Treewidth distance on phylogenetic trees

Steven Kelk, Georgios Stamoulis, and Taoyang Wu

Abstract

In this article we study the treewidth of the display graph, an auxiliary graph structure obtained from the fusion of phylogenetic (i.e., evolutionary) trees at their leaves. Earlier work has shown that the treewidth of the display graph is bounded if the trees are in some formal sense topologically similar. Here we further expand upon this relationship. We analyse a number of reduction rules which are commonly used in the phylogenetics literature to obtain fixed parameter tractable algorithms. In some cases (the subtree reduction) the reduction rules behave similarly with respect to treewidth, while others (the cluster reduction) behave very differently, and the behaviour of the chain reduction is particularly intriguing because of its link with graph separators and forbidden minors. We also show that the gap between treewidth and Tree Bisection and Reconnect (TBR) distance can be infinitely large, and that unlike, for example, planar graphs the treewidth of the display graph can be as much as linear in its number of vertices. On a slightly different note we show that if a display graph is formed from the fusion of a phylogenetic network and a tree, rather than from two trees, the treewidth of the display graph is bounded whenever the tree can be topologically embedded (“displayed”) within the network. This opens the door to the formulation of the display problem in Monadic Second Order Logic (MSOL). A number of other auxiliary results are given. We conclude with a discussion and list a number of open problems.

1 Introduction

Phylogenetic trees are used extensively within computational biology to model the history of a set of species $X$; the internal nodes represent evolutionary diversification events such as speciation [38]. Within the field of phylogenetics there has long been interest in quantifying the topological dissimilarity of phylogenetic trees and understanding whether this dissimilarity is biologically significant. This has led to the development of many incongruency measures such as Subtree Prune and Rergraft (SPR) distance and Tree Bisection and Reconnect (TBR) distance [1]. These measures are often NP-hard to compute. More recently such measures have also attracted attention because of their importance in methods which merge dissimilar trees into phylogenetic networks; phylogenetic networks are the generalization of trees to graphs [31].

Parallel to such developments there has been growing interest in the role of the graph-theoretic parameter treewidth within phylogenetics. Treewidth is an intensely studied parameter in algorithmic graph theory and it indicates, at least in an algorithmic sense, how far an undirected graph is from being a tree (see e.g. [8, 11, 12] for background). The enormous focus on treewidth is
closely linked to the fact that a great many NP-hard optimization problems become (fixed parameter) tractable on graphs of bounded treewidth [19]. A seminal paper by Bryant and Lagergren [16] linked phylogenetics to treewidth by demonstrating that, if a set of trees (not necessarily all on the same set of taxa $X$) can simultaneously be topologically embedded within a single “supertree” - a property known as compatibility - then an auxiliary graph known as the display graph has bounded treewidth. Since this paper a small but growing number of papers at the interface of graph theory and phylogenetics have explored this relationship further. Much of this literature focuses on the link between compatibility and (restricted) triangulations of the display graph (e.g. [19, 20, 41]), but more recently the algorithmic dimension has also been tentatively explored [6, 27, 32]. In the spirit of the original Bryant and Lagergren paper, which used heavy meta-theoretic machinery to derive a theoretically efficient algorithm for the compatibility problem, Kelk et al. [33] showed that the treewidth of the display graph of two trees is linearly bounded as a function of the TBR distance (equivalently, the size of a Maximum Agreement Forest - MAF [1]) between the two trees, and then used this insight to derive theoretically efficient algorithms for computation of many different incongruency measures. In this article it was empirically observed that in practice the treewidth of the display graph is often much smaller than the TBR distance (and thus also of the many incongruency measures for which TBR is a lower bound). This raised two natural questions. First, in how far can this apparently low treewidth be exploited to yield genuinely practical dynamic programming algorithms running over low-width tree decompositions? There has been some progress in this direction in the compatibility literature (notably, [6]) but there is still much work to be done. Second, how exactly does the treewidth of the display graph behave, both in the sense of extremal results (e.g. how large can the treewidth of a display graph get?) and in the sense of understanding when and why the treewidth differs significantly from measures such as TBR.

Here we focus primarily on the second question. We start by analyzing how reduction rules often used in the computation of incongruency measures impact upon the treewidth of the display graph. Not entirely surprisingly the common pendant subtree reduction rule [1] is shown to preserve treewidth. The cluster reduction [5, 35, 14], however, behaves very differently for treewidth than for many other incongruency measures. Informally speaking, if both trees can be split by deletion of an edge into two subtrees on $X'$ and $X''$, many incongruency measures combine additively around this common split, while treewidth behaves (up to additive terms) like the maximum function. We use this later in the article to explicitly construct a family of tree pairs such that the treewidth of the display graph is 3, but the TBR distance of the trees (and their MP distance - a function. We use this later in the article to explicitly construct a family of tree pairs such that the treewidth of the display graph is 3, but the TBR distance of the trees (and their MP distance - a measure based on the phylogenetic principle of parsimony [24, 36, 32]) grows to infinity. The third reduction rule we consider is the chain rule, which collapses common caterpillar-like regions of the trees into shorter structures. For incongruence measures it is often the case that truncation of such chains to $O(1)$ length preserves the measure [11, 15, 46], although sometimes the weaker result of truncation to length $f(k)$ [44, 42] (for some function that depends only on the incongruency parameter $k$) is the best known. We show that truncation of common chains to length $f(tw)$, where $tw$ is the treewidth of the display graph, indeed preserves treewidth; this uses asymptotic results on the number of vertices and edges in forbidden minors for treewidth. Proving that truncation to $O(1)$-length preserves treewidth remains elusive; we prove the intermediate result that truncation to length 2 can cause the treewidth to decrease by at most 1. The case when the chain is not a separator of the display graph seems to be a particularly challenging bottleneck in removing the “−1” term from this result. Although intuitively reasonable, it remains unclear whether truncation to length $O(1)$ is treewidth-preserving, for any universal constant.

In the next section we adopt a more structural perspective. We show that, given an arbitrary (multi)graph $G$ on $n$ vertices with maximum degree $k$, one can construct two unrooted binary trees $T_1(G)$ and $T_2(G)$ such that their display graph $D = D(T_1(G), T_2(G))$ has at most $O(nk)$ vertices and edges and $G$ is a minor of $D$. We combine this with the known fact that cubic expanders (a special family of 3-regular graphs) on $n$ vertices have treewidth $Ω(n)$ to yield the result that display graphs on $n$ vertices can also (in the worst case) have treewidth linear in $n$. This contrasts, for example, with planar graphs on $n$ vertices which have treewidth at most $O(\sqrt{n})$ [20]. We also show how a more specialized construction can be used to embed arbitrary grid minors [17] into
display graphs with a much smaller inflation in the number of vertices and edges.

Moving on, we then switch to the topic of phylogenetic networks. In our context, networks can be considered to be connected undirected graphs whose internal nodes all have degree 3 and whose leaves are bijectively labelled by a set of labels \( X \). Due to the interpretation of phylogenetic networks as species networks that contain multiple embedded gene trees, a major algorithmic question in that field is to determine whether a network displays (i.e., topologically embeds) a tree \( T \). Here we show that constructing a display graph from a network and a tree (rather than two trees) also has potential applications. Specifically, we show that if \( N \) displays \( T \) the display graph of \( N \) and \( T \) has bounded treewidth (as a function of the treewidth of \( N \) or, alternatively, as a function of the reticulation number of \( N \)). This then allows us to pose the question “does \( N \) display \( T \)?” in Monadic Second Order Logic (MSOL) which yields a logical-declarative version of earlier, combinatorial fixed parameter tractability results. This once again shows that the flexibility of Courcelle’s Theorem in the context of phylogenetics; the details of the MSOL formulation are technical and are deferred to the appendix. For completeness we show that treewidth alone is not sufficient to distinguish between YES and NO instances of the algorithmic question in that field is to determine whether a network displays or, alternatively, as a function of the reticulation number of \( N \). This then allows us to pose the question “does \( N \) display \( T \)” in Monadic Second Order Logic (MSOL) which yields a logical-declarative version of earlier, combinatorial fixed parameter tractability results. This once again shows that the flexibility of Courcelle’s Theorem in the context of phylogenetics; the details of the MSOL formulation are technical and are deferred to the appendix. For completeness we show that treewidth alone is not sufficient to distinguish between YES and NO instances of the display problem: we show a network \( N \) and a tree \( T \) such that \( N \) does not display \( T \), but the treewidth of \( N \) does not increase when merged into a display graph with \( T \).

In the last two mathematical sections of the paper we prove that, if two trees have TBR distance 1, or MP-distance 1, then the treewidth of their display graph is 3. However, the converse certainly does not hold: we construct the aforementioned “infinite gap” examples where the display graph has treewidth 3 but both TBR distance and MP-distance spiral off to infinity.

Finally, we reflect on the wider context of these results and discuss a number of open problems.

In conclusion, we observe that for (algorithmic) graph theorists the interface between treewidth and phylogenetics continues to yield many new questions which will likely require a new “phylo-algorithmic” graph theory to be answered. For phylogeneticists the appeal remains structural-algorithmic: can we convert the apparently low treewidth of display graphs into competitive, or even superior, algorithms for computation of incongruency measures?

### 2 Preliminaries

An unrooted binary phylogenetic tree \( T \) on a set of leaf labels (known as taxa) \( X \) is an undirected tree where all internal vertices have degree three and the leaves are bijectively labeled by \( X \). If we (exceptionally) allow some internal vertices of \( T \) to have degree two, then we call these vertices roots (abusing slightly the usual root meaning). Similarly, an unrooted binary phylogenetic network \( N \) on a set of leaf labels \( X \) is a simple, connected, undirected graph that has \( |X| \) degree-1 vertices that are bijectively labeled by \( X \) and any other vertex has degree 3. The reticulation number \( r(N) \) of \( N \) is defined as \( r(N) := |E| - (|V| - 1) \), i.e., the number of edges we need to delete from \( N \) in order to obtain a tree that spans \( V \). A network \( N \) with \( r(N) = 0 \) is simply an unrooted phylogenetic tree. When it is understood from the context we will often drop the prefix “unrooted binary phylogenetic” for brevity.

Let \( Y \subseteq X \). Then, for a tree \( T \) we denote by \( T[Y] \) the tree which is obtained by forming a minimal subgraph \( T' \) of \( T \) that spans all leaves labeled by \( Y \), and suppressing any vertices of degree 2.

Let \( T_1, T_2 \) be two trees (or networks, or combination of the trees and networks), both on the same set of leaf labels \( X \). The display graph of \( T_1, T_2 \), denoted by \( D(T_1, T_2) \), is formed by identifying vertices with the same leaf label and forming the disjoint union of these two trees. This can be extended in a straightforward way to more than 2 trees/networks.

If \( N \) is a network and \( T \) a tree on a common set of taxa \( X \) we say that \( N \) displays \( T \) if there exists a subtree \( N' \) of \( N \) that is a subdivision of \( T \). In other words, \( T \) can be obtained by a series of edge contractions on a subgraph \( N' \) of \( N \). \( N' \) is a minimal connected subgraph of \( N \) that spans all the taxa \( X \). We say that \( N' \) is an image of \( T \). We can easily see that every vertex of \( T \) is mapped to a vertex of \( N' \), and that edges of \( T \) potentially map to paths in \( N' \), leading us to the following observation (see also [16]):

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Observation 2.1. If an unrooted binary network $N$ displays an unrooted binary tree $T$, where both are defined on a common set of leaves (taxa) $X$, then there exists a surjection $f$ from a subtree $N'$ of $N$ to $T$ such that: (1) $f(t) = t, \forall t \in X$, (2) the subsets of $V(N')$ induced by $f^{-1}$ are mutually disjoint, and each such subset induces a connected subtree of $V(N')$, and (3) $\forall \{u, v\} \in E(T), \exists \{\alpha, \beta\} \in E(N') : f(\alpha) = u$ and $f(\beta) = v$.

This observation will be crucial when we study the treewidth of $D(N, T)$ as a function of the treewidth of $N$. We say that two (or more) trees are compatible if there exists another tree on $X$ that displays all the trees. Note that for two unrooted binary phylogenetic trees on the same set of labels $X$ compatibility is simply equivalent to the existence of a label-preserving isomorphism between the two trees.

A tree decomposition of an undirected graph $G = (V, E)$ is a pair $(B, \mathbb{T})$ where $B = \{B_1, \ldots, B_q\}$, $B_i \subseteq V(G)$, is a collection of bags and $\mathbb{T}$ is a tree whose nodes are the bags $B_i$ satisfying the following three properties:

1. $\forall_{i=1}^q B_i = V(G)$;
2. $\forall e = \{u, v\} \in E(G), \exists B_i \in B$ s.t. $\{u, v\} \subseteq B_i$;
3. $\forall v \in V(G)$ all the bags $B_i$ that contain $v$ form a connected subtree of $\mathbb{T}$.

The width of $(B, \mathbb{T})$ is equal to $\max_{i=1}^q |B_i| - 1$. The treewidth of $G$ is the smallest width among all possible tree decompositions of $G$. For a graph $G$, we denote $\text{tw}(G)$ the treewidth of $G$. Given a tree decomposition $\mathbb{T}$ for some graph $G$, we denote by $V(\mathbb{T})$ the set of its bags and by $E(\mathbb{T})$ the set of its edges (connecting bags). Property (tw3) is also known as running intersection property.

