Hybridization in Non-Binary Trees

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Abstract

Reticulate evolution—the umbrella term for processes like hybridization, horizontal gene transfer, and recombination—plays an important role in the history of life of many species. Although the occurrence of such events is widely accepted, approaches to calculate the extent to which reticulation has influenced evolution are relatively rare. In this paper, we show that the NP-hard problem of calculating the minimum number of reticulation events for two (arbitrary) rooted phylogenetic trees parameterized by this minimum number is fixed-parameter tractable.

Index Terms

Rooted phylogenetic tree, reticulate evolution, hybridization network.

I. INTRODUCTION

Using mathematical models to reconstruct a tree of life from nucleotide or protein sequences is subject of many phylogenetic studies that aim at analyzing the complex evolutionary processes that have occurred during the development of the current diversity of species. Under the usual assumption that each species arises from its ancestor by a simple speciation event, tree-based methods have contributed significantly to approaching this task. However, due to non-tree-like events, not all groups of taxa are suited to this type of presentation. Such processes, collectively referred to as reticulation events, include hybridization, horizontal gene transfer, and recombination. Since reticulate evolution results in genomes that are mosaics of distinct ancestral genomes, there has been an increased interest in modeling evolutionary relationships using phylogenetic networks rather than phylogenetic trees.

In this paper, we focus our attention on hybridization and its impact on evolution. This has been an active and controversially discussed field of research for many years and even several definitions of the term hybridization have been suggested [?]. For the purposes of this article, we refer to the origin of a new species through a mating between two individuals of different species as a hybridization event. Hybridization is widely accepted to play an important role in the evolutionary history of certain groups of plants and fish. For a review of hybrid species, we refer the reader to [?].

To provide insight into the extent to which hybridization has influenced the evolution of a set of present-day species, this paper addresses the following fundamental problem: Given a collection
of rooted phylogenetic trees that are correctly reconstructed for different genetic loci, what is the smallest number of hybridization events needed to simultaneously explain the evolutionary scenarios of the gene trees under consideration?

Bordewich and Semple [?] showed that the above problem is NP-hard even when the initial collection consists of two rooted binary phylogenetic trees. However, the same authors showed [?] that in the case of two binary trees the problem is fixed-parameter tractable. In particular, they showed that the minimum number of hybridization events can be computed in time $O(f(k) + p(n))$, where $k$ is the actual minimum number, $f$ is some computable function, $n$ is the number of species, and $p$ is a fixed polynomial. Due to the NP-hardness of the problem, such a result is of importance, since for many practical instances, the minimum number of hybridization events is small and, therefore, the problem may be tractable, even for a large number of taxa. This can be seen by considering the separation of the variables $k$ and $n$. For more details about fixed-parameter tractability, we refer the interested reader to [?].

Despite the above fixed-parameter tractable algorithm, for many biological data sets in practice (e.g. [?], [?]), the reconstructed phylogenetic trees are not fully resolved; that is, they contain polytomies. For example, this may be due to either the tree reconstruction method or the use of consensus trees for a certain analysis. Polytomies—alternatively called multifurcations—refer to vertices that have more than two direct descendants. A polytomy is hard if it refers to an event during which an ancestral species gave rise to more than two offspring species at the same time, whereas a soft polytomy represents ambiguous evolutionary relationships as a result of insufficient information [?].
Since simultaneous speciation events only occur rarely, we typically assume that all polytomies in a phylogenetic tree are soft. The reconstruction of a strictly bifurcating (binary) tree may consequently force refinements that are not necessarily optimal in terms of the hybridization number. An example for that is depicted in Fig. ??, where two binary refinements $S_1$ and $S_2$ of the tree $T'$ are shown. While the hybridization number for $S_1$ and $T$ is 0, this number for $S_2$ and $T$ is 1.

In this paper, we show that the decision problem of asking whether the minimum number of hybridization events to explain two (arbitrary) rooted phylogenetic trees is at most $k$ is fixed-parameter tractable. We now describe the above-mentioned problem formally beginning with several definitions.

A rooted phylogenetic $X$-tree $T$ is a rooted tree with no degree-$2$ vertices except possibly the root which has degree at least two, and with leaf set $X$. The set $X$ is called the label set of $T$ and is denoted by $L(T)$. In addition, $T$ is binary if, apart from the root which has degree two, all interior vertices have degree three.

Let $Y$ be a subset of $X$. We call $Y$ an (edge) cluster of $T$ if there is an edge $e$, or equivalently a vertex $v$, whose set of descendants in $X$ is precisely $Y$. We denote this cluster by $C_T(v)$, or simply $C(v)$ if there is no ambiguity. The set of clusters of $T$ is denoted by $C(T)$. Furthermore, the most recent common ancestor of $Y$ is the vertex $v$ in $T$ with $Y \subseteq C_T(v)$ such that there exists no vertex $v'$ with $Y \subseteq C_T(v')$ and $C_T(v') \subset C_T(v)$. We denote $v$ by $\text{mrca}_T(Y)$.

Let $T$ and $T'$ be two rooted phylogenetic $X$-trees. We say that $T'$ refines $T$, or equivalently $T'$ is a refinement of $T$, if $C(T) \subseteq C(T')$. In addition, $T'$ is a binary refinement if $T'$ is binary. Note that $T$ is a refinement of itself. Graphically speaking, it is straightforward to see that if $T'$ refines $T$, then $T$ can be obtained from $T'$ by contracting interior edges.

Hybridization networks are a generalization of evolutionary trees that allow for a simultaneous visualization of several conflicting or alternating histories of life. Such a network embeds a collection of gene trees representing a set of present-day species, where each vertex whose in-degree is greater than 1 represents a hybrid species. Mathematically speaking, a hybridization network $H$ (on $X$) is a rooted acyclic digraph with root $\rho$ in which

(i) $X$ is the set of vertices of out-degree zero,
(ii) the out-degree of $\rho$ is at least 2, and
(iii) for each vertex with out-degree 1, its in-degree is at least 2.

To quantify the number of reticulation events, the hybridization number of a hybridization network $\mathcal{H}$ with root $\rho$ is

$$h(\mathcal{H}) = \sum_{v \neq \rho} (d^-(v) - 1),$$

where $v$ is a vertex of $\mathcal{H}$ and $d^-(v)$ denotes the in-degree of $v$.

Let $T$ be a rooted phylogenetic $X$-tree, and let $\mathcal{H}$ be a hybridization network. We say that $\mathcal{H}$ displays $T$ if there is a rooted subtree of $\mathcal{H}$ that is a refinement of $T$. In other words, $T$ can be obtained from $\mathcal{H}$ by first deleting a subset of the edges of $\mathcal{H}$, deleting and contracting any resulting degree-0 and degree-2 vertices, respectively, apart from the root, and then contracting edges. For a collection $\mathcal{P}$ of rooted phylogenetic trees, $\mathcal{H}$ displays $\mathcal{P}$ if each tree in $\mathcal{P}$ is displayed by $\mathcal{H}$. Furthermore, extending the definition of the hybridization number of a network to $\mathcal{P}$, we set

$$h(\mathcal{P}) = \min\{h(\mathcal{H}) : \mathcal{H} \text{ is a hybridization network that displays } \mathcal{P}\}.$$

If $\mathcal{P}$ contains precisely two rooted phylogenetic $X$-trees $T$ and $T'$, then we denote the hybridization number $h(\mathcal{P})$ by $h(T, T')$ and remark that the beforehand given definition is equivalent to

$$h(T, T') = \min\{h(S, S') : S \text{ and } S' \text{ are binary refinements of } T \text{ and } T', \text{ respectively}\}.$$

Throughout the paper, both definitions are used interchangeably.

We can now formally state the decision problem HYBRIDIZATION NUMBER for when $\mathcal{P} = \{T, T'\}$:

**HYBRIDIZATION NUMBER**

**Instance:** Two rooted phylogenetic $X$-trees $T$ and $T'$, and an integer $k$.

**Question:** Is $h(T, T') \leq k$?

Since computing $h(T, T')$ is NP-hard when $T$ and $T'$ are binary [?], calculating this value for when $T$ and $T'$ are arbitrary rooted phylogenetic $X$-trees is also NP-hard.

The main result of this paper is the following theorem.

**Theorem 1.1:** The decision problem HYBRIDIZATION NUMBER is fixed-parameter tractable with $h(T, T')$ being the parameter.

