4 Beyond Treewidth 2

Two incompatible quartets induce a display graph with treewidth 3, so treewidth 3 cannot guarantee compatibility. However, it is natural to ask whether treewidth 3 guarantees compatibility if the number of input trees becomes sufficiently large. Unfortunately, the answer to that question is no. Namely, for any number of trees there exists a compatible instance with \(tw(D) = 3\) and an incompatible instance with \(tw(D) = 3\), as we now demonstrate.

Consider figures 5 and 6. They both show the display graph of \(k\) trees with leaves indicated by black circles and inner nodes of each tree indicated by filled circles in the same color as that of the tree they correspond to. Both graphs contain \(K_4\) as a minor. Thus, the treewidth of the graphs is at least 3. As it can be easily verified either by any available software or by giving a tree decomposition of width 3, the key structural bags of which are depicted in Figure 7, the treewidth of both of these display graphs is exactly 3.

The display graph in figure 5 however shows an instance that is compatible. This can be verified without too much difficulty. We already argued that the cleaning up procedure preserves (in)compatibility; we will use this now. Notice then that we can remove two leaves of \(T_k\) with degree 1, making \(T_k\) a tree on three leaves. We can thus remove the whole tree, thereby making \(T_{k-1}\) and \(T_{k-2}\) trees on three leaves. Removing \(T_{k-1}\) and \(T_{k-2}\) makes \(T_{k-3}\) a tree on three leaves etc. In the end we are only left with a single tree, \(T_1\). Since a single tree is trivially compatible it follows that all \(k\) trees are compatible.

Figure 6 on the other hand shows an incompatible instance. We can again
start cleaning up this instance from $T_k$ backwards until we are left with $T_1$, $T_2$ and $T_3$. Figure 8, first panel, shows the display graph of $T_1$, $T_2$ and $T_3$. We can do one more cleaning up step and end up with a graph in the middle panel (we abuse the notation slightly and call the cleaned up version of $T_3$, $T_3$ again). We argue that the three trees in the middle panel of Figure 8 are incompatible.

In the third panel of Figure 8 we try to build a supertree of the three trees in order to reach a contradiction. We start with $T_3$ and add $T_1$ to it. $T_3$ already contains leaves 1, 2, 3 of $T_1$ so we only have to decide where to add leaves 6 and 7. Notice that $T_1$ requires paths $p(1, 6)$ and $p(2, 7)$ to be disjoint. Furthermore, an inner vertex $k$ of $T_1$ is (by definition of a tree) the only vertex with a property that paths $p(1, k), p(2, k), p(3, k)$ are edge-disjoint. If we want to map it to $T_3$ there is only one place where it can be (as indicated in the third panel of the Figure 8). From the condition that paths $p(1, 6)$ and $p(2, 7)$ must be disjoint, it follows that leaf 6 has to be attached somewhere on the path $p(1, k)$ and leaf 7 has to be attached somewhere on the path $p(2, k)$. Since these two paths are in fact edges in $T_3$ it follows that there only one place where we can attach leaves 6 and 7 respectively. So the supertree of $T_1$ and $T_3$ is unique. Furthermore, it contains a quartet $45|67$ which in incompatible with tree $T_2 = 47|56$. So the
Figure 7: Tree decomposition of display graph of \( k \) compatible trees given in figure 5 such that each bag contains exactly four vertices. Due to the symmetry of the graph, we only give decomposition for the first part.

Figure 8: A display graph of three incompatible trees; A cleaned-up display graph of the same three trees; A unique supertree of \( T_1 \) and \( T_3 \)

three trees \( T_1, T_2 \) and \( T_3 \) are incompatible, and thus all \( k \) trees from Figure 6 must be incompatible.

5 Conclusion

Figure 9 summarizes our results. The red area is due to result of Bryant and Lagergren which proves that any instance on \( k \) trees whose display graph has treewidth strictly greater than \( k \) must be incompatible. The green area is due to our result. What we are left with is the gray area in which (as demonstrated by the constructions in the previous section) we cannot conclude anything about compatibility of the instances based only on treewidth of the display graph and the number of trees, at least not with the current results. An obvious open question is whether existing characterizations (such as legal triangulations [16]) can be specialized to yield simple and efficient combinatorial algorithms in the case of treewidth 3 or higher.
Figure 9: The green (respectively, red) area shows which combinations of (number of input trees, treewidth of display graph) are always compatible (respectively, incompatible). The gray area indicates that both compatible and incompatible instances exist for this combination of parameters.

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