We note that the treewidth of any graph $G$ is at most $|V(G)| - 1$: consider a bag with all vertices of $G$. This is a valid tree decomposition of width $|V(G)| - 1$. Thus the treewidth is always a finite parameter for any graph.

Another, equivalent, definition of treewidth is based on chordal graphs. We remind that a graph $G$ is chordal if every induced cycle in $G$ has exactly three vertices. The treewidth of $G$ is the minimum, ranging over all chordal completions of $G$ (we add edges until $G$ becomes a chordal graph), of the size of the maximum clique in $c(G)$ minus one. Under this definition, each bag of a tree decomposition of $G$ naturally corresponds to a maximal clique in the chordal completion of $G$.

For a graph $G = (V, E)$ and an edge $e = \{u, v\} \in E(G)$, the deletion of $e$ is the operation which simply deletes $e$ from $E(G)$ and leaves the rest of the graph $G$ the same. The contraction of $e$, denoted $G/e$, is the operation where edge $e$ is deleted and its incident vertices $u, v$ are identified. We say that a graph $H$ is a minor of another graph $G$ if $H$ can be obtained by repeated applications of edge deletions and/or edge contraction, followed possibly by deleting isolated vertices, on $G$.

The order that these operations are performed does not matter and it will result always $H$ in any performed order.

## 2.1 Phylogenetic distances and measures

Several distances have been proposed to measure the incongruence between two (or more) phylogenetic trees on the same set of taxa. The high-level problem is to propose a measure that quantifies the dissimilarity of a given set of phylogenetic trees.

The most relevant distances for the purpose of this article are the so-called Tree Bisection and Reconnect distance and the Maximum Parsimony Distance which are defined in the following.

Given an unrooted binary phylogenetic tree $T$ on $X$, a Tree Bisection and Reconnect (TBR) move is defined as follows \footnote{Equivalently we can say that $H$ is a minor of $G$ if $H$ can be obtained by vertex deletions, edge deletions and edge contractions in $G$.}: (1) we delete an edge of $T$ to obtain two subtrees $T'$ and $T''$. (2) Then we select two edges $e_1 \in T', e_2 \in T''$, subdivide them with two new vertices $v_1$ and $v_2$ respectively, add an edge from $v_1$ to $v_2$, and suppress all vertices of degree 2. In case either $T'$ or
A single leaf, then the new edge connecting $T'$ and $T''$ is incident to that leaf. Let $T_1, T_2$ be two unrooted binary phylogenetic trees on the same set of leaf-labels. The TBR-distance from $T_1$ to $T_2$, denoted $d_{TBR}(T_1, T_2)$, is the minimum number of TBR moves required to transform $T_1$ into $T_2$ (or, equivalently, $T_2$ to $T_1$).

Computing the TBR-distance is essentially equivalent to the Maximum Agreement Forest (MAF) problem: Given an unrooted binary phylogenetic tree on $X$ and $X' \subseteq X$ we let $T(X')$ denote the minimal subtree that connects all the elements in $X'$. An agreement forest of two unrooted binary trees $T_1, T_2$ on $X$ is a partition of $X$ into non-empty blocks $\{X_1, \ldots, X_k\}$ such that (1) for each $i \neq j$, $T_1(X_i)$ and $T_1(X_j)$ are node-disjoint and $T_2(X_i)$ and $T_2(X_j)$ are node-disjoint, (2) for each $i$, $T_1|X_i = T_2|X_i$. A maximum agreement forest is an agreement forest with a minimum number of components (such that it maximizes the agreement), and this minimum is denoted $d_{MAF}(T_1, T_2)$. In 2001 it was proven by Allen and Steel that $d_{MAF}(T_1, T_2) = d_{TBR}(T_1, T_2) + 1$.

In order to define the Maximum Parsimony Distance [24][30][32] between two unrooted binary phylogenetic trees $T_1, T_2$ both on $X$, we need first to define the concept of character on $X$ which is simply a surjection $f : X \rightarrow C$ where $C$ is a set of states. Given a tree $T$ on $X$, and a character $f$ also on $X$, an extension of $f$ to $T'$ is a mapping $f'$ from $V(T(T'))$ to $C$ such that $f'(v) = f(v)$, $\forall v \in X$. An edge $e = \{u, v\}$ with $(u) \neq f'(v)$ is known as a mutation induced by $f'$. The minimum number of mutations ranging over all extensions $f'$ of $f$ is called the parsimony score of $f$ on $T$ and is denoted by $l_f(T)$. Given two trees $T_1, T_2$ their maximum parsimony distance $d_{MP}(T_1, T_2)$ is equal to $\max_f |l_f(T_1) - l_f(T_2)|$.

Both the TBR and MP distances are NP-hard to compute and they are also metric distances i.e., they satisfy the four axioms of metric spaces: (a) non-negativity, (b) identity of indiscernibles (c) symmetry and (d) triangle inequality.

Given an unrooted binary phylogenetic tree $T$ and a distance $d$ (such as TBR and MP), we define the unit ball or the unit neighborhood of $T$ under $d$ to be $u_d(T) = \{T' : d(T, T') = 1\}$ i.e., the set of all trees $T'$ that are within distance one from $T$ under the distance $d$. Such neighborhoods are important because usually they are building blocks of “local search” algorithms that try to find trees that optimize some particular criterion. Moreover, the diameter $\Delta_d(d)$ is defined as the maximum value $d$ taken over all pairs of phylogenetic trees with $n$ taxa (see [39] Section 2.5) for a recent review on various results on the unit ball and the diameter of several tree rearrangement metrics.

3 Treewidth Distance

The main purpose of this manuscript is to define and study the properties of the treewidth distance between two phylogenetic trees. As mentioned in the introduction, the study of treewidth in the context of phylogenetics was triggered by the pioneering work of Bryant & Lagergren [16] who proved that a necessary condition for a set of trees (not necessarily on the same set of taxa) to be compatible, is that their display graph has bounded treewidth. They used this insight to leverage a (theoretical) positive algorithmic result. Here we are interested in the question: in how far does the treewidth of the display graph itself function directly as a measure of phylogenetic incongruence? Hence the following natural definition:

Definition 3.1 (Treewidth Distance). Given two unrooted binary phylogenetic trees $T_1, T_2$, both on the same set of leaf labels $X$, where $|X| \geq 3$, their treewidth distance is defined to be $tw(D(T_1, T_2)) - 2$ and is denoted as $d_{tw}(T_1, T_2)$.

It is easy to see that for two unrooted binary phylogenetic trees $T_1, T_2$ we have that $d_{tw}(T_1, T_2) \geq 0$, for $|X| \geq 3$. This is a direct consequence of the fact that if $|X| \geq 3$ then the display graph contains at least one cycle and hence $tw(D(T_1, T_2)) \geq 2$. If $|X| < 3$ then $T_1, T_2$ are trivially isomorphic (they are either a single edge or a single vertex) and it does not make much sense to define a distance between such trees. So we can discard these boundary cases without any loss of generality in our study. (Of course, the treewidth of the display graph is still well-defined.
of that it was shown in [33] that $\text{tw}(D(T_1, T_2)) = 2$ for two unrooted binary phylogenetic trees on $X$, $|X| \geq 3$, if and only if $T_1$ and $T_2$ are compatible (see e.g. [27]). As mentioned earlier compatibility in this context is the same as label-preserving isomorphism, so it is natural to speak of equality and write $T_1 = T_2$. Note that it was shown in [33] that $\text{tw}(D(T_1, T_2)) \leq d_{\text{MAF}}(T_1, T_2) + 1 = d_{\text{TBR}}(T_1, T_2) + 2$, and hence $d_{\text{tw}}(T_1, T_2) \leq d_{\text{TBR}}(T_1, T_2)$.

We remark that, because computation of treewidth is fixed parameter tractable [10, 22], so too is $d_{\text{tw}}$. As we discuss in the final section of the paper it is not known whether $d_{\text{tw}}$ can be computed in polynomial time, but ongoing research efforts by the algorithmic graph theory community to compute treewidth efficiently in practice (see e.g. [10]) will naturally strengthen the appeal of $d_{\text{tw}}$ as a phylogenetic measure.

An easy, but important, observation that we will use extensively in the rest of the manuscript is that treewidth (and treewidth distance) are unchanged by edge subdivision and degree-2 vertex suppression operations - with one trivial exception. We say that a graph is a unique triangle graph if it contains exactly one cycle such that this cycle has length 3 and at least one of the cycle suppression operations - with one trivial exception. We say that a graph is a unique triangle graph if it contains exactly one cycle such that this cycle has length 3 and at least one of the cycle vertices has degree 2. A unique triangle graph has treewidth 2.

Given a graph $G = (V,E)$, let $e = \{u_1, u_2\} \in E$ be any edge of $G$ and $v$ be any degree-2 vertex of $G$ (if there exists any) with neighbors $v_1, v_2$. We define the following two operations:

Subdivision of an edge $e$: This defines a new graph $G' = (V', E')$ where $V' = V \cup \{w\}, w \notin V$ and $E' = (E \setminus \{e\}) \cup (\{u_1, w\}, \{w, u_2\})$.

Suppression of a degree-2 vertex $v$: This defines a new graph $G'' = (V'', E'')$ where $V'' = V \setminus \{v\}, E'' = E \setminus (\{v_1, v\} \cup \{v, v_2\}) \cup \{v_1, v_2\}$.

Observation 3.1. Let $G = (V,E)$ be a graph, which is not a unique triangle graph and let $e = \{u_1, u_2\} \in E$ be any edge of $G$ and $v$ be any degree-2 vertex of $G$ (if any) with neighbors $v_1, v_2$. Consider the following two graphs:

1. $G' = (V', E')$ where we obtain $G'$ after a single application of the edge subdivision step on $e \in E(G)$, and

2. $G'' = (V'', E'')$ where $G''$ is obtained from $G$ after suppressing a degree-2 vertex $v \in V(G)$.

Then we have that: $\text{tw}(G) = \text{tw}(G') = \text{tw}(G'').$

Proof. For the subdivision of an edge case, let $G'$ be the resulting graph after the subdivision of some edge $e$. It is immediate that the treewidth of $G'$ is at least $q = \text{tw}(G)$ since $G$ is a minor of $G'$ and treewidth is non-increasing under minor operations. To show that the treewidth cannot increase we argue as follows. If $G$ is a tree, then $G'$ is also a tree and $\text{tw}(G) = \text{tw}(G') = 1$ and we are done. So, we assume that $G$ is not a tree so $q \geq 2$. Take a bag $B$ of an optimal tree decomposition $T$ of $G$ with largest bag size at least 3, which contains the endpoints $u_1, u_2$ of $e$. Create a new bag $B' \notin B(T) : B' = \{u_1, u_2, w\}$ and attach it to $B$. This operation cannot increase the treewidth of the tree decomposition and it is immediate that the new tree decomposition is a valid one for $G'$.

Now we will handle the degree-2 vertex suppression operation. This can be simulated by two edge contraction operations, which are minor operations, so the treewidth cannot increase. In the other direction (i.e. proving that the treewidth cannot decrease), we see that if $G$ is a tree the treewidth is immediately preserved. If $G$ is not a tree, let $G''$ be the resulting graph after a single degree-2 vertex suppression operation on a vertex $v$ with neighbors, in $G$, $v_1, v_2$ such that in $G'' \{v_1, v_2\} \in E''$. Take an optimal tree decomposition of $G''$, let this be $T''$. By assumption that $G$ is not a tree and that $G$ is not a unique triangle graph, $G''$ contains at least one cycle. Hence, $\text{tw}(G'') \geq 2$ i.e., the size of the largest bag is at least 3. In $T''$, locate a bag $A$ that contains the pair of vertices $v_1, v_2$. Such a bag must exists by definition. Create a new bag $A' = \{v_1, v, v_2\}$ and attach it to $A$ thus creating a new tree decomposition $T'''$. It is immediate that $T'''$ is a valid tree decomposition for $G$ with width the same as the width of $T''$, and the claim follows.

\[ \square \]
Recall that if two unrooted binary trees $T_1, T_2$ are incompatible, then $tw(D(T_1, T_2)) \geq 3$, so the display graph cannot be a unique triangle graph. Hence:

**Observation 3.2.** Let $T_1$ and $T_2$ be two unrooted binary phylogenetic trees on the same set of taxa $X$. If $T_1$ and $T_2$ are incompatible, then the following operations can be applied arbitrarily to $D(T_1, T_2)$ without altering its treewidth: suppression of degree-2 vertices, and subdivision of edges.

In subsequent sections we will often use Observation 3.2 to (in particular) suppress some or all of the taxa in the display graph without altering its treewidth.

### 3.1 Metric properties of $d_{tw}$

Given the definition of the treewidth distance, it is tempting to see if indeed such a distance is a metric distance e.g., it satisfies the four axioms of metric distances. We already argued that it satisfies the non-negativity condition and trivially it satisfies the identity of indiscernibles because $T_1 = T_2 \iff d_{tw}(T_1, T_2) = 0$ as demonstrated in the previous discussion. The symmetry condition is also trivially satisfied because $D(T_1, T_2) = D(T_2, T_1)$ i.e., the display graph is identical in both cases and thus has the same treewidth.