The overall approach in proving Theorem ?? is similar to that used to show that HYBRIDIZATION NUMBER is fixed-parameter tractable when the initial two trees are binary. Basically, we use three reductions to kernalize the problem instance in a regulated way before calculating...
exactly the minimum number of hybridization events using an exhaustive search. The reason that this is sufficient to prove Theorem ?? is that the size of the label set of the trees $S$ and $S'$ obtained from $T$ and $T'$ by repeatedly applying the three reductions is linear in $h(T, T')$.

The paper is organized as follows. The next section contains some additional preliminaries that are used throughout the paper. In Sections ?? and ??, we characterize HYBRIDIZATION NUMBER in terms of a particular type of agreement forest. This characterization is essential to getting the main result of the paper. Section ?? describes the three reductions that are used to kernalize the problem instance and also includes three key lemmas that are needed for the proof of Theorem ??). This proof is given in Section ??). The paper ends with some brief remarks in Section ??.

We end the introduction by remarking that despite the similarities between the approaches used to prove Theorem ?? and the analogous result for binary trees, we see no obvious way that this latter result can be used to directly establish Theorem ??). Part of the reason for this is that a number of additional and non-trivial complications arise in the non-binary case.

II. PRELIMINARIES

In this section, we give some preliminary definitions that are used throughout the paper. Unless stated otherwise, the notation and terminology follows [?].

For a rooted phylogenetic $X$-tree $T$, a subset $Y$ of $X$ is called a vertex cluster of $T$ if there is a refinement of $T$ in which $Y$ is an edge cluster. For example, considering Fig. ??, the taxa set $\{1, 2\}$ is an edge cluster in $T$, but a vertex cluster (and not an edge cluster) in $T'$. Note that edge clusters are special types of vertex clusters.

Let $T$ be a rooted phylogenetic $X$-tree. Several types of rooted subtrees of $T$ play a central role in this paper. Let $Y$ be a subset of $X$. The minimal rooted subtree of $T$ that connects the leaves in $Y$ is denoted by $T(Y)$. Furthermore, the restriction of $T$ to $Y$, denoted $T|Y$, is the subtree obtained from $T(Y)$ by contracting all non-root vertices of degree two. Furthermore, a subtree of $T$ is pendant if it can be obtained from a refinement of $T$ by deleting a single edge. Lastly, a subtree is non-trivial if it contains at least two leaves.

III. AGREEMENT FORESTS

Various types of agreement forests have recently been used to analyze reticulate evolution for a set of gene trees and its impact on evolution [?], [?], [?], [?], [?]. All of these approaches
are restricted to the case when the trees under consideration are binary. Here, we extend the
definition of agreement forests to arbitrary rooted phylogenetic trees. For the reader familiar with
agreement forests, we note that the following definitions coincide with those previously given
for rooted binary phylogenetic trees.

Let \( T \) and \( T' \) be two rooted phylogenetic \( X \)-trees. For the purposes of the upcoming defini-
tions, we regard the root of both \( T \) and \( T' \) as a vertex labeled \( \rho \) at the end of a pendant edge
adjointed to the original root. Furthermore, we also regard \( \rho \) as part of the label set of
\( T \) and \( T' \), thus we view their label sets as \( X \cup \{ \rho \} \).

A forest of \( T \) is a partition \( \{ L_{\rho}, L_1, L_2, \ldots, L_k \} \) of its label set \( X \cup \{ \rho \} \), where
\( L_{\rho} \) contains \( \rho \), no part is empty, and the trees in \( \{ T(L_i) : i \in \{ \rho, 1, 2, \ldots, k \} \} \) are edge-disjoint rooted subtrees
of \( T \). An agreement forest \( F \) for \( T \) and \( T' \) is a forest \( \{ L_{\rho}, L_1, L_2, \ldots, L_k \} \) of \( T \) and \( T' \) such
that, for all \( i \in \{ \rho, 1, 2, \ldots, k \} \), the trees \( T|L_i \) and \( T'|L_i \) have a common binary refinement. To
illustrate these concepts, two examples of agreement forests \( F_1 \) and \( F_2 \) are shown in Fig. ??
for the two rooted phylogenetic trees \( T \) and \( T' \) also shown in that figure. Considering \( F_1 \), it is
easily checked that, for each label set \( L_i \), the restrictions of \( T \) and \( T' \), respectively, to
\( L_i \) have a common binary refinement.

The subtree prune and regraft distance between two rooted binary phylogenetic \( X \)-trees can
be characterized in terms of agreement forests. However, the corresponding characterization for
the minimum number of hybridization events for the same pair of trees requires an additional
condition. This condition excludes the possibility that species inherit genetic material from their
own descendants. Let \( F = \{ L_{\rho}, L_1, L_2, \ldots, L_k \} \) be an agreement forest for two arbitrary rooted
phylogenetic \( X \)-trees \( T \) and \( T' \). Let \( G_F \) be the directed graph that has vertex set \( F \) and an arc
\((L_i, L_j)\) from \( L_i \) to \( L_j \) precisely if \( i \neq j \) and either

(I) the path from the root of \( T(L_i) \) to the root of \( T(L_j) \) contains an edge of \( T(L_i) \), or
(II) the path from the root of \( T'(L_i) \) to the root of \( T'(L_j) \) contains an edge of \( T'(L_i) \).

We say that \( F \) is an acyclic-agreement forest for \( T \) and \( T' \) if \( G_F \) contains no directed cycles,
that is, \( G_F \) is acyclic. For the example depicted in Fig. ??, \( F_2 \) is an acyclic-agreement forest for
\( T \) and \( T' \) since \( G_{F_2} \) is acyclic, whereas \( F_1 \) is not an acyclic-agreement forest for \( T \) and \( T' \). If
\( F \) contains the smallest number of parts over all acyclic-agreement forests for \( T \) and \( T' \), we say
that \( F \) is a maximum-acyclic-agreement forest for \( T \) and \( T' \), in which case, we denote this value
of \( k \) by \( m_a(T, T') \). In the case that both \( T \) and \( T' \) are binary, these definitions again extend
Fig. 2. Two agreement forests $F_1$ and $F_2$ for the two rooted trees $T$ and $T'$ and their associated digraphs $G_{F_1}$ and $G_{F_2}$.

those typically given for two rooted binary phylogenetic trees. Baroni et al. [?] established the following characterization for binary trees.

**Theorem 3.1:** Let $T$ and $T'$ be two rooted binary phylogenetic $X$-trees. Then

$$h(T, T') = m_a(T, T').$$

**IV. CHARACTERIZING $h(T, T')$ IN TERMS OF AGREEMENT FORESTS**

In this section, we prove the following analog of Theorem ?? for arbitrary rooted phylogenetic trees. This analog is crucial in proving the main result of the paper.

**Theorem 4.1:** Let $T$ and $T'$ be two rooted phylogenetic $X$-trees. Then

$$h(T, T') = m_a(T, T').$$

Essentially, all of the work in establishing this theorem is done in proving the next two lemmas.

**Lemma 4.2:** Let $T$ and $T'$ be two rooted phylogenetic $X$-trees, and let $F$ be an acyclic-agreement forest for $T$ and $T'$. Then there exist binary refinements $S$ and $S'$ of $T$ and $T'$, respectively, such that $F$ is an acyclic-agreement forest for $S$ and $S'$.
Proof: Suppose that $\mathcal{F} = \{L_1, L_2, \ldots, L_k\}$ is an acyclic-agreement forest for $T$ and $T'$, and let $B_i$ be a common binary refinement of $T|L_i$ and $T'|L_i$ for all $i$. The proof of the lemma is by induction on $k$. Clearly, the result holds if $k = 0$. Now suppose that the result holds for all acyclic-agreement forests of $T$ and $T'$ of size at most $k$. Since $\mathcal{F}$ is acyclic, $G_{\mathcal{F}}$ contains a vertex, $L_m$ say, with out-degree zero. Since $L_m$ has out-degree zero, $T(L_m)$ is a pendant subtree of $T$ and $T'(L_m)$ is a pendant subtree of $T'$.