The only case left is to see if $d_{tw}$ satisfies the triangle inequality property: given three unrooted binary phylogenetic trees $T_1, T_2, T_3$ all on $X$ is it the case that $d_{tw}(T_1, T_3) \leq d_{tw}(T_1, T_2) + d_{tw}(T_2, T_3)$? Unfortunately, this is false as shown in Figure 1. By using appropriate software, for example QuickBB [26], we can see that $d_{tw}(T_1, T_2) = 1, d_{tw}(T_2, T_3) = 2$ and $d_{tw}(T_1, T_3) = 4 > d_{tw}(T_1, T_2) + d_{tw}(T_2, T_3)$. We remark that, although mathematically disappointing, the absence of the triangle inequality is not a great hindrance in practice. Some other well-known phylogenetic measures, such as hybridization number, also do not obey the triangle inequality [37].
4 The treewidth of the display graph under phylogenetic reduction rules

In this section we investigate the effect of several common phylogenetic reduction rules on the treewidth of the display graph. We will study the following three rules: (i) common pendant subtree, (ii) common chain and (iii) cluster reduction rule. Such rules constitute the building block of many FPT algorithms for computing phylogenetic distances. We will see that the three reduction rules behave somewhat differently with respect to the treewidth of the display graph.

In particular, we will show how the subtree reduction operation, where compatible subtrees are collapsed to a single taxon, preserves the treewidth of the display graph. For the second case, the collapsing of a common chain (a maximal “caterpillar-like” region) in both trees down to length 2, could potentially decrease the treewidth of the display graph by at most one. On the other hand we show that if we collapse common chains down to length that is a function of the treewidth of the display graph, then we preserve the treewidth. The open question here is if this gap can be understood better i.e., if we can collapse the common chains to a constant length and preserve the treewidth. Finally, we investigate the cluster reduction rule where clusters are formed if in each tree there is an edge (called a common split) the deletion of which results that both trees are split into two subtrees on $X'$ and $X''$. We will see that the treewidth of the display graph is (up to additive terms) equal to the maximum of the treewidth of the two clusters. We note that this is in contrast to other phylogenetic distance measure which usually behave additively with respect to the distances of the two clusters.

It is well-known that compatibility is preserved under the described reductions. For this reason we will assume that the two input trees $T_1, T_2$ on $X$ are not compatible. This immediately gives us a lower bound on the cardinality of the taxon set, namely $|X| \geq 3$ since any two trees on 2 taxa are by definition compatible (both trees are single edges). Moreover the treewidth of their display graph is at least 3.

We start with the common pendant subtree rule.

4.1 Subtree Reduction Rule

Let $T_1, T_2$ be two unrooted binary phylogenetic trees on the same set of taxa $X$. A subtree $T$ is called a pendant subtree of $T_i$, $i \in \{1, 2\}$ if there exists an edge $e$ the deletion of which detaches $T$ from $T_i$. A subtree $T$, which induces a subset of taxa $X' \subseteq X$, is called common pendant subtree of $T_1$ and $T_2$ if $T_1|X' = T_2|X'$ and if the additional following condition holds:

> Let $e_i$ be the edge of tree $T_i$, $i \in \{1, 2\}$ the deletion of which detaches $T$ from $T_i$ and let $v_i \in e_i, i \in \{1, 2\}$ be the endpoint of $e_i$ “closest” to the taxon set $X'$. Let’s say that we root each $T_i|X'$ at $v_i$, thus inducing a rooted binary phylogenetic tree $(T_i|X')^o$ on $X'$. We require that $(T_1|X')^o = (T_2|X')^o$.

The previous condition formalizes the idea that the point of contact of the pendant subtree with the rest of the tree should explicitly be taken into account when determining whether a pendant subtree is common. (This is consistent with the definition of common pendant subtree elsewhere in the literature.)

In the following we will show that the treewidth of the display graph $D(T_1, T_2)$ of the two phylogenetic trees $T_1, T_2$ is preserved under the common pendant subtree reduction rule:

Common Pendant Subtree (CPS) reduction: Find a maximal common pendant subtree in $T_1, T_2$. Let $T$ be such a common subtree with at least two taxa and let $X_T$ be its set of taxa. Clip $T$ from $T_1$ and $T_2$. Attach a single label $x$ not $X$ in place of $T$ on each $T_i$. Set $X := (X \setminus X_T) \cup \{x\}$ and let $T'_1, T'_2$ be the two resulting trees and $D(T'_1, T'_2) = D'$ be their resulting display graph.

**Theorem 4.1.** Suppose that $T_1$ and $T_2$ are a pair of incompatible unrooted binary phylogenetic trees on $X$ and the pair $(T'_1, T'_2)$ is obtained from $(T_1, T_2)$ by one application of the Common Pendant Subtree reduction. Then $d_{tw}(T_1, T_2) = d_{tw}(T'_1, T'_2)$. 

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Figure 2: An illustration of the concept of common pendant subtree. If \( X' = \{a, b, c, d\} \) we see that \( T_1|X' = T_2|X' \) (because of the suppression of the parent of a in \( T_2 \)) but this is not true if we take into account the “root” location (in bold squares). Here both \( \{e, f\} \) and \( \{c, d\} \) induce maximal common pendant subtrees.

\[
\begin{align*}
\text{Figure 3: Reduction of a common cherry } \{x, y\} \text{ as described in the proof of Theorem 4.1.}
\end{align*}
\]

Proof. A cherry is simply a size-2 subset of taxa \( \{x, y\} \) that have a common parent, and a cherry \( \{x, y\} \) is common if it is in both trees. Let us first consider the case that the pair \( \{T'_1, T'_2\} \) is obtained from a subtree reduction on a common cherry \( \{x, y\} \) whose parent is \( u_i \) in \( T_i \) and the parent of \( u_i \) is \( v_i \), \( i = 1, 2 \). Then the display graph \( D' = D(T'_1, T'_2) \) is obtained from \( D = D(T_1, T_2) \) by replacing the vertex subset \( \{u_1, x, y, u_2\} \) with a single vertex \( r \) which is connected to \( v_1 \) and \( v_2 \) and these are the only neighbors of \( r \) (see Figure 3). Note that \( v_1 \neq v_2 \) and \( \{v_1, v_2\} \) is not an edge in \( D \) because \( T_1 \) and \( T_2 \) are incompatible. \( D' \) can be obtained from \( D \) by applying Observation 3.2: suppress \( x \), suppress \( y \) (and delete the created multi-edge) and then suppress \( u_2 \). Hence \( tw(D') = tw(D) \). (The surviving vertex \( u_1 \) assumes the role of \( r \), since labels are irrelevant to treewidth.) For the more general case: it is easy to see that applying the CPS reduction rule to a subtree that is not a cherry, can be achieved by iteratively applying the CPS reduction to common cherries. This is correct because collapsing a common cherry cannot make two incompatible trees compatible. The result follows.

\[
\begin{align*}
4.2 \text{ Chain Reduction Rule}
\end{align*}
\]

Let \( T \) be an unrooted binary tree on \( X \). For each taxon \( x_i \in X \), let \( p_i \) be its unique parent in \( T \). Let \( C = (x_1, x_2, \ldots, x_t) \) be an ordered sequence of taxa and let \( P = (p_1, p_2, \ldots, p_t) \) be the corresponding ordered sequence of their parents, If \( P \) is a path in \( T \) and the \( p_i \) are all mutually distinct then \( C \) is called a chain of length \( t \). A chain \( C \) is a common chain of two binary phylogenetic trees \( T_1, T_2 \) on a common set of taxa, if \( C \) is a chain in each one of them. See Figure 4 for an example. Note that our insistence that the \( p_i \) are mutually distinct differs from
the definition of chain encountered elsewhere in the literature, in which \( p_1 = p_2 \) and \( p_{i-1} = p_i \) is permitted. However, our more restrictive definition of chain is only a very mild restriction, since a chain of length \( t \) under the traditional definition yields a chain of length at least \((t - 4)\) under our definition. Our definition ensures that in both trees neither end of the chain is a cherry, which avoids a number of annoying (and uninteresting) technicalities. Let \( v_i \) denote the parent of \( x_1 \) in \( T_1 \) and \( u_i \) its parent in \( T_2 \).

We now define the common chain reduction rule.

**Common \( d \)-Chain Reduction Rule (\( d \)-cc):** Let \( T_1, T_2 \) be two incompatible unrooted binary phylogenetic trees on a common set of taxa \( X \). Let \( C' \) be a common chain of \( T_1, T_2 \) of length \( t \geq 3 \). On each \( T_i, i \in \{1, 2\} \) clip the chain down to length \( d \in \{2, \ldots, t-1\} \) as follows: Keep the first \([d/2]\) and the last \([d/2]\) taxa and delete all the intermediate ones (i.e., delete all the taxa with indexes in \( \{[d/2]+1, \ldots, t-[d/2]\} \)), suppress any resulting vertex of degree 2 and delete any resulting unlabelled leaves of degree 1. Let \( C' \) be the new clipped common chain on both trees.

Observe that \( C' \) has \([d/2]+t-(t-[d/2])=[d/2]+[d/2]=d\) taxa and that in each \( T_1, T_2 \) the parents of the taxa \( x_{[d/2]}, x_{-[d/2]+1} \) are connected by an edge. Let \( D(T_1, T_2) = D \) be the display graph of \( T_1, T_2 \) and \( D'(T'_1, T'_2) = D' \) be the display graph of \( T'_1, T'_2 \) after the application of one chain reduction rule. Equivalently, \( D' \) can be obtained directly from \( D \) by deleting the \((t-d)\) pruned taxa and suppressing unlabelled degree-2 vertices. In fact, due to the fact that \( T_1, T_2 \) are incompatible (and thus so are \( T'_1, T'_2 \)) we can (by Observation \[B.3\]) safely suppress (in \( D \)) all the degree-2 nodes labelled by taxa in \( C' \), and (in \( D' \)) all the degree-2 nodes labelled by taxa in \( C' \), without altering the treewidth of \( D \) or \( D' \). Without loss of generality we assume that this suppression has taken place.

Observe that the part of \( D \) that corresponds to the common chain \( C \) now resembles a \( 2 \times t \) grid and in \( D' \) is a \( 2 \times d \) grid. For a common chain \( C \) of length \( t \), let \( g(C) \) be the corresponding \( 2 \times t \) grid in \( D \) and similarly define \( g(C') \) in \( D' \) for the clipped common chain of length \( d \).

Now, assume that we have an optimal tree decomposition \( T \) of \( D \) of width \( k \), i.e., the maximum bag size in \( T \) is \( k+1 \). First of all, by a standard minor argument, it is immediate that application of the cc-reduction rule cannot increase the treewidth: the resulting display graph \( D' \) is a minor of \( D \).

Our strategy will be as follows: Given an optimal tree decomposition \( T' \) for \( D' \), we will modify it to construct a tree decomposition for \( D \) that in the worst case has width at most \( tw(D') + 1 \), thus proving \( tw(D') \geq tw(D) - 1 = k - 1 \). (In some cases we will be able to prove the stronger result that \( tw(D) = tw(D') \)).

We distinguish two cases.

**Case 1:** *The common chain \( g(C) \) is a separator in \( D \).* In other words, deleting \( g(C) \) from \( D \) will result in two connected components. In this case we will show that clipping the common chain \( C \) down to length 2 by applying a 2-cc step preserves the treewidth of \( D \). We note that an application of a 2-cc step causes \( g(C) \) to resemble a \( C_4 \) in \( D' \), where as usual, \( C_4 \) is a cycle of length 4.

**Lemma 4.1.** Let \( T'_1, T'_2 \) be two incompatible unrooted binary phylogenetic trees that are obtained after a single application of the operation 2-cc(\( C \)) on \( T_1 \) and \( T_2 \) where \( g(C) \) is a separator in \( D(T_1, T_2) \). Then \( d_{tw}(T_1, T_2) = d_{tw}(T'_1, T'_2) \).

**Proof.** Let \( D \) be the display graph of \( T_1, T_2 \) and \( D' \) the display graph after we clipped the common chain \( C \) down to length 2 and let \( g(C') \) be the \( 2 \times 2 \) grid induced by the common chain in \( D' \). Remember that \( g(C') \) has 4 vertices \( \{v_1, u_1, v_2, u_2\} \) such that \( \{v_1, v_2\} \subset V(T_1) \) and \( \{u_1, u_2\} \subset V(T_2) \). Let \( T' \) be an optimal tree decomposition for \( D' \).

Consider the grid \( g(C') \) in \( D' \) corresponding to the clipped chain \( C' \) of length \( d = 2 \). We will expand \( g(C') \) inductively by first inserting the parents \( v_2, u_2 \) of the clipped taxon \( x_2 \) (and an edge between them): These two vertices will be inserted in the \( C_4 \) induced by \( \{v_1, v_2, u_1, u_2\} \). After the \( j \)-th step, \( j \leq t - d \), of this process, we will have retrieved the parents of taxa \( x_2, \ldots, x_{j+1} \).
Step \((j + 1)\) continues by expanding the current \(g(C')\) of length \(j + 2\) by inserting the parents \(v_{j+2}, u_{j+2}\) in the \(C_4\) induced by \(v_{j+1}, v_t, u_{j+1}, u_t\). We will show how, at each step, we can update the tree decomposition \(T'\), without increasing its width, so that the new one will be a valid tree decomposition for the updated display graph.

We will start by proving the base case. For this, we will find helpful the following claim about the structure of \(T'\).

**Claim 4.1.** There exists an optimal tree decomposition \(T''\) of \(D'\) such that \(T''\) contains two adjacent degree-2 bags \(A_1\) and \(A_2\) where \(A_1 = \{v_1, u_1, v_t\}\), \(A_2 = \{v_t, u_1, u_t\}\).

**Proof.** Observe that since \(g(C)\) is a separator in \(D\), then so is \(g(C')\) in \(D'\). In \(D'\) we delete the edges \(\{v_1, v_t\}\) and \(\{u_1, u_t\}\) and we obtain, wlog, two connected components \(D'_1\) and \(D'_2\) such that \(\{v_1, u_1\} \subset V(D'_1)\) and \(\{v_t, u_t\} \subset V(D'_2)\). Consider optimal tree decompositions \(t_1, t_2\) of \(D'_1, D'_2\) respectively. Note that \(\text{tw}(D'_1) \leq \text{tw}(D'), \text{tw}(D'_2) \leq \text{tw}(D')\) and \(\text{tw}(D') \geq 3\). Since \(\{v_1, u_1\} \in E(D'_1)\), there must be a bag \(B_1 \in V(t_1)\) that contains \(\{v_1, u_1\}\). Similarly, there must be a bag \(B_2 \in V(t_2)\) that contains \(\{v_t, u_t\}\). Attach to \(B_1\) a new bag \(A_1 = \{v_1, u_1, v_t\}\) and attach to \(B_2\) bag \(A_2 = \{v_t, u_1, u_t\}\) and join \(A_1, A_2\) by an edge to create a new tree decomposition \(T''\) for \(D'\); indeed, it is immediate to see that \(T''\) satisfies all the tree width conditions. Moreover, the width of this tree decomposition is \(\max(\text{tw}(D'_1), \text{tw}(D'_2), 2)\). Noting that \(3 \leq \text{tw}(D') \leq \max(\text{tw}(D'_1), \text{tw}(D'_2), 2) \leq \max(\text{tw}(D'_1), \text{tw}(D'_2)) \leq \text{tw}(D')\) it follows that it is an optimal tree decomposition of \(D'\).

\[\square\]

![Figure 4: An example of the inductive construction of Lemma 4.1](image)

We construct a new tree decomposition which facilitates the extra links added by increasing the length of \(g(C')\) by one, corresponding to adding the parents of the current missing taxon (in this case \(x_2\)). The grey edges are not in the display graph \(D'\) but they indicate the maximal cliques induced by the size-3 bags that we add in Lemma 4.1.

Given \(T''\) as described in the previous claim, delete bags \(A_1, A_2\) and consider the following set of bags: \(J_1 = \{v_1, v_2, u_1\}\), \(J_2 = \{v_2, u_1, u_2\}\), \(J_3 = \{v_2, v_t, u_2\}\) and \(J_4 = \{v_2, u_1, u_t\}\). Attach \(J_1\) to \(B_1\) (the bag that was adjacent to \(A_1\)) and \(J_4\) to \(B_2\) (the bag that was adjacent to \(A_2\)) and create a path of bags from \(J_1\) to \(J_4\). It is easy to argue that this is a valid tree decomposition \(D''\), defined as the display graph after the parents of \(x_2\) have been added; see Figure 4. First of all, for conditions (tw1) and (tw2) this is immediate by construction. Indeed, \(v_2\) belongs to \(J_1, J_2, J_3, J_4\), \(u_t\) belongs to \(J_2, J_3, J_4\). For (tw2) observe that the edges \(\{v_1, v_t\}, \{u_1, u_t\}\) are not present in \(g(C'')\) so we do not need to consider them. For the new edges we have that \(\{v_1, v_2\} \in J_1, \{u_1, u_2\} \in J_2, \{v_2, u_2\} \in J_3, \{v_2, v_t\} \in J_4\) and \(\{u_1, u_2\} \in J_4\). Also, by leveraging the explicit construction of \(T''\) (in particular: \(v_1, u_1 \notin B_1\) and \(u_1, v_t \notin B_2\)) we can easily verify that (tw3) is true for \(T''\). Finally, the width of this new tree decomposition is no greater than the width of \(T''\) because we only add bags of size 3 and, by construction, \(T''\) already contains at least one bag of size 4.

This proves that, for the base case, the treewidth of the new display graph remains unchanged. For the \(j\)-th step, we apply the arguments above where as \(A_1\) and \(A_2\) we use the bags \(\{v_j, u_j, v_t\}\) and \(\{v_t, u_j, u_t\}\) which by induction exist and are adjacent. Delete them and replace them with the following chain of bags, as before: \(J_1 = \{v_j, v_{j+1}, u_t\}\), \(J_2 = \{v_{j+1}, u_j, u_{j+1}\}\), \(J_3 = \{v_{j+1}, v_t, u_{j+1}\}\) and \(J_4 = \{v_t, u_{j+1}, u_t\}\). We continue until we add the last missing piece of \(g(C)\).

\[\square\]

**Case 2: The common chain \(C\) is not a separator in \(D\).** We say that the \(2 \times t\) grid \(g(C)\) in \(D\) that corresponds to the common chain \(C\) is not a separator if the deletion of \(g(C)\) from \(D\)
leaves the display graph $D$ connected. See Figure 1 as an example of such a case and Figure 2 for an example of their display graph. It is easy to observe that if $g(C)$ is not a separator in $D$ then neither is $g(C')$ in $D'$. We will show that in this case the treewidth of $D$ after clipping $g(C)$ down cannot decrease by more than a unit term.

**Lemma 4.2.** Let $T'_1, T'_2$ be the two incompatible unrooted binary phylogenetic trees that are obtained after a single application of the $d$-cc reduction rule with $d = 2$ on $T_1$ and $T_2$ on a common chain $C$ such that $g(C)$ is not a separator in $D(T_1, T_2)$. Then we have $d_{tw}(T'_1, T'_2) \leq d_{tw}(T_1, T_2) \leq d_{tw}(T'_1, T'_2) + 1$.

**Proof.** As in the separator case, we will alter the tree decomposition $T''$ for $D'$ to obtain a new tree decomposition $T'''$ that will be valid for $D''$ (the display graph with the expanded $2 \times 3$ grid $g(C')$) and which has width at most $tw(D') + 1$. Then, we will argue how we can increase the length of this $2 \times 3$ grid $g(C')$ to any arbitrary length without further increasing the width. So, the +1 term might be incurred only when we transfer from the $2 \times 2$ to the $2 \times 3$ grid but when we retrieve the rest of $C$ we do not have to pay again in terms of increasing the width. The reason for this is that in the transition from length 2 to 3 we guarantee that the tree decomposition for the updated situation has a certain invariant property that we can exploit in order to further increase the length of the grid “for free.” The initial tree decomposition might however not possess this property and we have to pay potentially a unit increase in the width of the decomposition to establish it.

Consider the grid $g(C')$ in $D'$ corresponding to the clipped chain $C'$ of length $d = 2$. It contains 4 vertices: $\{v_1, v_t\} \in V(T_1)$ and $\{u_1, u_t\} \in V(T_2)$. As in the separator case we will expand this $g(C')$ inductively by first inserting the parents $v_2, u_2$ of the clipped taxon $x_2$ and after the $j$-th step, $j \leq t - d$ of this process we will have already retrieved the parents of taxa $x_2, \ldots, x_{j+1}$. The $(j + 1)$-th step proceeds by expanding the current $g(C'')$ of length $j + 2$ by inserting the parents $v_{j+2}, u_{j+2}$ in the $C_4$ induced by $v_{j+1}, v_t, u_{j+1}, u_t$.

For the base case, we will distinguish three cases. In all cases we assume without loss of generality that $T'$ is an optimal small tree decomposition of $D'$. A small tree decomposition is a tree decomposition where no bag in the tree decomposition is a subset of another (which thus also excludes the possibility of having two copies of the same bag). It is well-known that there exist optimal tree decompositions that are also small.

$|V(D')| > 4$ and $\exists$ bag $B \in V(T')$ such that $B$ contains $\{v_1, v_t, u_1, u_t\}$. As a first step, we claim that $|B| \geq 5$. Indeed, assume for the sake of contradiction that $B$ contains only these four vertices and take any bag $A \in V(T')$ that is adjacent to $B$ in the tree decomposition $T'$. (Such a bag must exist because $|V(D')| > 4$.) Consider their intersection $A \cap B$. By the smallness assumption on $T'$ we have that $|A \cap B| \leq 3$. By standard properties of tree decompositions (see e.g., [12]) we know that $A \cap B$ is a separator in $D'$ of the following two sets of vertices: $F_A = \cup_{e \in V(T_A)} B_e$, $F_B = \cup_{e \in V(T_B)} B_e$, where $T_A$ is the connected component of $T'$ that contains bag $A$ and $T_B$ is the connected component of $T'$ that contains $B$ if we delete the edge $\{A, B\}$ from $E(T')$. But observe that $A \cap B$ cannot be a separator for separation $F_A, F_B$ because $A \cap B \subset g(C')$ and $g(C')$ is not a separator of $D'$. A contradiction.

Now we proceed as follows: Create a new bag $H_1 = \{v_1, v_t, u_1, u_t, v_2\}$ and attach it to $B$ with an edge. Create a second bag $H_2 = H_1 \cup \{u_2\} \setminus \{u_1\}$ and attach it to $H_1$.

We claim this is a valid tree decomposition for $D''$ (which is $D'$ where $g(C')$ has increased its length by 1). Indeed, property (tw1) is immediate by construction, as is (tw3). For (tw2) observe that bag $H_1$ takes care of the new edges $\{v_1, v_2\}, \{v_2, v_1\}$ of $g(C'')$ and the bag $H_2$ of the new edges $\{v_2, u_2\}, \{v_1, u_2\}, \{u_2, u_t\}$. Note that, because $|B| \geq 5$, the new bags $H_1$ and $H_2$ do not increase the width of the decomposition.

$|V(D')| = 4$ and $\exists$ bag $B \in V(T')$ such that $B$ contains $\{v_1, v_t, u_1, u_t\}$. This situation can only occur if $D'$ is the complete graph on 4 vertices $K_4$ (since we know $tw(D') \geq 3$). This exceptional case can be dealt with similarly to the previous case, except that the addition of
bags $H_1$ and $H_2$ increase the width of the decomposition by exactly one. That is, we obtain a decomposition of $D'$ of width $\text{tw}(D') + 1$.

$\exists B \in V(T')$ that contains all of $\{v_1, v_t, u_1, u_t\}$. Note that every chordal completion of $D'$ must introduce the chord $\{v_1, u_1\}$ and/or the chord $\{v_t, u_t\}$. It is well-known that each maximal clique in a chordal completion induces a bag in a corresponding tree decomposition, and each bag in a tree decomposition induces a maximal clique in a corresponding chordal completion. Assume without loss of generality that the chord $\{v_t, u_1\}$ is present. Then $\{v_1, u_t\}$ is not present (because otherwise the corresponding bag would contain all of $\{v_1, v_t, u_1, u_t\}$, violating the case assumption.) Hence there exist two bags $A \neq B$ of $T'$ that contain the sets of vertices $\{v_1, u_1, v_t\}$ and $\{u_1, u_t, v_1\}$ respectively (and possibly other vertices). Add the element $v_1$ to $B$ and, in order to guarantee the running intersection property for $v_1$, add it also to each of the bags in the unique path from $A$ to $B$ in the tree decomposition $T'$ (all these bags contain $\{u_1, v_1\}$ by the running intersection property). This might increase the width of the decomposition by at most one. We introduce $H_1$ next to $B \cup \{v_1\}$ and $H_2$ next to $H_1$.

- If adding $v_1$ does increase the width, it is because $v_1$ is added to a bag that already has maximum size. All maximum-size bags in $T'$ contain at least 4 vertices (because $\text{tw}(D') \geq 3$) so after adding $v_1$ the maximum-size bags in the decomposition contain at least 5 vertices. Specifically, adding $H_1$ and $H_2$ cannot further increase the width of the decomposition and we obtain a decomposition of width at most $\text{tw}(D') + 1$.

- If adding $v_1$ does not increase the width, then the maximum bag size in our new $v_1$-augmented decomposition is at least 4 (because $|B \cup \{v_1\}| \geq 4$). Hence, adding $H_1$ and $H_2$ cannot increase the width of the decomposition by more than 1. So we again have a decomposition of width at most $\text{tw}(D') + 1$.