Let $T_m$ and $T'_m$ be the rooted phylogenetic trees $T|((X \cup \{\rho\}) - L_m)$ and $T'|((X \cup \{\rho\}) - L_m)$, respectively, and let $\mathcal{F}_m = \mathcal{F} - \{L_m\}$. Since $\mathcal{F}$ is an acyclic-agreement forest of $T$ and $T'$, it is easily checked that, as $T(L_m)$ is a pendant subtree of $T$ and $T'(L_m)$ is a pendant subtree of $T'$, the collection $\mathcal{F}_m$ is an acyclic-agreement forest of $T_m$ and $T'_m$. Therefore, by the induction assumption, there are binary refinements $S_m$ and $S'_m$ of $T_m$ and $T'_m$, respectively, such that $\mathcal{F}_m$ is an acyclic-agreement forest for $S_m$ and $S'_m$.

We now construct a binary refinement of $T$ from $S_m$. Let $u$ be the vertex of $T$ with the property that $C(u)$ is the minimal cluster of $T$ that properly contains $L_m$. By construction, $C(u) - L_m$ is a cluster of $T_m$. Furthermore, as $S_m$ is a binary refinement of $T_m$, the set $C(u) - L_m$ is a cluster of $S_m$. Let $u_m$ be the vertex of $S_m$ such that $C(u_m) = C(u) - L_m$. Let $S$ be the rooted binary phylogenetic tree obtained from $S_m$ by subdividing the edge coming into $u_m$ with a new vertex $v$ and adjoining the root of $B_m$ to this new vertex $v$ via a new edge. Observing that $C(v) = C(u)$, it is easily checked that $S$ is a binary refinement of $T$. Furthermore, by construction and because of the induction assumption, it follows that $\mathcal{F}$ is a forest of $S$ and, for all $i$, we have $S|L_i = B_i$.

By the same construction and argument, there is a binary refinement $S'$ of $T'$ such that $\mathcal{F}$ is a forest of $S'$ and, for all $i$, we have $S'|L_i = B_i$. It now follows that $\mathcal{F}$ is an agreement forest for $S$ and $S'$. Moreover, as $\mathcal{F}_m$ is an acyclic-agreement forest for $S_m$ and $S'_m$, it is easily seen that $\mathcal{F}$ is an acyclic-agreement forest for $S$ and $S'$. This completes the proof of the lemma.

Lemma 4.3: Let $T$ and $T'$ be two rooted phylogenetic $X$-trees, and let $S$ and $S'$ be binary refinements of $T$ and $T'$, respectively. If $\mathcal{F}$ is an agreement forest for $S$ and $S'$, then $\mathcal{F}$ is an acyclic-agreement forest for $T$ and $T'$.

Proof: Let $\mathcal{F} = \{L_1, L_2, \ldots, L_k\}$ be an acyclic-agreement forest of $S$ and $S'$. Since $S$ and $S'$ are both binary, it is easily seen, for all $i$, that $S|L_i$ and $S'|L_i$ are binary. Therefore, as $S$ and $S'$ are binary refinements of $T$ and $T'$, respectively, $S|L_i$ is a common binary refinement of $T|L_i$ and $T'|L_i$ for all $i$. To see that the trees in $\{T(L_i) : i \in \{\rho, 1, 2, \ldots, k\}\}$ are edge-disjoint.
rooted subtrees of $T$, suppose that this is not the case. Then, for some $r \neq s$, the subtrees $T(L_r)$ and $T(L_s)$ are not edge-disjoint. That is, $T(L_r)$ and $T(L_s)$ have an edge $e = \{u, v\}$ in common. Let $u$ be the end vertex of $e$ closest to $\rho$. Since $S$ is a binary refinement of $T$, there are vertices $u'$ and $v'$ of $S$ with $C_S(u') = C_T(u)$ and $C_S(v') = C_T(v)$. Now it is easily seen that $S(L_r)$ contains $u'$ and $v'$, and $S(L_s)$ contains $u'$ and $v'$. In other words, $S(L_r)$ and $S(L_s)$ are not edge-disjoint in $S$, contradicting that $F$ is an agreement forest of $S$ and $S'$. Thus the trees in $\{T(L_i) : i \in \{\rho, 1, 2, \ldots, k\}\}$ are edge-disjoint rooted subtrees of $T$ and, similarly, the trees in $\{T'(L_i) : i \in \{\rho, 1, 2, \ldots, k\}\}$ are edge-disjoint rooted subtrees of $T'$. Hence, $F$ is an agreement forest of $T$ and $T'$.

Now relative to $S$ and $S'$, the graph $G_F$ is acyclic. With respect to $F$, consider the analogous graph, $G'_F$ say, for $T$ and $T'$. Noting that both graphs have the same vertex set, it is clear that if $(L_r, L_s)$ is an arc in $G'_F$, then $(L_r, L_s)$ is an arc in $G_F$. Thus the arc set of $G'_F$ is a subset of the arc set of $G_F$. Since $G_F$ is acyclic, it follows that $G'_F$ is acyclic. This completes the proof of the lemma.  

Proof of Theorem ??: Let $S$ and $S'$ be binary refinements of $T$ and $T'$ that satisfy the hypothesis of Lemma ??, then, by that lemma, $m_a(T, T') \geq m_a(S, S')$. But, by Theorem ??, $m_a(S, S') = h(S, S')$. It now follows that, as $h(S, S') \geq h(T, T')$, we have $m_a(T, T') \geq h(T, T')$.

To establish the converse, now let $S$ and $S'$ be binary refinements of $T$ and $T'$ such that $h(S, S') = h(T, T')$. Then, by Theorem ??, there is an acyclic-agreement forest $F$ of $S$ and $S'$ such that

$$|F| - 1 = h(S, S') = h(T, T').$$

By Lemma ??, $F$ is an acyclic-agreement forest for $T$ and $T'$, so

$$m_a(T, T') \leq |F| - 1 = h(T, T').$$

It now follows that $h(T, T') = m_a(T, T')$. This completes the proof of the theorem.  

V. Reducing the Size of the Problem Instance

In this section, we introduce three reductions which kernalize HYBRIDIZATION NUMBER. The subtree and long-chain reductions extend the subtree and chain reductions described in [?]. Additionally, we introduce the short-chain reduction which—in combination with the other
two reductions—guarantees that all problem instances can be kernalized. We begin with some preliminaries.

Let $T$ be a rooted phylogenetic $X$-tree, and let $x$ be an element of $X$. Viewing $T$ as a directed graph with edges directed away from its root, the unique vertex, $u$ say, of $T$ such that $(u, x)$ is an arc of $T$ is called the parent of $x$ and is denoted by $p_T(x)$.

For all $n \geq 2$, an $n$-chain of $T$ is an ordered tuple $(a_1, a_2, \ldots, a_n)$ of distinct elements of $X$ that satisfies the following properties:

(i) for all $i \in \{1, 2, \ldots, n-1\}$, either $p_T(a_i) = p_T(a_{i+1})$ or $p_T(a_i)$ is a child of $p_T(a_{i+1})$, and

(ii) there is an ordering, $p_1, p_2, \ldots, p_m$ say, of the parents of $a_1, a_2, \ldots, a_n$ such that, for all $i \in \{1, 2, \ldots, m-1\}$, the vertex $p_i$ is a child of $p_{i+1}$ and, apart from $p_1$ and $p_m$, each of the vertices $p_2, p_3, \ldots, p_{m-1}$ has exactly one child not in $\{a_1, a_2, \ldots, a_n\}$.

If $p$ is a parent of an element in $A = \{a_1, a_2, \ldots, a_n\}$, then $p$ is called internal if it has at most one child not in $A$; otherwise $p$ is said to be external. An element of $A$ is internal if its parent is internal, otherwise it is external. Note that $p_2, \ldots, p_{m-1}$ are always internal, but that $p_1$ and $p_m$ can be internal or external. Thus if $a_i$ is external, then it is a child of $p_1$ or $p_m$. Furthermore, if $T$ is binary, then all elements of $A$ are internal. Throughout the paper, we will assume that if $(a_1, a_2, \ldots, a_n)$ is an $n$-chain of both $T$ and $T'$, where $T$ and $T'$ are rooted phylogenetic $X$-trees, then $T$ and $T'$ have no common non-trivial pendant subtree whose label set is a subset of $\{a_1, a_2, \ldots, a_n\}$. As we will soon see, this assumption does not restrict the results in this paper; it is simply for convenience and to avoid repetition in the statements. As an illustration, $(a_1, a_2, \ldots, a_n)$ is an $n$-chain of the two rooted phylogenetic trees $T$ and $T'$ shown in Fig. ??, where triangles represent subtrees outside of the chain.