In all the above three cases we end up with a (not necessarily optimal) tree decomposition in which $H_1$ and $H_2$ are two adjacent size 5 bags (of degree 2 and 1 respectively). This process can now be iterated without further raising the width of the decomposition because all added bags will have size at most 5. For example, to add the parents of $x_3$: add a new bag $\{v_2, u_2, v_t, u_t\}$ next to $H_2$ (“forget” $u_1$ from bag $H_2$) and then add two new bags $\{v_2, v_3, v_t, u_2, u_t\}$ (“introduce” $v_3$) and $\{v_3, v_t, u_2, u_3, u_t\}$ (“forget” $v_2$ and “introduce” $u_3$).

In conclusion, from a clipped chain $C'$ and its corresponding grid $g(C')$ in $D'$ we can retrieve the whole original chain by increasing the treewidth of the resulting display graph by at most 1. Equivalently, clipping a common chain down to length 2 where in the display graph $D(T_1, T_2)$ the common chain is not a separator, cannot decrease the treewidth of the resulting display graph by more than 1.

Figure 6 shows that shortening a chain to length 2 might indeed reduce the treewidth of the display graph by 1. A natural question therefore arises: is there a constant $d > 2$ such that, if we clip a chain down to length $d$, the treewidth of the display graph is guaranteed to not decrease? This seems like a highly non-trivial question with deep connections to forbidden minors. But, at least in the case where the common chain is very large with respect to a function of the treewidth of the display graph $D$, we can show that shortening chains to a length dependent on the treewidth of $D$ does preserve the treewidth.

**Theorem 4.2.** Let $T_1, T_2$ be two incompatible unrooted binary trees and $D(T_1, T_2)$ their display graph such that $\text{tw}(D(T_1, T_2)) = k$. Then, there is a function $f(k)$ such that if there exists a common chain $C$ of length $t > f(k)$ then we can clip $C$ down to length $f(k)$ such that $\text{tw}(D') = \text{tw}(D)$ (where as usual $D'$ is the display graph of the trees with the shortened chains).

\footnote{If $\{v_1, u_1\}$ is present and not $\{v_t, u_1\}$ then by topological symmetry of the chain the argument still goes through: conceptually we are then simply reconstructing the chain in the “opposite” direction.}
Proof. Give that \( tw(D(T_1,T_2)) = k \geq 3 \) we can as usual without loss of generality suppress all taxa in the display graph. Now, \( D(T_1,T_2) \) must have as a minor one of the forbidden minors for treewidth \( k-1 \). Forbidden minors for treewidth \( k-1 \) (where \( k-1 \geq 2 \)) are all connected simple graphs with minimum degree 3. By the work of Lachgren [34] we know that the number of edges (and vertices) in forbidden minors for treewidth \( k-1 \) is bounded by a function \( f' \) of \( k \) which is doubly exponential in \( O(k^5) \). Let \( d' = f'(k-1) \). Now, fix the image of a forbidden minor for treewidth \( k-1 \) inside \( D \). Each vertex \( v \) of the minor has degree at most \( d' \), and (crudely) a degree \( d' \) vertex \( v \) can be split into at most \( \leq d' \) degree-3 vertices on the image inside \( D \) (these are the vertices which via edge contractions will merge to form \( v \)). Hence a common chain longer than \( (d')^2 \) must necessarily contain ever more vertices which are not on the image at all, or which are degree-2 vertices on the image. For a sufficiently large function \( f \) the point is reached that, if the chain is longer than \( f((d')^2) \), reducing the length of the chain by 1 cannot destroy the forbidden minor: either the image survives or a slight modification of it (with fewer degree-2 vertices) can be embedded in the graph. Hence, shortening the chain to length \( f((d')^2) \) cannot reduce the treewidth below \( k \). \( \square \)

![Figure 5: An example of two trees with a common chain indexed by taxa \( x_5, x_6, x_7 \).](image)

![Figure 6: The display graph (after the suppression of all vertices of degree two) of the two trees \( T_1, T_2 \) from Figure 5. Observe that the final graph is in fact one of the forbidden minors for treewidth 3, the Möbius graph, and \( tw(D) = 4 \). Observe also that if we clip the common chain down to length 2, then the treewidth of \( D \) decreases to 3.](image)

4.3 Cluster Reduction Rule

In this subsection we will study how the treewidth of the display graph relates to the treewidth of its clusters which are related to common splits:

**Definition 4.1.** Let \( T_1 \) and \( T_2 \) be two unrooted binary phylogenetic trees on the same set of taxa \( X \). We say that \( T_1 \) and \( T_2 \) have a common split \( X^* \upharpoonright X^{**} \) if \( X^* \) and \( X^{**} \) together form a bipartition of \( X \) and, for \( i \in \{1,2\} \), \( T_i \) has some edge \( e_i \) such that deleting \( e_i \) separates \( X^* \) from \( X^{**} \) in that tree.

In the following proofs we will refer extensively to Figure[7]

**Lemma 4.3.** Let \( T_1 \) and \( T_2 \) be two incompatible unrooted binary phylogenetic trees on the same set of taxa \( X \) and let \( X^* \upharpoonright X^{**} \) be a common split of \( T_1 \) and \( T_2 \). Let \( p = tw(D(T_1|X^*,T_2|X^*)) \) and \( q = tw(D(T_1|X^{**},T_2|X^{**})) \). Then

\[
\max(p,q) \leq tw(D(T_1, T_2)) \leq \max(p,q) + 1
\]
Proof. First we observe that the lower bound $\max(p,q) \leq tw(D(T_1,T_2))$ is immediate, since both $D(T_1|X^*,T_2|X^*)$ and $D(T_1|X^{**},T_2|X^{**})$ are minors of $D(T_1,T_2)$.

For the upper bound, we will first deal with the case when $|X^*|,|X^{**}| \geq 3$. Let $e_1 = \{u_1,v_1\}$ be the edge that induces the $X^*|X^{**}$ split in $T_1$, and let $e_2 = \{u_2,v_2\}$ be the edge which induces the split in $T_2$. If we delete both the edges $\{u_1,v_1\}$ and $\{u_2,v_2\}$ from $D(T_1,T_2)$ then we obtain a graph with two connected components. Each one of these two components has two degree-2 vertices, the endpoints of the two deleted edges. One of these components is a “rooted” version of $D(T_1|X^*,T_2|X^*)$, which we call $G^*$, and the other is a “rooted” version of $D(T_1|X^{**},T_2|X^{**})$, which we call $G^{**}$ where, in contrast with $D(T_1|X^*,T_2|X^*)$, $D(T_1|X^{**},T_2|X^{**})$, we do not suppress the degree-2 vertices $v_1,v_2,u_1,u_2$. Note that, due to the cardinality constraints on $X^*$ and $X^{**}$, $p = tw(G^*)$ and $q = tw(G^{**})$ because $D(T_1|X^*,T_2|X^*)$ can be obtained from $G^*$ by suppressing the degree-2 vertices which does not alter the treewidth (because the pathological case of Observation 3.1 does not apply). Similarly for the other component. Assume without loss of generality that $u_1$ and $u_2$ are in $G^*$, and $v_1$ and $v_2$ are in $G^{**}$. Let $\mathbb{T}^*$ and $\mathbb{T}^{**}$ be minimum-width tree decompositions of $G^*$ and $G^{**}$ respectively. Locate a bag $B^*$ of $\mathbb{T}^*$ that contains $u_1$ and a bag $B^{**}$ of $\mathbb{T}^{**}$ that contains $v_1$. Introduce a bag $\{u_1,v_1\}$ and insert it between $B^*$ and $B^{**}$. Clearly, the width in this merged tree decomposition is not altered. It remains only to ensure that the decomposition covers the edge $\{u_2,v_2\}$. This can be achieved simply by adding (say) $u_2$ to every bag in the tree decomposition of $G^{**}$, which increases the size of all bags by at most one. The result follows.

Now, we deal with the case where $|X^*| \leq 2$ and/or $|X^{**}| \leq 2$. First of all, we observe that since $T_1,T_2$ are incompatible by assumption, it is not the case that $|X^*|,|X^{**}| \leq 2$ at the same time. So, at least one of $|X^*|,|X^{**}|$ must be at least 3. Suppose $|X^*|=2$ and $|X^{**}| \geq 3$. Observe that in this case $tw(G^*) = 2 \neq p = 1$ but $tw(G^{**}) = q \geq 2$, so $\max(p,q) \geq 2$. Hence the construction from the previous case - adding bag $\{u_1,v_1\}$ and then adding $u_2$ to all bags - again cannot increase the width of the decomposition by more than 1. The case $|X^*|=1$ is somewhat strange because then $D(T_1|X^*,T_2|X^*)$ is just a single vertex. However, the upper bound still goes through because $tw(G^{**}) = q \geq 2$ and $D(T_1,T_2)$ can be obtained from $G^{**}$ by connecting the two roots of $G^{**}$ by an edge and then subdividing this new edge with a single degree-2 vertex. Adding an edge to a graph can increase its treewidth by at most 1, and edge subdivision is treewidth invariant.

Now, let $[G^*]$ be the graph obtained from $G^*$ by adding the edge $\{u_1,u_2\}$, and $[G^{**}]$ be obtained from $G^{**}$ by adding the edge $\{v_1,v_2\}$. See again Figure 7.

**Observation 4.1.** $tw(G^*) \leq tw([G^*]) \leq tw(D(T_1,T_2))$ and $tw(G^{**}) \leq tw([G^{**}]) \leq tw(D(T_1,T_2))$.
Proof. The lower bounds are immediate by a standard minor argument. The upper bounds are also obtained via minors. Specifically, observe that \([G^*]\) can be obtained from \(D = D(T_1, T_2)\) by completely contracting the part of \(D\) that lies between \(v_1\) and \(v_2\) (i.e., the \(X^*\) part of \(D\)). A symmetrical argument holds for \([G^{**}]\) by completely contracting the \(X^*\) part of \(D\).

The following theorem strengthens Lemma 4.3 by adding necessary and sufficient conditions for the lower bound to hold.

**Theorem 4.3.** Consider Lemma 4.3. Assume without loss of generality that \(p \leq q\). Then \(tw(D(T_1, T_2)) = \max(p, q)\) if and only if the following holds:

1. (Case \(p < q\)): \(tw([G^{**}]) = tw(G^{**})\).
2. (Case \(p = q\)): \(tw([G^{**}]) = tw(G^{**})\) and \(tw([G^*]) = tw(G^*)\).

Proof. We consider both cases and both directions of implication.

1. (Case \(p < q\), \(\Rightarrow\)) Assume \(p < q\) and \(tw(D(T_1, T_2)) = \max(p, q) = q\). Now, by Observation 4.1 \(tw([G^{**}]) \leq tw(D(T_1, T_2)) = q = tw(G^{**})\). The bound \(tw(G^{**}) \leq tw([G^{**}])\) also follows from Observation 4.1 so \(tw([G^{**}]) = tw(G^{**})\).

2. (Case \(p = q\), \(\Rightarrow\)) Assume \(p = q\) and \(tw(D(T_1, T_2)) = \max(p, q) = p = q\). Both \(tw([G^{**}]) = tw(G^{**})\) and \(tw([G^*]) = tw(G^*)\) follow from Observation 4.1

3. (Case \(p < q\), \(\Leftarrow\)) Observe that the statement \(tw([G^{**}]) = tw(G^{**})\) holds if and only if there exists a minimum-width tree decomposition of \(G^{**}\) in which \(v_1\) and \(v_2\) are both in the same bag \(B^{**}\). So, let us assume the existence of such a tree decomposition \(T^{**}\) and bag \(B^{**}\). Construct a minimum-width tree decomposition \(T^*\) of \(G^*\). Suppose \(T^*\) contains a bag \(B^*\) that contains both \(u_1\) and \(u_2\). We can merge \(T^*\) and \(T^{**}\) by inserting bags \(\{u_1, v_1, u_2\}\) and \(\{u_2, v_1, v_2\}\) between \(B^*\) and \(B^{**}\). The size-3 bags do not influence the width of the decomposition, so \(tw(D(T_1, T_2)) \leq \max(p, q)\), and \(tw(D(T_1, T_2)) = \max(p, q)\) then follows from Lemma 4.3. If no such bag \(B^*\) exists then create it by first adding (say) \(u_2\) to every bag of \(T^*\). The addition of \(u_2\) to every bag potentially increases the width of \(T^*\) by 1, but due to the fact that \(p < q\) we have \(p + 1 \leq q\), so \(\max(p + 1, q) \leq \max(p, q)\) and the earlier argument goes through.

4. (Case \(p = q\), \(\Leftarrow\)) This is very similar to the (Case \(p < q\), \(\Leftarrow\)) argument. The main difference is that, due to the strengthened starting assumption, both bags \(B^{**}\) and \(B^*\) are guaranteed to exist. Hence the “If no such bag \(B^*\)” part of the argument will never be required.