Let $T$ and $T'$ be two rooted phylogenetic $X$-trees. Let $P$ be a disjoint collection of subsets $\{a_1, a_2, \ldots, a_n\}$ of $X$ each being the set of elements of a chain $(a_1, a_2, \ldots, a_n)$ common to both $T$ and $T'$ such that either

(i) $(a_1, a_2, \ldots, a_n)$ has exactly three elements that are internal in both $T$ and $T'$, or

(ii) for one of the trees, $(a_1, a_2, \ldots, a_n)$ has exactly two internal elements while, in the other tree, $(a_1, a_2, \ldots, a_n)$ has exactly one parent.

Depending on whether the chain satisfies (i) or (ii), it is assigned a triple of weights or a single weight from $\mathbb{Z}^+ \times \mathbb{Z}^+ \times \mathbb{Z}^+$ and $\mathbb{Z}^+$, respectively. We call such a pair of trees with associated
weighted set $P$ a pair of weighted rooted phylogenetic $X$-trees.

We now describe the three reductions. Let $\mathcal{T}$ and $\mathcal{T}'$ be a pair of weighted rooted phylogenetic $X$-trees with an associated set $P$, and let $A$ be a subset of $X$. We say that $A$ does not cross $P$ if, for each member $S$ of $P$, the intersection $S \cap A$ is empty.

**Subtree Reduction:** For $|A| \geq 2$, if $A$ is the label set of a maximal pendant subtree in $\mathcal{T}$ and $\mathcal{T}'$ with the properties that $\mathcal{T}|A$ and $\mathcal{T}'|A$ have a common binary refinement and $A$ does not cross $P$, then replace these subtrees with either a single new leaf labeled $a$ or a pendant edge ending in a new leaf labeled $a$ depending on whether the subtree can be obtained without or with refinement, respectively. In all cases, the new label is the same in both resulting trees.

**Long-Chain Reduction:** For $n \geq 4$, let $(a_1, a_2, \ldots, a_n)$ be a maximal $n$-chain of $\mathcal{T}$ and $\mathcal{T}'$ that does not cross $P$ and has the following properties:

(i) The chain has at least three internal parents in both $\mathcal{T}$ and $\mathcal{T}'$, and at least three elements that are internal in both $\mathcal{T}$ and $\mathcal{T}'$.

(ii) If $a_1$ is external in one of the trees, then $a_2$ is internal in the same tree and $a_1$ is internal in the other tree.

(iii) If $a_n$ is external in one of the trees, then $a_{n-1}$ is internal in the same tree while, in the other tree, $a_n$ is internal and there are not exactly three internal parents of which one has $a_n$ as its only child in $\{a_1, a_2, \ldots, a_n\}$.

Depending upon whether $\emptyset$, $\{a_1\}$, $\{a_n\}$, or $\{a_1, a_n\}$ is the subset of elements of $\{a_1, a_2, \ldots, a_n\}$ that are external in either $\mathcal{T}$ or $\mathcal{T}'$, respectively replace this chain in $\mathcal{T}$ and $\mathcal{T}'$ with the chain $(a, b, c)$, $(e_1, a, b, c)$, $(a, b, c, e_2)$, or $(e_1, a, b, c, e_2)$ as follows:

(i) In $\mathcal{T}$,

$$p_\mathcal{T}(e_1) \neq p_\mathcal{T}(a) = p_\mathcal{T}(b) \neq p_\mathcal{T}(c) \neq p_\mathcal{T}(e_2),$$

where $e_1$ is external if $a_1$ is external in $\mathcal{T}$, otherwise $e_1$ is internal; and where $e_2$ is external if $a_n$ is external in $\mathcal{T}$, otherwise $e_2$ is internal.

(ii) In $\mathcal{T}'$,

$$p_\mathcal{T}'(e_1) \neq p_\mathcal{T}'(a) \neq p_\mathcal{T}'(b) = p_\mathcal{T}'(c) \neq p_\mathcal{T}'(e_2),$$

where $e_1$ is external if $a_1$ is external in $\mathcal{T}'$, otherwise $e_1$ is internal; and where $e_2$ is external if $a_n$ is external in $\mathcal{T}'$, otherwise $e_2$ is internal.
Relative to \((a_1, a_2, \ldots, a_n)\), if \(m\) denotes the number of internal parents in \(T\) and \(m'\) denotes the number of internal parents in \(T'\), then respectively add the new set \(\{a, b, c\}\), \(\{e_1, a, b, c\}\), \(\{a, b, c, e_2\}\), or \(\{e_1, a, b, c, e_2\}\) to \(P\) and, calling this set \(S\), assign it a tuple of weights in which the first coordinate \(w_1\) is \(n - |S|\), the second coordinate \(w_2\) is \(m\) minus the number of internal parents of the resulting chain in \(T\), and the third coordinate \(w_3\) is \(m'\) minus the number of internal parents of the resulting chain in \(T'\). Intuitively, the reduction results in replacing \(a_1\) and \(a_n\) with \(e_1\) and \(e_2\), respectively, if \(a_1\) or \(a_n\) is external in either \(T\) or \(T'\), and replacing the
elements of the chain that are internal in both trees with \(a, b,\) and \(c\). Fig. ?? depicts an example of the long-chain reduction, where \(T\) and \(T'\) are the trees before, and \(S\) and \(S'\) are the trees after applying the long-chain reduction. In this example, \(a_1\) is external in \(T\), while \(a_n\) is external in \(T'\), and so the chain \((a_1, a_2, \ldots, a_n)\) is replaced with the chain \((e_1, a, b, c, e_2)\).

**Short-Chain Reduction:** For \(n \geq 3\), let \((a_1, a_2, \ldots, a_n)\) be a maximal \(n\)-chain of \(T\) and \(T'\) that does not cross \(P\) and has the property that in one of the trees, say \(T\), this chain has exactly one parent, while in the other tree \(T'\) this chain has at least three internal parents. (Due to the assumption that no element of an \(n\)-chain is part of a common non-trivial pendant subtree of \(T\) and \(T'\), note that \(p_T(a_1), \ldots, p_T(a_n)\) are pairwise distinct vertices in \(T'\) and so only \(a_1\) or \(a_n\) may be external in \(T'\).) Depending upon whether \(\emptyset, \{a_1\}, \{a_n\},\) or \(\{a_1, a_n\}\) is the subset of external elements of this chain in \(T'\), respectively replace this chain in \(T\) and \(T'\) with the chain \((a, b), (e_1, a, b), (a, b, e_2)\), or \((e_1, a, b, e_2)\) as follows:

(i) In \(T\),

\[
p_T(e_1) = p_T(a) = p_T(b) = p_T(e_2).
\]

(ii) In \(T'\),

\[
p_T'(e_1) \neq p_T'(a) \neq p_T'(b) \neq p_T'(e_2),
\]

where \(e_1\) is external if \(a_1\) is external in \(T'\) and \(e_2\) is external if \(a_n\) is external in \(T'\). Furthermore, add the new set \(\{a, b\}, \{e_1, a, b\}, \{a, b, e_2\},\) or \(\{e_1, a, b, e_2\}\) to \(P\) and, calling this set \(S\), assign it weight \(w = n - |S|\). Intuitively, the reduction results in replacing \(a_1\) and \(a_n\) with \(e_1\) and \(e_2\), respectively, if either \(a_1\) or \(a_n\) is external in \(T'\) and, relative to \(T'\), replacing the internal elements with \(a\) and \(b\). Fig. ?? depicts an example of the short-chain reduction, where \(T\) and \(T'\) are the trees before, and \(S\) and \(S'\) are the trees after applying the short-chain reduction. Here \(a_1\) is external in \(T'\), but \(a_n\) is internal in \(T'\), and so the chain \((a_1, a_2, \ldots, a_n)\) is replaced with the chain \((e_1, a, b)\).

An agreement forest \(\mathcal{F}\) for a pair of weighted rooted phylogenetic \(X\)-trees \(T\) and \(T'\) is **legitimate** if \(\mathcal{F}\) is acyclic and satisfies the following property, where, depending on the set in \(P\), the elements \(e_1\) and \(e_2\) may or may not exist:

**\(P\):** If \(\{e_1, a, b, c, e_2\} \in P\), then exactly one of the following holds:

(i) \(\{e_1, a, b, c, e_2\}\) is a subset of a label set in \(\mathcal{F}\),

(ii) \(\{a\}, \{b\},\) and \(\{c\}\) are label sets in \(\mathcal{F}\), and \(e_1\) and \(e_2\) are in separate label sets in \(\mathcal{F}\),
Fig. 4. Two rooted phylogenetic $X$-trees $T$ and $T'$ reduced under the short-chain reduction, where $S$ and $S'$ are the resulting trees. Dotted lines indicate regions of the chain $(a_1, a_2, \ldots, a_n)$. Note that $a_1$ is external in $T'$ while $a_n$ is internal in $T'$.

(iii) $\{a, b\}$ and $\{e\}$ are label sets in $F$, $e_1$ and $e_2$ are in separate label sets in $F$ and, relative to $(e_1, a, b, c, e_2)$, if $e_1$ or $e_2$ is internal in $T$, then $\{e_1\}$ or $\{e_2\}$ is a label set in $F$, respectively,

(iv) $\{a\}$ and $\{b, c\}$ are label sets in $F$, $e_1$ and $e_2$ are in separate label sets in $F$ and, relative to $(e_1, a, b, c, e_2)$, if $e_1$ or $e_2$ is internal in $T'$, then $\{e_1\}$ or $\{e_2\}$ is a label set in $F$, respectively,

while if $\{e_1, a, b, e_2\} \in P$, then exactly one of the following holds:

(I) $\{e_1, a, b, e_2\}$ is a subset of a label set in $F$,

(II) $\{a\}$ and $\{b\}$ are label sets in $F$, and $e_1$ and $e_2$ are in separate label sets in $F$.

Furthermore, referring to property (P), for an arbitrary agreement forest of $T$ and $T'$, we define
the weight of $\mathcal{F}$, denoted by $w(\mathcal{F})$, to be

$$w(\mathcal{F}) = |\mathcal{F}| - 1 + \sum_{S = \{e_1, a, b, c, e_2\} \in P; S \text{ satisfies (ii) in } \mathcal{F}} w_1(S)$$
$$+ \sum_{S = \{e_1, a, b, c, e_2\} \in P; S \text{ satisfies (iii) in } \mathcal{F}} w_2(S)$$
$$+ \sum_{S = \{e_1, a, b, c, e_2\} \in P; S \text{ satisfies (iv) in } \mathcal{F}} w_3(S)$$
$$+ \sum_{S = \{e_1, a, b, c, e_2\} \in P; S \text{ satisfies (II) in } \mathcal{F}} w(S).$$

We denote the minimum weight of a legitimate-agreement forest for $\mathcal{T}$ and $\mathcal{T}'$ by $f(\mathcal{T}, \mathcal{T}')$. Observe that $f(\mathcal{T}, \mathcal{T}') \geq h(\mathcal{T}, \mathcal{T}')$ as the weightings are non-negative, and $f(\mathcal{T}, \mathcal{T}') = h(\mathcal{T}, \mathcal{T}')$ whenever $P$ is empty.

Lemmas ??, ??, and ?? are key lemmas in proving that HYBRIDIZATION NUMBER is fixed-parameter tractable. Each lemma describes how particular common configurations in $\mathcal{T}$ and $\mathcal{T}'$ behave in a legitimate-agreement forest for $\mathcal{T}$ and $\mathcal{T}'$ of minimum weight. For convenience in the proofs of these lemmas, we will frequently refer to the property of a forest $\mathcal{F}$ that the trees in $\{\mathcal{T}(\mathcal{L}_i) : i \in \{p, 1, 2, \ldots, k\}\}$ are edge-disjoint rooted subtrees of $\mathcal{T}$ as no two label sets in $\mathcal{F}$ edge-overlap in $\mathcal{T}$.

Much of the proofs in the rest of this section involve taking a given legitimate-agreement forest $\mathcal{F}$, modifying it slightly, and showing that the resulting partition $\mathcal{F}'$ is also a legitimate-agreement forest. Two of the repetitive tasks is to show that $\mathcal{F}'$ is an agreement forest and acyclic. To avoid some of the repetition and to provide some intuition, let $\mathcal{L}_i \in \mathcal{F}$ and $\mathcal{L}_i' \in \mathcal{F}'$ with $\mathcal{L}_i' \subseteq \mathcal{L}_i$. First observe that if $\mathcal{L}_i'$ is the label set of a pendant subtree of $\mathcal{T}|\mathcal{L}_i$, then $\mathcal{L}_i'$ is the label set of a pendant subtree of $\mathcal{T}'|\mathcal{L}_i$. Analogously, if $\mathcal{L}_i'$ is the label set of a pendant subtree of $\mathcal{T}'|\mathcal{L}_i$, then $\mathcal{L}_i'$ is the label set of a pendant subtree of $\mathcal{T}|\mathcal{L}_i$. Second, as $\mathcal{T}|\mathcal{L}_i$ and $\mathcal{T}'|\mathcal{L}_i$ have a common binary refinement, $\mathcal{T}|\mathcal{L}_i'$ and $\mathcal{T}'|\mathcal{L}_i'$ have a common binary refinement. Third, if $\mathcal{L}_r, \mathcal{L}_s \in \mathcal{F} \cap \mathcal{F}'$, then $(\mathcal{L}_r, \mathcal{L}_s)$ is an arc in $G_{\mathcal{F}}$ if and only if it is an arc in $G_{\mathcal{F}'}$. Since $\mathcal{F}$ is acyclic, it follows that if $G_{\mathcal{F}'}$ contains a directed cycle, then this cycle must use a vertex in $\mathcal{F}' - \mathcal{F}$. Furthermore, if $\mathcal{L}_i \neq \mathcal{L}_r$, then, as $\mathcal{L}_r$ and $\mathcal{L}_i$ are edge-disjoint in $\mathcal{T}$ and $\mathcal{T}'$, we have $(\mathcal{L}_r, \mathcal{L}_i')$ is an arc in $G_{\mathcal{F}}$ if and only if $(\mathcal{L}_r, \mathcal{L}_i)$ is an arc in $G_{\mathcal{F}}$. Also, if $(\mathcal{L}_i', \mathcal{L}_s)$ is an arc in $G_{\mathcal{F}'}$, then $(\mathcal{L}_i, \mathcal{L}_s)$ is an arc in $G_{\mathcal{F}}$. Specializing these observations to when $\mathcal{F}'$ is a refinement of $\mathcal{F}$, that is, for each $\mathcal{L}_i' \in \mathcal{F}'$, we have $\mathcal{L}_i' \subseteq \mathcal{L}_i$ for some $\mathcal{L}_i \in \mathcal{F}$, it is straightforward to prove
the following lemma.

**Lemma 5.1:** Let $\mathcal{T}$ and $\mathcal{T}'$ be a pair of weighted rooted phylogenetic $X$-trees, and let $\mathcal{F}$ be an acyclic-agreement forest for $\mathcal{T}$ and $\mathcal{T}'$. Let $\mathcal{F}'$ be an agreement forest of $\mathcal{T}$ and $\mathcal{T}'$ that is a refinement of $\mathcal{F}$. Then $\mathcal{F}'$ is acyclic.

The above observations will be freely used in the rest of this section. The next lemma is repeatedly used in the key lemmas to show that our modified agreement forest satisfies (P).

**Lemma 5.2:** Let $\mathcal{T}$ and $\mathcal{T}'$ be a pair of weighted rooted phylogenetic $X$-trees, and let $\mathcal{F}$ be a legitimate-agreement forest for $\mathcal{T}$ and $\mathcal{T}'$ of minimum weight. Let $S$ be an element of $P$ such that $S$ contains elements of the form $e_1$ and $e_2$, and let $A$ be the label set of either a pendant subtree of $\mathcal{T}$ and $\mathcal{T}'$ that could be used for a subtree reduction or a chain of $\mathcal{T}$ and $\mathcal{T}'$ that could be used for a long-chain or short-chain reduction. Then there are no distinct label sets $\mathcal{L}_1$, $\mathcal{L}_2 \in \mathcal{F}$ such that $e_1 \in \mathcal{L}_1$, $e_2 \in \mathcal{L}_2$, and $\mathcal{L}_1 \cap A$ and $\mathcal{L}_2 \cap A$ both non-empty.