The above results show that the treewidth of the display graph behaves rather differently around common splits than other phylogenetic incongruence measures. Many such measures are (essentially) additive (i.e., the distance is the sum of the \(X^*\) and \(X^{**}\) parts) \([5, 35, 44]\), contrasting with the maximum function used in treewidth. As we demonstrate later in Section 8 this is one of the reasons why treewidth distance can be substantially lower than, for example, \(d_{MAF}\). A second point worth noting is that, while Theorem 4.3 describes necessary and sufficient conditions for the treewidth of the display graph to achieve the lower bound, it is not yet clear what (phylogenetic) properties of \(T_1\) and \(T_2\) actually create these conditions. Expressed differently, and for simplicity focusing on the case \(p < q\): what properties do \(T_1\) and \(T_2\) need to have to ensure \(tw([G^{**}]) = tw(G^{**})\)? It is perhaps relevant to observe that the graphs \([G^*], [G^{**}]\) can themselves be viewed, modulo a treewidth-invariant suppression of a single degree-2 vertex, as display graphs of appropriately rooted phylogenetic trees. Taking \([G^*]\) as an example: take the two trees \(T_1[X^*]\) and \(T_2[X^{**}]\) and attach a new placeholder taxon \(p\) at points \(u_1\) and \(u_2\), respectively.
5 Diameters on \( d_{tw} \)

In this section we explore the question of how large can the treewidth of the display graph of two unrooted binary phylogenetic trees, both on \( X \), can get. More precisely, we consider the diameter \( \Delta_n(d_{tw}) \) defined as the maximum value of \( d_{tw} \) taken over all pairs of phylogenetic trees with \( n \) taxa. Somewhat surprisingly, we show that \( \Delta_n(d_{tw}) \) is bounded below and above by linear functions on \( n \). To prove this, we first present a general result showing how we can embed an arbitrary graph into display graphs (as minors) without adding too many extra edges or vertices.

**Theorem 5.1.** Let \( G = (V, E) \) be an undirected (multi)graph with \( n \) vertices and maximum degree \( d \geq 2 \). Then we can construct two unrooted binary phylogenetic trees \( T_1 \) and \( T_2 \) such that both trees have \( O(nd) \) taxa, \( O(nd) \) nodes and \( O(nd) \) edges (and hence their display graph has \( O(nd) \) nodes and edges) and \( G \) is a minor of \( D(T_1, T_2) \).

**Proof.** The construction can easily be computed in polynomial time. We start by selecting an arbitrary unrooted binary tree \( T \) on \( n + 2 \) taxa. Set \( T_1 := T \) and \( T_2 := T \). The idea is that the \( n \) internal nodes of \( T_1 \) are in bijection with the \( n \) vertices of \( G \). We will add the edges of \( G \) one at a time, in the following manner. If an edge \( e = \{u, v\} \) of \( G \) already exists within \( T_1 \), the edge is already encoded so there is nothing to do. If not, we subdivide an arbitrary edge in \( T_2 \) and let \( y \) be the subdivision node. We then introduce two new taxa \( x_1^y \) and \( x_2^y \) and a new vertex \( z \) in \( T_2 \), and add the following edges: \( \{u, x_1^y\}, \{x_1^y, z\}, \{z, y\}, \{z, x_2^y\} \) and \( \{x_2^y, v\} \). The first and last of these edges is in \( T_1 \), the rest are in \( T_2 \). In the display graph the path \( u, x_1^y, z, x_2^y, v \) will become the image of the edge \( \{u, v\} \) (in the embedding of the minor). After encoding all the edges, \( T_1 \) and \( T_2 \) will each have at most \( k = (n + 2) + 2|E| \) taxa, so (because \( T_2 \) remains binary) each will have at most \( k - 2 \) internal nodes and each at most \( 2k - 3 \) edges. Now, observe that the \( n \) internal nodes of \( T_1 \) might have degree as large as \( d + 3 \). To turn \( T_1 \) into a binary tree we replace each vertex \( u \), where \( \text{deg}(u) > 3 \), by a path of \( t = \text{deg}(u) - 2 \) vertices \( u_1, \ldots, u_t \). The first two edges incident to \( u \) are now made incident to \( u_1 \), the final two edges incident to \( u \) are made incident to \( u_t \), and each of the remaining edges is made incident to exactly one of the nodes \( u_2, \ldots, u_{t-1} \). (When obtaining \( u \) from the embedding of \( G \), the idea is that the edges of the path will be contracted to retrieve \( u \)). This transformation does not alter the number of taxa, so \( T_1 \) and \( T_2 \) now have both the same number of internal nodes and edges (i.e. at most \( k - 2 \) and \( 2k - 3 \) respectively). Due to the fact that \( G \) has maximum degree \( d \), \( |E| \leq nd/2 \). We conclude that both trees each has at most \( (n + 2) + nd \) taxa, at most \( n(d + 1) \) internal nodes and at most \( 2n + 4 + 4|E| - 3 \leq 2n + 1 + 2nd \) edges. It follows that \( D(T_1, T_2) \) has at most \( 2n(d + 1) + ((n + 2) + nd) \) nodes in total and at most \( 4n + 2 + 4nd \) edges.

Applying the last theorem on complete graphs leads to a lower bound on \( \Delta_n(d_{tw}) \) which grows linearly on \( \sqrt{n} \). To get a better lower bound, below we use the fact that there are cubic expanders on \( n \) vertices with treewidth at least \( \epsilon n \), for some constant \( \epsilon > 0 \) (see, for example, [28, 29]).

**Corollary 5.1.** We have \( \Delta_n(d_{tw}) = \Theta(n) \) for \( n \geq 4 \), that is, \( \Delta_n(d_{tw}) \) is bounded below by a linear function on \( n \) and above by a linear function on \( n \).

**Proof.** As mentioned above, it is a well known fact that there are cubic expanders on \( n \) vertices with treewidth linear in \( n \). The maximum degree of such graphs is 3, so for every cubic expander \( G \) there exists (by the previous theorem) a display graph on \( O(n) \) vertices that contains \( G \) as a minor. Hence, the treewidth of the display graph is at least that of the expander, which is linear in \( n \). This establish the linear lower bound on \( \Delta_n(d_{tw}) \). The upper bound follows from \( \Delta_n(d_{tw}) \leq \Delta_n(d_{TBK}) \leq n - 3 - \left\lceil \frac{\sqrt{n - 2} - 1}{2} \right\rceil \),

where the second inequality follows from [21, Theorem 1.1].
Figure 8: Embedding grid minors in the display graphs of two unrooted binary trees: grids with even side length (left; \(k = 4\)) and odd side length (right; \(k = 5\)). Taxa are shown as small dots inside the grid. Both trees have exactly \((k - 1)^2 + 3\) taxa.

The construction (and bounds) described in Theorem 5.1 can be refined significantly in specific cases. Consider the \(k \times k\) grid graph, which has maximum degree 4 and \(k^2\) nodes. When taking \(n = k^2\) the theorem yields a bound of \(\approx 13n\) nodes. However, consider the construction shown in Figure 8, which distinguishes the cases \(k\) even and \(k\) odd. The two sides of the curve indicate the two trees that are needed and the points at which the curve touches the grid become the taxa of the two trees. Note that the red edges are added simply to ensure that all 4 corners of the grid (which have degree-2) can be correctly retrieved when taking minors; 2 of the corners are already present (because the curve intersects a neighbouring edge) but the other 2 require the addition of the red edges. As in the theorem the degree-4 nodes can be split into two degree-3 nodes. In both the odd and even cases it can be verified that both the resulting unrooted binary trees have \((k - 1)^2 + 3\) taxa and thus that the display graph has \(3(k - 1)^2 + 5\) nodes in total. This is \(\approx 3n\), a significant improvement on the generic bound. In fact it is not far from “best possible”. A \(k \times k\) grid contains \((k - 1)^2\) chordless 4-cycles, and because a tree cannot contain a cycle the embedding of each cycle must pass through at least 2 taxa in the display graph. Each taxon can be shared by at most two 4-cycles (because the display graph has maximum degree 3) yielding a lower bound on the number of taxa required of \((k - 1)^2\).

6 Display graphs formed from trees and networks

In this section we will consider the display graph formed by an unrooted binary phylogenetic network \(N = (V, E)\) and an unrooted binary phylogenetic tree \(T\) both on the same set of taxa \(X\). We will show upper bounds on the treewidth of \(D(N, T)\) in terms of the reticulation number \(r(N) = |E| - (|V| - 1))\) and the treewidth \(tw(N)\) of \(N\).

We begin with the first result that gives a sharp upper bound on the treewidth of the display graph in terms of the reticulation number of \(N\).

**Lemma 6.1.** Let \(N = (V, E)\) be an unrooted binary phylogenetic network and \(T\) an unrooted binary phylogenetic tree, both on \(X\), where \(|X| \geq 3\). If \(N\) displays \(T\) then \(tw(D(N, T)) \leq r(N) + 2\).

**Proof.** Due to the fact that \(N\) displays \(T\), there is a subgraph \(T'\) of \(N\) that is a subdivision of \(T\). If \(T'\) is a spanning tree of \(N\), then let \(N' = T'\). Otherwise, construct a spanning tree \(N'\) of \(N\) by greedily adding edges to \(T'\) until all vertices of \(N\) are spanned. At this point, \(N'\) contains exactly \(|V| - 1\) edges and consists of a subdivision of \(T\) from which possibly some unlabelled pendant subtrees (i.e. pendant subtrees without taxa) are hanging. We argue that \(D(N', T)\) has treewidth 2, as follows. First, note that \(D(T, T)\) has treewidth 2, because \(T\) is trivially compatible.

---

Note that if we “round off” the 4 corners of the grid its treewidth (which is \(k\)) is unaffected and the red edges are not required.
with $T$ (and $|X| \geq 3$). Now, $D(T,T)$ can be obtained from $D(N',T)$ by repeatedly deleting unlabelled vertices of degree 1 and suppressing unlabelled degree 2 vertices. These operations cannot increase or decrease the treewidth (because $tw(D(N',T')) = 2$ and because the pathological case of Observation 5.1 does not apply here). Hence, $D(N',T)$ has treewidth 2. Now, $D(N,T)$ can be obtained from $D(N',T)$ by adding back the $r(N) = |E| - (|V| - 1)$ missing edges. The addition of each edge can increase the treewidth by at most 1, so $tw(D(N,T)) \leq 2 + r(N)$. 

We note that this bound is sharp, since if $N = T$ then $r(N) = 0$ and $D(N,T)$ has treewidth 2. Also, observe that an essentially unchanged argument shows that if two networks $N_1$ and $N_2$, both on $X$, both display some tree $T$ on $X$, then $tw(D(N_1, N_2)) \leq r(N_1) + r(N_2) + 2$.

Now we derive a second upper bound in terms of the treewidth of the network $N$.

Lemma 6.2. Let $N = (V, E)$ be an unrooted binary phylogenetic network and $T$ an unrooted binary phylogenetic tree, both on $X$, where $|X| \geq 3$. If $N$ displays $T$ then $tw(D(N,T)) \leq 2tw(N) + 1$.

Proof. Since $N$ displays $T$ there is a subgraph $N'$ of $N$ that is a subdivision of $T$. We consider the surjection function $f$ defined in the preliminaries (which maps from vertices of $N'$ to vertices of $T$). Informally, $f$ maps taxa to taxa and degree-3 vertices of $N'$ to the corresponding vertex of $T$. Each degree-2 vertex of $N'$ lies on a path corresponding to an edge $\{u,v\}$ of $T$; such vertices are mapped to $u$ or $v$, depending on how exactly the surjection was constructed.

Now, consider any tree decomposition $t$ of $N$. Let $k$ be the width of the tree decomposition i.e., the largest bag in the tree decomposition has size $k + 1$. We will construct a new tree decomposition $t'$ for $D(N,T)$ as follows. For each vertex $u' \in V(N')$ we add $f(u')$ to every bag that contains $u'$. To show that $t'$ is a valid tree decomposition for $D(N,T)$ we will show that it satisfies all the treewidth conditions. Condition (tw1) holds because $f$ is a surjection. For property (tw2) we need to show that for every edge $e = \{u,v\} \in E(T)$, there exists some bag $B \in V(t) : \{u,v\} \subset B$. For this we use the third property of $f$ described in our observation: $\forall \{u,v\} \in E(T), \exists \alpha, \beta \in E(N') : f(\alpha) = u$ and $f(\beta) = v$. For each $e = \{u,v\} \in E(T)$, let $\alpha, \beta \in E(N')$ be the edge which is mapped through $f$ to $e$. Since $\alpha, \beta \in E(N)$, there must be a bag $B \in V(t)$ that contains both of $\alpha, \beta$. Since $f(\alpha) = u$ and $f(\beta) = v$, both of $u, v$ will be added into $B$. For the last property (tw3) we need to show that the bags of $t$ where $u \in V(T)$ have been added form a connected component. For this, we use property (2) of the function $f$: $\forall u \in V(T)$, the set $\{u \in V(N') : f(u) = v\}$ forms a connected subtree in $N'$. Hence, the set of bags that contain at least one element from $\{u \in V(N') : f(u) = v\}$ form a connected subtree in the tree decomposition. These are the bags to which $v$ is added, ensuring that (tw3) indeed holds for $v$.

We now calculate the width of $t'$: Observe that the size of each bag can at most double. This can happen when every vertex in the bag is in $V(T')$, and $f(u') \neq f(u')$ for every two vertices $u', v'$ in the bag. This causes the largest bag after this operation to have size at most $2(k+1)$ i.e., the width of the new decomposition is at most $2k + 1$.