**Proof:** Suppose that there exist such label sets $\mathcal{L}_1$ and $\mathcal{L}_2$. Clearly, $S$ does not satisfy either (i) or (I) in the definition of (P). Assume $S$ satisfies (ii). Most of the work in the proof is involved in eliminating this particular case. Since there exist such label sets $\mathcal{L}_1$ and $\mathcal{L}_2$, and $\mathcal{L}_1$ and $\mathcal{L}_2$ are edge-disjoint in $\mathcal{T}$ and $\mathcal{T}'$, it is easily checked that $e_1$ is external in one of the trees, while $e_2$ is external in the other tree. The upcoming argument is independent of whether or not $a$ and $b$ have the same parent or $b$ and $c$ have the same parent, thus, without loss of generality, we may assume $e_1$ is external in $\mathcal{T}$, while $e_2$ is external in $\mathcal{T}'$. Thus $e_1$ is internal in $\mathcal{T}'$ and $e_2$ is internal in $\mathcal{T}$. Furthermore, $\mathcal{T}(\mathcal{L}_2)$ contains the parents of $a$, $b$, and $c$ in $\mathcal{T}$, and $\mathcal{T}'(\mathcal{L}_1)$ contains the parents of $a$, $b$, and $c$ in $\mathcal{T}'$. As $\mathcal{F}$ is acyclic, it follows that either the roots of $\mathcal{T}'(\mathcal{L}_1)$ and $\mathcal{T}'(\mathcal{L}_2)$ coincide in $\mathcal{T}'$, in particular, both roots are $p_{\mathcal{T}'}(e_2)$, or the root of $\mathcal{T}'(\mathcal{L}_2)$ is an ancestor of the root of $\mathcal{T}'(\mathcal{L}_1)$.

If $A$ is the label set of a pendant subtree, then, as $\mathcal{L}_1 \cap A$ and $\mathcal{L}_2 \cap A$ are both non-empty, the paths in $\mathcal{T}$ from any element in $\mathcal{L}_1 \cap A$ to $\rho$ and from any element in $\mathcal{L}_2 \cap A$ to $\rho$ meet at $p_{\mathcal{T}}(e_1)$, while the paths in $\mathcal{T}'$ from any element in $\mathcal{L}_1 \cap A$ to $\rho$ and from any element in $\mathcal{L}_2 \cap A$ to $\rho$ meet at $p_{\mathcal{T}'}(e_2)$. This set-up is depicted in Fig. ???. Let $\mathcal{L}_2'$ denote the subset of elements of $\mathcal{L}_2$ for which $p_{\mathcal{T}}(e_1)$ is an ancestor. Since $\mathcal{T} | \mathcal{L}_2$ and $\mathcal{T}' | \mathcal{L}_2$ have a common binary refinement and $\mathcal{L}_2 \cap A$ is non-empty, each of the elements in $\mathcal{L}_2'$ is a descendant of $p_{\mathcal{T}'}(e_2)$ in $\mathcal{T}'$. Let $\mathcal{L}_1'$ denote the subset of elements of $\mathcal{L}_1$ for which $p_{\mathcal{T}'}(e_1)$ is not an ancestor in $\mathcal{T}'$. Let $\mathcal{F}'$ be the partition obtained from $\mathcal{F}$ by replacing $\mathcal{L}_1$, $\mathcal{L}_2$, $\{a\}$, $\{b\}$, and $\{c\}$ with $(\mathcal{L}_2 - \mathcal{L}_2') \cup \{e_1, a, b, c\}$,
for a long-chain reduction. Since $L$ cycle in $G$ label set of a pendant subtree. subtree of $T$, forest of $(P)$, it is easily checked that $F$ binary refinement, except for $A$ $F$. Also, $L$ $G$ $T$ the root of $T$. Using the observations prior to Lemma $L$, and if $F$ is acyclic, note that, up to $A$ $T$, no element in $L$ is a descendant of $2$, $(L, L_2) = (e_1, a, b, c)$, $F'$ is a refinement of $F$. Moreover, for $L_1, L_s \in F \cap F'$, $(L_r, (L_2 - L_2) \cup \{e_1, a, b, c\})$ is an arc in $G_{F'}$ if and only if $(L_r, L_2)$ is an arc in $G_F$, and if $((L_2 - L_2) \cup \{e_1, a, b, c\}, L_s)$ is an arc in $G_F$, then $(L_2, L_s)$ is an arc in $G_F$ unless the root of $T'(L_2)$ is not a strict ancestor of $p_{T}(e_2)$. In this exceptional instance, $(L_1, L_s)$ is an arc in $G_F$ and, whenever $(L_r, (L_2 - L_2) \cup \{e_1, a, b, c\})$ is an arc in $G_F$, $(L_r, L_1)$ is an arc in $G_F$. Using the observations prior to Lemma $L$, a routine check shows that if there is a directed cycle in $G_{F'}$, then there is a directed cycle in $G_F$. It follows that $F'$ is a legitimate-agreement forest of $T$ and $T'$. But $w(F') < w(F)$, contradicting the minimality of $F$, and so $A$ is not the label set of a pendant subtree.

Now assume that $A$ is the set of elements of a chain $(a_1, a_2, \ldots, a_n)$ that could be used for a long-chain reduction. Since $L_1 \cap A$ and $L_2 \cap A$ are both non-empty, $p_{T}(a_n) = p_{T}(e_1)$, $p_{T}(a_1) = p_{T}(e_2)$, $a_1 \in L_1$, and $a_n \in L_2$. Thus $a_1$ is external in $T'$ and $a_n$ is external in $T$. Also, $L_1 \cap A = \{a_1\}$ and $L_2 \cap A = \{a_n\}$. Furthermore, as $T|L_2$ and $T'|L_2$ have a common binary refinement, except for $a_n$, no element in $L_2$ is a descendant of $p_{T}(e_1)$ in $T$ and, except for $e_2$, no element in $L_2$ is a descendant of $p_{T'}(e_2)$ in $T'$. Let $L_1'$ denote the subset of elements

Fig. 5. Set-up in the proof of Lemma $L$ for when $S$ satisfies (ii) in the definition of $(P)$ and $A$ is the label set of a pendant subtree of $T$ and $T'$. The roots of $T(L_1)$ and $T'(L_1)$ are indicated by $mrca_{T}(L_1)$ and $mrca_{T'}(L_1)$, respectively.
of \( L_1 \) for which \( p_T'(e_1) \) is not an ancestor. Let \( F' \) be the partition obtained from \( F \) by replacing \( L_1, L_2, \{a\}, \{b\}, \) and \( \{c\} \) with \( (L_2 - \{a_n\}) \cup \{e_1, a, b, c\}, (L_1 - L'_1) - \{e_1\}, \{a_n\}, \) and \( L'_1 \).

The set-up is similar to that of the last paragraph where we assumed \( A \) was a pendant subtree. Indeed, a similar argument now leads to the desired contradiction.

Next assume that \( A \) is the set of elements of a chain \((a_1, a_2, \ldots, a_n)\) that could be used for a short-chain reduction. Since \( L_1 \cap A \) and \( L_2 \cap A \) are both non-empty, \( p_T(a_n) = p_T(e_1) \) and \( p_T(a_1) = p_T(e_2) \) regardless in which tree the chain has a single parent. If the chain has a single parent in \( T \), then \( L_1 \cap A = \{a_1\} \) and \( T'(L_2) \) contains a parent of one of the elements in \( \{a_2, \ldots, a_n\} \). Now \( |L_2 \cap A| = 1 \) otherwise \( T|L_2 \) and \( T'|L_2 \) do not have a common binary refinement, and so each of the at least two internal elements of the chain in \( T' \) that is not the element in \( L_2 \cap A \) is a singleton in \( F \). It is now easily checked that the partition

\[
F' = \{L_i - A : L_i \in F - \{L_2\}\} \cup \{L_2 \cup A\}
\]

is a legitimate-agreement forest of \( T \) and \( T' \). But \( w(F') < w(F) \), contradicting the minimality of \( F \). Therefore assume that the chain has a single parent in \( T' \). Let \( L'_2 \) denote the subset of elements of \( L_2 \) for which \( p_T'(e_1) \) is an ancestor. As \( T|L_2 \) and \( T'|L_2 \) have a common binary refinement and \( L_2 \cap A \) is non-empty, each of the elements in \( L'_2 \) is a descendant of \( p_T'(e_2) \) in \( T' \).

Let \( L'_1 \) denote the subset of elements of \( L_1 \) for which \( p_T'(e_1) \) is not an ancestor. Let \( F' \) be the partition obtained from \( F \) by replacing \( L_1, L_2, \{a\}, \{b\}, \) and \( \{c\} \) with \( (L_2 - L'_2) \cup \{e_1, a, b, c\}, (L_1 - L'_1) - \{e_1\}, L'_2, \) and \( L'_1 \). This set-up is again similar to that when we assumed \( A \) was a pendant subtree and, as above, a similar argument leads to the desired contradiction. It now follows that \( S \) does not satisfy (ii).