Combining these two lemmas yields the following:

Corollary 6.1. Let $N$ be an unrooted binary phylogenetic network and $T$ be an unrooted binary phylogenetic tree, both on $X$. Then if $N$ displays $T$, $tw(D(N,T)) \leq \min\{2tw(N) + 1, r(N) + 2\}$.

The above results raise a number interesting points. First, consider the case where a binary network $N$ does not display a given binary phylogenetic network $T$. As we can see in Figure 9 there is a network $N$ and a tree $T$ such that $N$ does not display $T$ and yet the treewidth of their display graph is equal to the treewidth of $N$ which (as can be easily verified) is equal to three. Hence “does not display” does not necessarily cause an increase in the treewidth. On the other hand, the results in Section 5 show that for two incompatible unrooted binary phylogenetic trees (vacuously: neither of which displays the other, and both of which have treewidth 1) the treewidth of the display graph can be as large as linear in the size of the trees. The increase in treewidth in this situation is asymptotically maximal. So the relationship between “does not display” and treewidth is rather complex. Contrast this with the bounded growth in treewidth articulated

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Such bounded growth opens the door to algorithmic applications. In Section A (in the Appendix) we leverage this bounded growth to obtain a (theoretical) FPT result for determining whether a network displays a tree.

Second, observe that $tw(N)$ is equal to the maximum treewidth ranging over all biconnected components of $N$. An upper bound on the treewidth of a biconnected component $K$ is $r(K)$ i.e. the number of edges that need to be deleted from $K$ to obtain a spanning tree of the component. In phylogenetics the maximum value of $r(K)$ ranging over all biconnected components $K$ of $N$ is a well-studied parameter known as level [25, 31]. So $tw(N) \leq$ level$(N)$. Hence, if $N$ displays $T$, then the treewidth of $D(N, T)$ is also bounded as a function of the level of $N$.

7 The unit ball of $d_{tw}$ compared to that of $d_{TBR}$ and $d_{MP}$

In this section we will compare the unit ball neighborhood of $d_{tw}$ with those of $d_{TBR}$ and $d_{MP}$. Recall that given a distance $d$ and a phylogenetic tree $T$ on $X$ the unit neighborhood of $T$ under $d$ is the set of all phylogenetic trees $T'$ on $X$ with the property that $d(T, T') = 1$ (see, e.g.[30, 36], for results that characterise the unit ball neighbourhoods of $d_{TBR}$ and $d_{MP}$). We will begin by comparing treewidth with Maximum Parsimony (MP) unit neighborhoods.

**Theorem 7.1.** Suppose that $T$ and $T'$ are a pair of unrooted binary phylogenetic trees on $X$ with $d_{MP}(T, T') = 1$ or $d_{TBR}(T, T') = 1$. Then we also have $d_{tw}(T, T') = 1$.

**Proof.** Note that, because both TBR and MP distance are metrics (and thus satisfy the identity of indiscernibles property) we can assume that $T_1$ and $T_2$ are incompatible. We will first show that the claim is true for the TBR distance. Take two (necessarily incompatible) binary phylogenetic trees $T, T'$ such that $d_{TBR}(T, T') = 1$. By combining the results of [1] where it was shown that $d_{TBR}(T_1, T_2) = d_{MAF}(T_1, T_2) + 1$ and the result of [33] where it was shown that $tw(D(T_1, T_2)) \leq d_{MAF}(T_1, T_2) + 1$ we have that

$$tw(D(T_1, T_2)) \leq d_{TBR}(T_1, T_2) + 2.$$

Now if $T, T'$ are such that $d_{TBR}(T, T') = 1$ we conclude by the above that $tw(D(T, T')) \leq 3$ and by the assumption that $T, T'$ are incompatible we have that $d_{tw}(T, T') = 1$.
Now we will deal with the Maximum Parsimony distance. Let $T,T'$ be two (necessarily incompatible) unrooted binary phylogenetic trees such that $d_{MP}(T,T') = 1$. Using Theorem 4.1, we assume without any loss of generality that $T$ and $T'$ share no common pendant subtrees. Therefore, we can apply [36, Theorem 6.4] on $T,T'$ which characterizes the unit ball neighborhood of the maximum parsimony distance. There it was shown that $d_{MP}(T,T') = 1$ if and only if either (1) $d_{TBR}(T,T') = 1$, in which case we are done since we are in the TBR case or (2) $d_{TBR}(T,T') = 2$ and using common pendant subtree (CPS) reductions we can transform $T$ and $T'$ into a pair of trees with precisely five taxa. (All unrooted binary phylogenetic trees on 5 taxa are caterpillars and modulo relabelling of taxa there is only one caterpillar topology on 5 taxa.) Since $d_{tw}$ is preserved by CPS reduction in view of Theorem 4.1, we can assume without loss of generality that $T$ and $T'$ both have 5 taxa, and $T$ is the tree $T_1$ depicted in Fig. 11. Let $D = D(T,T')$ be the display graph formed from $T$ and $T'$ in which we subsequently suppress all vertices of degree-2. (Suppression does not alter the treewidth, by Observation 3.2.) It is easy to observe that $D$ has at most (in fact, exactly) 6 vertices.

Now, assume that $tw(D) > 3$ so that $d_{tw}(T,T') > 1$. Then, $D$ must have as a minor one of the forbidden minors for treewidth 3. In other words, one of the forbidden minors for treewidth 3 can be obtained by a series of edge deletions/contractions on $D$. There are precisely 4 forbidden minors for treewidth 3 [3], 2 of which are on 6 vertices or less: the $K_5$ and the Octahedron graph. Both of them have uniform degree 4. On the other hand, recall that the degree of each vertex of $D$ is 3 (because $T,T'$ are unrooted binary phylogenetic trees), so each degree-4 vertex of the minor maps to at least 2 vertices of $D$. This is clearly impossible. So $D$ cannot contain as a minor any of the forbidden minors for treewidth 3 which shows that $tw(D) \leq 3$. By assumption, $T,T'$ are incompatible so $tw(D(T,T')) = 3 \Rightarrow d_{tw}(T,T') = 1$.

In the following section we will show that the converse of the above claim, namely that $d_{tw}(T_1,T_2) = 1 \Rightarrow d_{MP}(T_1,T_2) = 1$ is certainly not true (and that the same holds for the TBR distance.)

8 On the gap between $d_{tw}$ and $d_{TBR}$, $d_{MP}$

The purpose of this section is to explore how far treewidth distance $d_{tw}$ can be from the other two distances considered in this manuscript, namely maximum parsimony distance $d_{MP}$ and TBR distance $d_{TBR}$. In particular we will provide an example of a sequence of pairs of trees whose treewidth distance is as low as 1 (i.e., the treewidth of their display graph is at most 3) but such that the corresponding TBR and MP distances can be arbitrarily large.

The construction starts with the 2 incompatible quartets (unrooted binary trees on 4 taxa) $T_1 = ab|cd$ and $T_2 = ac|bd$. Without any loss of generality, we assume that both of the quartets contain a degree-2 vertex in the “middle” namely, vertices $u,v$ respectively. (See Figure 11.) Note that with or without these degree-2 vertices the display graph has treewidth exactly 3 (by Observation 3.2).

Given a tree $T$ with a single degree-2 vertex we define the following doubling operation as follows:

**Doubling tree operation**: Given a tree $T$, with a unique degree-2 vertex $v$, the doubling of $T$, denoted by $(T,T)$, is constructed as follows: we take 2 copies of $T$ and we join with an edge their unique degree-2 vertices. We subdivide this new edge such that $(T,T)$ has a unique degree-2 vertex.

This operation will be the base of our construction. We will construct trees $T^i_1$ and $T^i_2$, for any step $i$, inductively as follows: $T^i_1 = (T_1,T_1)$ and $T^{i+1}_1 = (T^i_1,T^i_1)$. Similarly for $T^i_2$ and subsequently for $T^{i+1}_2 = (T^i_2,T^i_2)$. Let $D^i$ be the display graph of $T^i_1$ and $T^i_2$. Observe that since we start from $T_1,T_2$ on a common set of 4 taxa \{a,b,c,d\}, all the new doubled trees are on the same taxon set by labelling the new leaves appropriately, and so their display graph is well defined.
and unique. Initially, let $D = D^0$ be the display graph of $T_1^0 = T_1$ and $T_2^0 = T_2$. We will show that $\text{tw}(D) = 3$, for all $i$.

**Claim 8.1.** For every step $i$ we have that $d_{\text{tw}}(T_1^i, T_2^i) = 1$. Equivalently, we have that $\text{tw}(D^i) = 3$.

**Proof.** The proof is by an inductive argument. For the base of the induction, we first construct a tree decomposition of width 3 with specific properties: see Figure II.

As is apparent from the base case, we can assume without any loss of generality that the two degree-2 vertices $u, v$ in $T_1, T_2$ respectively, are in the same bag of the tree decomposition of their display graph $D$. We will exploit this fact in the following. For the induction step we assume that the display graph $D^i$ formed by $T_1^i$ and $T_2^i$ has treewidth 3. We will show a tree decomposition for $D^{i+1}$ of width equal to the width of the tree decomposition of $D^i$. We can construct $D^{i+1}$ from $D^i$ as follows: take two copies of $D_i$, let’s call them $D_1^i$ and $D_2^i$. Each copy $D_j^i$, $j \in \{1, 2\}$ has two degree-2 vertices: one, let’s call it $u_j^i$ is the degree-2 vertex resulting after repeated doubling of the $T_1$ tree and the other, let’s call it $v_j^i$ from doubling the $T_2$ tree. For each display graph $D_j^i$ let $T_j^i$ be its tree decomposition which by the inductive hypothesis has width 3. Moreover, as explained, we can assume without any loss of generality that the two degree-2 vertices $u_j^i$ and $v_j^i$ are in the same bag $B_j$. Observe that $D^{i+1}$ has two new degree two vertices, $u^*, v^*$: $u^*$ will be connected
with each $u^*_j$ and $v^*_j$ with each $v_j$, $j \in \{1, 2\}$. Construct $T^{i+1}$ as follows: locate the bags $B_j$ that contain $\{u^*_j, v^*_j\}$, $j \in \{1, 2\}$. Such bags exist by the inductive hypothesis. Create the following chain of bags: $B_1 = \{u^*_1, v^*_1\} - \{u^*_1, v^*_1\} - \{u^*_1, v^*_1\} - \{u^*_1, v^*_1\} - B_2$. It is immediate that $T^{i+1}$ is a valid tree decomposition for $D^{i+1}$ of width no higher than the width of $T^i$ (and $u^*$ and $v^*$ are in the same bag) so the claim follows. 

So the treewidth distance $d_{tw}$ of $T^i_1$ and $T^i_2$ remains 1 for any $i$. We will now give lower bounds on $d_{TBR}(T^i_1, T^i_2)$. We claim that $d_{TBR}(T^i_1, T^i_2) > d_{TBR}(T^{i+1}_1, T^{i+1}_2)$ for $i > j$. In particular $d_{TBR}(T^{i+1}_1, T^{i+1}_2) > d_{TBR}(T^i_1, T^i_2)$, for all $i \geq 0$. We will prove the claim using the maximum agreement forest distance which, by the result of Allen and Steel [1], is equivalent to TBR: $d_{MAF}(T^i_1, T^i_2) = d_{TBR}(T^i_1, T^i_2) + 1$. (See the preliminaries for definitions pertaining to agreement forests).

First of all, it is not too difficult to verify that (after suppression of the two degree-2 vertices) $d_{MAF}(T^i_1, T^i_2) = \frac{4}{2}$.

Let $T^{i+1}_j$ be the two trees obtained after we double $T^i_j$, for $j \in \{1, 2\}$ and let $d_{MAF}(T^i_1, T^i_2) = p \in \mathbb{N}^+$. We assume without loss of generality that neither of $T^{i+1}_1, T^{i+1}_2$ has a degree-2 vertex.

We distinguish between two cases: Let $e_1(e_2)$ be the edge used to connect the two copies of $T^i_1(T^i_2)$ to construct $T^{i+1}_1(T^{i+1}_2)$. We say that an edge is deleted by an agreement forest if it is an edge that is deleted in order to obtain the agreement forest. It is easy to observe that if $e_1$ is deleted in an agreement forest, then so is $e_2$ because of the symmetric properties of the constructed graphs $T^{i+1}_1, T^{i+1}_2$. Now, fix $m$ to be an arbitrary maximum agreement forest.

Edges $e_1(e_2)$ are deleted by $m$: Note that by deleting $e_1(e_2)$ we obtain two disjoint copies of the trees $T^i_1(T^i_2)$. In this case we observe that $d_{MAF}(T^{i+1}_1, T^{i+1}_2) = 2d_{MAF}(T^i_1, T^i_2) = 2p$ since any maximum agreement forest that does not use $e_1(e_2)$ can and should select a maximum agreement forest for the pair of trees $T^i_1, T^i_2$, and do this twice (since there are two disjoint copies of these trees).