If \( S \) satisfies (iii), then either \( L_1 \) or \( L_2 \) edge-overlap with \( \{a, b\} \) in \( T' \); a contradiction. Therefore \( S \) does not satisfy (iii) and, similarly, \( S \) does not satisfy (iv). Lastly, assume \( S \) satisfies (ii). Then, using the fact that \( e_1, a, b, \) and \( e_2 \) have the same parent in \( T \), a routine check shows that the partition \( F' \) obtained from \( F \) by replacing \( L_1, L_2, \{a\}, \) and \( \{b\} \) with \( L_1 \cup \{a, b, e_2\} \) and \( L_2 - \{e_2\} \) or \( L_1 - \{e_1\} \) and \( L_2 \cup \{a, b, e_1\} \) depending on whether \( T'(L_1) \) or \( T'(L_2) \) includes the parents of \( a \) and \( b \) in \( T' \), respectively, is a legitimate-agreement forest of \( T \) and \( T' \). But \( w(F') < w(F) \), contradicting the minimality of \( F \). Thus there are no such distinct label sets \( L_1 \) and \( L_2 \).

Lemma 5.3: Let \( T \) and \( T' \) be a pair of weighted rooted phylogenetic X-trees. Let \( A \) be the
label set of a maximal pendant subtree in $T$ and $T'$ with the properties that $T|A$ and $T'|A$ have a common binary refinement and $A$ does not cross $P$. Then, for every legitimate-agreement forest $F$ for $T$ and $T'$ of minimum weight, $A$ is a subset of a label set in $F$.

Proof: Let $F = \{L_p, L_1, L_2, \ldots, L_k\}$ be a legitimate-agreement forest of $T$ and $T'$ of minimum weight. Suppose that two subsets, $L_i$ and $L_j$ say, have the property that $L_i \cap A$ and $L_j \cap A$ are both non-empty. If there are no such subsets $L_i$ and $L_j$ so that $L_i \cap ((X \cup \{\rho\}) - A)$ and $L_j \cap ((X \cup \{\rho\}) - A)$ are both non-empty, then it is easily checked that the partition

$$\{L_i : L_i \cap A = \emptyset, L_i \in F\} \cup \{L_A\},$$

where $L_A = \bigcup_{L_i \in F, L_i \cap A \neq \emptyset} L_i$, is legitimate-agreement forest of $T$ and $T'$ but with smaller weight than $F$; a contradiction. Therefore, we may assume that we can choose $L_i$ and $L_j$ such that $L_i \cap ((X \cup \{\rho\}) - A)$ and $L_j \cap ((X \cup \{\rho\}) - A)$ are both non-empty. Because of this assumption, the pendant subtree with label set $A$ cannot be obtained from $T$ or $T'$ by deleting a single edge. Let $e$ denote the edge of $T$ that is directed into the root of $T(A)$ and let $e'$ denote the edge of $T'$ that is directed into the root of $T'(A)$. Since no label sets in $F$ edge-overlap in $T$ or $T'$, at most one of $T(L_i)$ and $T(L_j)$ includes $e$ and at most one of $T'(L_i)$ and $T'(L_j)$ includes $e'$. Also, since $G_F$ is acyclic, if $T(L_i)$ includes $e$, then $T'(L_j)$ does not include $e'$. Similar conclusions hold for the other combinations including $e$ or $e'$. Let $F'$ be the partition of $X \cup \{\rho\}$ obtained from $F$ by replacing $L_i$ and $L_j$ with $L_i \cup L_j$. It follows from the above conclusions and the observations prior to Lemma ?? that $F'$ is an acyclic-agreement forest for $T$ and $T'$. Furthermore, as $F$ satisfies (P), it follows by Lemma ?? that $F'$ satisfies (P), and so $F'$ is a legitimate-agreement forest of $T$ and $T'$. But, as $w(F') < w(F)$, we obtain a contradiction to the minimality of $F$. This contradiction completes the proof of the lemma.

Lemma 5.4: Let $T$ and $T'$ be a pair of weighted rooted phylogenetic $X$-trees. Let $(a_1, a_2, \ldots, a_n)$ be a maximal chain of both $T$ and $T'$ that does not cross $P$ and has properties (i)-(iii) in the definition of the long-chain reduction. Then, for every legitimate-agreement forest $F$ for $T$ and $T'$ of minimum weight, one of the following holds:

(i) $\{a_1, a_2, \ldots, a_n\}$ is a subset of a label set in $F$,
(ii) no label set in $F$ contains at least two elements of the chain and, if $a_i$ is an internal element of both $T$ and $T'$, then $\{a_i\}$ is a singleton in $F$, or
(iii) for either $T$ or $T'$, say $T$, two elements of the chain are in the same label set precisely if they
have the same parent and, moreover, if that parent is internal in $\mathcal{T}$, then the corresponding set contains no other elements of $X \cup \{\rho\}$.

**Proof:** Let $\mathcal{F} = \{\mathcal{L}_1, \mathcal{L}_2, \ldots, \mathcal{L}_k\}$ be a legitimate-agreement forest for $\mathcal{T}$ and $\mathcal{T}'$ of minimum weight. Let $A = \{a_1, a_2, \ldots, a_n\}$. The proof is partitioned into two cases depending on which of the following properties, up to interchanging the roles of $\mathcal{T}$ and $\mathcal{T}'$, is satisfied by $\mathcal{F}$:

(A) For all $\mathcal{L}_i \in \mathcal{F}$ with $\mathcal{L}_i \cap A$ non-empty and $p_{\mathcal{T}}(a_1)$ an ancestor of all elements in $\mathcal{L}_i - A$ in $\mathcal{T}$, the vertex $p_{\mathcal{T}'}(a_1)$ is an ancestor of all elements in $\mathcal{L}_i - A$ in $\mathcal{T}'$.

(B) There is a label set, $\mathcal{L}_i$ say, in $\mathcal{F}$ with both $\mathcal{L}_i \cap A$ and $\mathcal{L}_i - A$ non-empty and such that, in $\mathcal{T}$, the vertex $p_{\mathcal{T}}(a_1)$ is an ancestor of all elements in $\mathcal{L}_i - A$, but, in $\mathcal{T}'$, the vertex $p_{\mathcal{T}'}(a_1)$ is not an ancestor of all elements in $\mathcal{L}_i - A$.

**Case (A).** Let $J$ index the label sets of $\mathcal{F}$ that contain elements of the chain. More precisely,

$$J = \{j \in \{\rho, 1, 2, \ldots, k\} : \mathcal{L}_j \cap \{a_1, a_2, \ldots, a_n\} \neq \emptyset\}.$$

Relative to the chain $(a_1, a_2, \ldots, a_n)$, we will call an edge of $\mathcal{T}$ or $\mathcal{T}'$ a **non-pendant chain edge** if the edge is not incident with an element in $A$, but it is incident with an internal parent in $\mathcal{T}$ or $\mathcal{T}'$, respectively. The analysis of (A) is partitioned into two subcases:

(I) There exists (not necessarily distinct) label sets $\mathcal{L}_i$ and $\mathcal{L}_i'$ in $\mathcal{F}$ such that $\mathcal{T}(\mathcal{L}_i)$ and $\mathcal{T}'(\mathcal{L}_i')$ contain a non-pendant edge of the chain $(a_1, a_2, \ldots, a_n)$ in $\mathcal{T}$ and $\mathcal{T}'$, respectively.

(II) $\mathcal{F}$ contains no such label sets $\mathcal{L}_i$ and $\mathcal{L}_i'$.