Neither of these edges is deleted by $m$: Then these edges are used by the image of some component $C$ of the agreement forest $m$. If we split $C$ into two pieces (at the edges $e_1$ and $e_2$) we increase the size of the agreement forest by 1 and obtain an agreement forest that does not use either edge $e_1$ or $e_2$. From the previous case we know that any agreement forest that does not use these edges has at least $2p$ components. Hence, $d_{MAF}(T^{i+1}_1, T^{i+1}_2) \geq 2p - 1$.

**Lemma 8.1.** The MAF distance between $T^{i+1}_1$ and $T^{i+1}_2$ is at least $2 \times d_{MAF}(T^i_1, T^i_2) - 1 > d_{MAF}(T^i_1, T^i_2)$.

**Theorem 8.1.** There is at least one infinite subfamily of trees $T_1, T_2$ such that $d_{tw}(T_1, T_2) = 1$ whereas $d_{TBR}(T_1, T_2)$ is unbounded.

Finally, we turn to $d_{MP}$.

**Theorem 8.2.** There is at least one infinite subfamily of trees $T_1, T_2$ such that $d_{tw}(T_1, T_2) = 1$ whereas $d_{MP}(T_1, T_2)$ is unbounded.

**Proof.** In fact, this is a strengthening of the previous theorem because $d_{MP}$ is always a lower bound on $d_{TBR}$. However, as $d_{MP}$ is less well-known we only sketch the construction. Observe that the tree $T^i_1$ contains $2^i$ copies of each taxon. We assign all the copies of taxa $a$ and $b$ the state 0, and all copies of taxa $c$ and $d$ the state 1. It can be easily verified (by applying e.g. Fitch’s algorithm) that the parsimony score of $T^i_1$ on such a character is at most $2^i$. However, on the same character the parsimony score of $T^i_2$ will be at least $2 \cdot 2^i$. Hence, $d_{MP}(T^i_1, T^i_2) \geq 2 \cdot 2^i - 2^i$ and this grows to infinity. 

\footnote{Agreement forests are unaffected by suppression of degree-2 vertices.}
9 Discussion and open problems

In this paper we presented several algorithmic and combinatorial results on the treewidth distance $d_{tw}$, including its behaviour under three commonly used tree reduction rules and its diameter and unit ball neighbourhood. There are a number of interesting problems remain open, and we discuss some of them below.

A major open question is whether it is $\text{NP}$-hard to compute the treewidth distance $d_{tw}$ between two trees. This is equivalent to compute the treewidth of the display graph of these two trees, which is a cubic graph after suppressing all degree-2 vertices. Although computing the treewidth of general graphs is $\text{NP}$-hard, even for graphs whose maximum degree is at most 9 [4, 13], it is still unknown whether the treewidth of cubic graphs can be computed in polynomial time. Hence it is also interesting to understand the complexity of computing the treewidth of cubic graphs, and whether it has the same complexity of computing that of display graphs. Moreover, irrespective of whether it is an $\text{NP}$-hard problem, it is of interest to explore whether the structure of display graphs can be leveraged to compute their treewidth quickly in practice.

Another question concerns the common chain reduction, that is, whether there exists a universal constant $d$ such that reducing common chains to length $d$, preserves the treewidth of the display graph? This is likely to require deep insights into forbidden minors - in particular the way they interact with chain-like regions of graphs (that are not separators).

Initial numerical experiments suggest that treewidth distance can be “low” compared to traditional phylogenetic distances, such as the well-known TBR distance. Is this phenomenon more widespread? In how far is this an artefact of the way treewidth distance decomposes around common splits? Are there traditional phylogenetic distances and measures which are verifiably (and/or empirically) close to treewidth distance - and, if so, why? Finally, could we leverage low treewidth distance to develop efficient algorithms (based on dynamic programming over tree decompositions) for other phylogenetic distances and measures?

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A Unrooted tree compatibility is FPT: an alternative proof via Courcelle’s Theorem

The Unrooted Tree Compatibility problem (UTC) is simply the problem of determining whether an unrooted binary phylogenetic network \( N \) on \( X \) displays an unrooted binary phylogenetic tree \( T \), also on \( X \).

In [33] a linear kernel is described for the UTC problem and, separately, a bounded-search branching algorithm. Summarizing, these yield FPT algorithms parameterized by \( r(N) \) i.e. algorithms that can solve UTC in time at most \( f(r(N)) \cdot \text{poly}(|N| + |T|) \) for some function \( f \) that depends only on \( r(N) \). Here we give an alternative proof of FPT using Courcelle’s Theorem. This leverages Corollary 6.1 from Section 6. We prove that UTC is not only FPT when parameterized by \( r(N) \), but also \( tw(N) \). We begin with a simple auxiliary observation.

**Observation A.1.** Let \( G = (V,E) \) be an undirected, connected graph and let \( k = |E| - (|V| - 1) \). For every \( E' \subseteq E \) such that \( |E'| = k \), if \( G' = (V,E \setminus E') \) is connected then \( G' = (V,E \setminus E') \) is a spanning tree.

**Proof.** Observe that \( G' = (V,E \setminus E') \) has exactly \( |V| - 1 \) edges. If \( G' \) contained at least one cycle then (due to the assumption that \( G' \) is connected) we could delete edges from \( G' \), whilst maintaining connectivity, to obtain a tree that has strictly fewer than \( |V| - 1 \) edges and which spans \( V \). However, this would contradict the standard result from graph theory that any connected spanning subgraph must contain at least \( |V| - 1 \) edges. Hence, \( G' \) is connected and acyclic i.e. it is a spanning tree. \( \square \)

The high-level idea of the following MSOL formulation is that, if \( N \) displays \( T \), then (rather like the proof of Lemma 6.1) \( N \) contains some subtree \( T' \) that is a subdivision of \( T \) and which can be “grown” into a spanning tree \( T'' \) of \( N \). Every spanning tree of \( N \) can be obtained by the deletion of \( |E| - (|V| - 1) \) edges from \( N \), and (from Observation A.1) any subset \( E' \subseteq E \) where \( |E'| = k \) and whose deletion from \( N \) yields a connected graph, must therefore yield a spanning tree. Note that the set of quartets (unrooted phylogenetic trees on subsets of exactly 4 taxa) displayed by \( T'' \) is identical to those displayed by \( T' \), which is identical to those displayed by \( T \). (In other words, subdivision operations, and pendant subtrees without taxa that possibly hang from \( T'' \), do not induce any extra quartets.)

For the benefit of readers not familiar with MSOL we now show how various basic auxiliary predicates can be easily constructed and combined to obtain more powerful predicates. (The article [33] gives a more comprehensive introduction to the use of these techniques in phylogenetics). The MSOL sentence will be queried over the display graph \( D(N,T) \) where we let \( V \) be the vertex set of \( D(N,T) \) and \( E \) its edge set. Here \( RD \) is the edge-vertex incidence relation on \( D(N,T) \). We let \( V_T,V_N,E_T,E_N \) denote those vertices and edges of \( D(N,T) \) which belong to \( T,N \) respectively (note that \( T_V \cap T_N = X \)). Alongside \( X,V,E \) all this information is available to the MSOL formulation via its structure.

- test that \( Z \) is equal to the union of two sets \( P \) and \( Q \):
  
  \[ P \cup Q = Z := \forall z (z \in Z \Rightarrow z \in P \lor z \in Q) \land \forall z (z \in P \Rightarrow z \in Z) \land \forall z (z \in Q \Rightarrow z \in Z). \]

- test that \( P \cap Q = \emptyset \):
  
  \[ \text{NoIntersect}(P,Q) := \forall u \in P (u \notin Q). \]

- test that \( P \cap Q = \{v\} \):
  
  \[ \text{Intersect}(P,Q,v) := (v \in P) \land (v \in Q) \land \forall u \in P (u \in Q \Rightarrow (u = v)). \]

- test if the sets \( P \) and \( Q \) are a bipartition of \( Z \):
  
  \[ \text{Bipartition}(Z,P,Q) := (P \cup Q = Z) \land \text{NoIntersect}(P,Q). \]
• test if the elements in \{x_1, x_2, x_3, x_4\} are pairwise different:
  \text{allDiff}(x_1, x_2, x_3, x_4) := \bigwedge_{i \neq j \in \{1, 2, 3, 4\}} x_i \neq x_j.
• check if the nodes p and q are adjacent:
  \text{adj}(p, q) := \exists e \in E(R^D(e, p) \land R^D(e, q)).

The predicate \(PAC(Z, x_1, x_2, K)\) asks: is there a path from \(x_1\) to \(x_2\) entirely contained inside vertices \(Z\) that avoids all the edges \(K\)? We model this by observing that this does not hold if you can partition \(Z\) into two pieces \(P\) and \(Q\), with \(x_1 \in P\) and \(x_2 \in Q\), such that the only edges that cross the induced cut (if any) are in \(K\).

\[
PAC(Z, x_1, x_2, K) := (x_1 = x_2) \lor \exists p, q \in P \land q \in Q \land (\forall p, q \in P \land q \in Q \Rightarrow \neg \text{adj}(p, q) \lor (\exists g \in K(R^D(g, p) \land R^D(g, q))))
\]

The following predicate \(QAC^i\), where \(i \in \{T, N\}\), returns true if and only if \(i\) contains an embedding of quartet \(x_a x_b x_c x_d\) that is disjoint from the edge cuts \(K\).

\[
QAC^i(x_a, x_b, x_c, x_d, K) := \exists u, v \in V_i((u \neq v) \land \exists A, B, C, D, P \subseteq V_i(x_u, u \in A \land x_b, u \in B \land x_c, v \in C \land x_d, v \in D \land u \in P \land v \in P \land \text{Intersect}(A, B, u) \land \text{Intersect}(A, P, u) \land \text{Intersect}(B, P, u) \land \text{Intersect}(C, D, v) \land \text{Intersect}(C, P, v) \land \text{NoIntersect}(A, C) \land \text{NoIntersect}(B, A) \land \text{NoIntersect}(B, C) \land \text{NoIntersect}(A, D) \land \text{NoIntersect}(B, D) \land \text{PAC}(A, u, x_a, K) \land \text{PAC}(B, u, x_b, K) \land \text{PAC}(C, v, x_c, K) \land \text{PAC}(D, v, x_d, K) \land \text{PAC}(P, u, v, K))
\]

The overall formulation is shown as below. The first line asks for a subset \(E'\) of cardinality exactly \(k\), the second line requires that the \(N\) part of \(D(N, T)\) remains connected after deletion of \(E'\) (and thus induces a spanning tree), and from the third line onwards we stipulate that, after deletion of \(E'\), the set of quartets that survive is exactly the same as the set of quartets displayed by \(T\). (This is leveraging the well-known result from phylogenetics that two trees are compatible if and only if they display the same set of quartets [38].)

\[
|E'| = k \land E' \subseteq E_N \land \\
\forall u, v \in V(N(PAC(V_N, u, v, E')) \land \\
\forall x_1, x_2, x_3, x_4 \in X(\text{allDiff}(x_1, x_2, x_3, x_4) \Rightarrow \\
((QAC^T(x_1, x_2, x_3, x_4, 0) \iff QAC^N(x_1, x_2, x_3, x_4, E')) \land \\
(QAC^T(x_1, x_3, x_2, x_4, 0) \iff QAC^N(x_1, x_3, x_2, x_4, E')) \land \\
(QAC^T(x_1, x_4, x_2, x_3, 0) \iff QAC^N(x_1, x_4, x_2, x_3, E'))).)
\]

**Theorem A.1.** Given an unrooted binary network \(N = (V, E)\) and an unrooted binary tree both on \(X\), we can determine in time \(O(f(k) \cdot n)\) whether \(N\) displays \(T\), where \(k = |E| - (|V| - 1)\) and \(n = |V|\).

**Proof.** We run Bodlaender’s linear-time FPT algorithm [9] to compute a tree decomposition of \(D(N, T)\) and return NO if the treewidth is larger than \(k + 2\). (This is correct by Lemma 6.1, 1). Otherwise, we construct the constant-length MSOL sentence described earlier and apply the Arnborg et al. [2] variant of Courcelle’s Theorem, from which the result follows. (Note that \(D(N, T)\) has \(O(n)\) vertices and \(O(n)\) edges). The result can be made constructive if desired i.e. in the event of a YES answer the actual set \(E'\) can be obtained. \(\blacksquare\)
Corollary A.1. Given an unrooted binary phylogenetic network \( N = (V, E) \) and an unrooted binary phylogenetic tree both on \( X \), we can determine in time \( O(f(t) \cdot n) \) whether \( N \) displays \( T \), where \( t \) is \( tw(N) \) and \( n = |V| \).

Proof. By Corollary 6.1 we know that, if \( N \) displays \( T \), then \( D(N, T) \) will have treewidth at most \( 2tw(N) + 1 \). Hence, if the treewidth of \( D(N, T) \) is larger than this, we can immediately answer NO. Otherwise, we have a bound on the treewidth of \( D(N, T) \) in terms of \( tw(N) \), so we can again leverage Courcelle’s Theorem.

Corollary A.1 is potentially interesting in cases where \( tw(N) \) is significantly smaller than \( r(N) \). Note also that \( tw(N) \) is a lower bound on the level of \( N \) (discussed earlier in the manuscript: see Section 5), so in fact UTC is also FPT when parameterized by the level of \( N \).