**Subcase (I).** Without loss of generality, we may assume that $\mathcal{L}_i$ and $\mathcal{L}_i'$ are chosen so that the roots of $\mathcal{T}(\mathcal{L}_i)$ and $\mathcal{T}'(\mathcal{L}_i')$ are as close to $\rho$ as possible in $\mathcal{T}$ and $\mathcal{T}'$. If neither $\mathcal{L}_i$ nor $\mathcal{L}_i'$ contains an element of $A$, then, as $A$ contains no common non-trivial pendant subtree, it is easily seen that $\mathcal{F}$ satisfies (ii) in the statement of the lemma. Thus, we may assume that either $\mathcal{L}_i$ or $\mathcal{L}_i'$, say $\mathcal{L}_i$, contains an element of $A$. If $\mathcal{L}_i'$ does not contain an element of $A$, then one of the following holds: (a) for some $a_j, a_{j'} \in (\mathcal{L}_i \cap A)$, we have $p_{\mathcal{T}}(a_j) \neq p_{\mathcal{T}}(a_{j'})$ but $p_{\mathcal{T}'}(a_j) = p_{\mathcal{T}'}(a_{j'})$; (b) $a_1 \in \mathcal{L}_i$, $a_n \notin \mathcal{L}_i$, and $a_1$ is an external element of the chain in $\mathcal{T}'$; or (c) $a_n \in \mathcal{L}_i$, $a_1 \notin \mathcal{L}_i$, and $a_n$ is an external element of the chain in $\mathcal{T}'$. Since $\mathcal{L}_i'$ does not contain an element of $A$, it follows that if a label set in $\mathcal{F}$ contains an element in $A$ and an element in $(X \cup \{\rho\}) - A$, then that label set contains either $a_1$ or $a_n$, in which case $a_1$ or $a_n$ are external in $\mathcal{T}'$, respectively, but no other elements from $A$. Furthermore, no label set in $\mathcal{F}$
contains two elements of $A$ that have different parents in $T'$. It is now easily checked that, as $F$ is a legitimate-agreement forest of minimum weight, $F$ satisfies (iii) if (a) holds and $F$ satisfies either (ii) or (iii) if (b) or (c) holds. In all cases, if (iii) holds, then $T'$ is the distinguished tree.

Now assume that $L_i$ and $L'_i$ contain an element of $A$. The rest of the analysis for (I) is partitioned into two parts. Let $L'_i$ denote the subset of elements in $L_i - A$ that are descendants of $p_T(a_1)$, and let $X'_i$ denote the subset of elements in $L_i - A$ that are descendants of $p_{T'}(a_1)$ in $T'$. Analogously, let $L_i'$ denote the subset of elements in $L_i - A$ that are descendants of $p_T(a_1)$, and let $X_i$ denote the subset of elements in $L_i - A$ that are descendants of $p_{T}(a_1)$ in $T$.

For the first part, suppose that $L'_i = X'_i$ and $L'_i = X_i$. Let $F'$ be the forest obtained from $F$ by removing each label set $L_j$ with $j \in J$ and inserting the new label set $L_a = \bigcup_{j \in J} L_j$. Since we are in case (A), $F'$ is an agreement forest for $T$ and $T'$. To see that $F'$ is acyclic, consider the directed graphs $G_F$ and $G_{F'}$. The vertex set of $G_{F'}$ is obtained from $G_F$ by deleting the vertices $L_j$ for all $j \in J$, and adding the new vertex $L_a$. Also, if $L_a, L_s \in F' - \{L_a\}$, then $(L_r, L_s)$ is an arc in $G_{F'}$ if and only if $(L_r, L_s)$ is an arc in $G_F$. Regarding the arcs in $G_{F'}$ incident with $L_a$, there are two instances to consider. First assume that $L_i - A$ is non-empty and contains an element that is not a descendant of $p_T(a_1)$ in $T$. Then $L_i - A$ contains an element that is not a descendant of $p_{T'}(a_1)$ in $T'$. Since $G_F$ is acyclic, there is no arc from $L_i'$ to $L_i$ in $G_{F'}$; otherwise, $G_F$ contains a directed 2-cycle. Therefore, either the roots of $T'(L_i)$ and $T'(L_i')$ coincide in $T'$ or the root of $T'(L_i')$ is a descendant of the root of $T'(L_i)$. Since the root of $T(L_a)$ is the same as the root of $T(L_i)$ in $T$, it follows that if $(L_r, L_a)$ is an arc in $G_{F'}$, then $(L_r, L_i)$ and $(L_r, L_i')$ are arcs in $G_F$. Moreover, if $(L_a, L_r)$ is an arc in $G_{F'}$, then either $(L_a, L_i)$ or $(L_a, L_i')$ is an arc in $G_F$. Thus, as $G_F$ is acyclic, $G_{F'}$ is also acyclic.

Second assume that either $L_i - A$ is empty or if $L_i - A$ is non-empty, then it only contains elements that are descendants of $p_T(a_1)$. Because of the first instance, we may assume that the analogous property holds for $L_i'$ and $T'$. Then the root of $T(L_a)$ is $p_T(a_n)$ in $T$ and the root of $T'(L_a)$ is $p_{T'}(a_n)$ in $T'$. Suppose that $G_{F'}$ contains the directed cycle $C$. Then, as $G_F$ is acyclic, $C$ must contain $L_a$. Let $L_i$ and $L_m$ denote the vertices in $C$ that immediately precede and succeed $L_a$, respectively, in this directed cycle. Except for $L_a$, all other vertices in $C$ are also vertices in $G_F$. Thus either $(L_i, L_m)$ or $(L_i', L_m)$ is an arc in $G_F$. But $(L_i, L_i)$ and $(L_i', L_i')$ are also arcs in $G_F$, implying that $G_F$ contains a directed cycle; a contradiction. Thus $G_{F'}$ is
acyclic. Hence $F'$ is an acyclic-agreement forest for $T$ and $T'$. Furthermore, as $F$ satisfies (P), it follows by Lemma ?? that $F'$ satisfies (P). Thus if $|J| \geq 2$, then $w(F') < w(F)$, contradicting the minimality of $F$. Therefore, $A$ is a subset of a label set in $F$ and so $F$ satisfies (i) in the statement of the lemma.

For the second part, suppose that either $L'_i \neq X'_1$ or $L''_i \neq X_1$. Without loss of generality, we may assume that $L'_i \neq X'_1$ and $a_i \in L_i \cap A$. Since we are in case (A), this implies that $p_T(a_1)$ is not an ancestor of all elements in $L_i - A$. Let $L''_i$ denote the subset of elements in $L_i - A$ that are not descendants of $p_T(a_1)$. Because we are in case (A), $X'_1 \neq L_i - A$, and so there is an element in $L_i - A$ that is not a descendant of $p_T(a_1)$ in $T'$. Furthermore, we may assume that $L'_i$ is non-empty. To see this, observe that if $L_i$ and $L''_i$ are distinct, then $X'_1$ is empty, and so $L'_i$ is non-empty. Also, if $L_i$ and $L''_i$ are the same, then, without loss of generality, we may assume that $L'_i$ is non-empty.

First assume that either $a_i$ is internal in both $T$ and $T'$, or $a_i = a_1$. If $(L_i - A) \cap X'_1$ is non-empty, then, as $T|L_i$ and $T'|L_i$ have a common binary refinement, $L'_i \subseteq X'_1$. Furthermore, if $a_i \neq a_1$ or $a_i = a_1$ and $a_1$ is internal in $T'$, then the same reasoning implies that $X'_1 \cap L''_i$ is empty. But then $X'_1 = L'_i$; a contradiction. Therefore, assume that $a_i = a_1$ and $a_1$ is external in $T'$. If $a_n \notin L_i$, then, as $F$ is a legitimate-agreement forest of minimum weight, $F$ satisfies (ii) in the statement of the lemma. So assume that $a_n \in L_i$. If $a_n$ is internal in $T$, then, as $T|L_i$ and $T'|L_i$ have a common binary refinement, another check shows that $X'_1 \cap L''_i$ is empty and so $X'_1 = L'_i$. So now assume that $a_n$ is external in $T$, and therefore internal in $T'$. Again as $T|L_i$ and $T'|L_i$ have a common binary refinement, it is straightforward to check that, for any two elements in $L''_i \cap X'_1$ the path in $T$ from each of these elements to $\rho$ meets the path from $a_n$ to $\rho$ in exactly one place. With this in hand, let $F'$ be the partition of $X \cup \{\rho\}$ obtained from $F$ by removing each label set $L_j$ with $j \in J$ and inserting the new label sets $\bigcup_{j \in J} L_j - (L''_i \cap X'_1)$ and $L''_i \cap X'_1$. Clearly, $F'$ is an agreement forest for $T$ and $T'$, and it is easily checked that, as $F$ is acyclic, $F'$ is acyclic. Furthermore, by Lemma ??, $F'$ satisfies (P). Thus $F$ is a legitimate-agreement forest for $T$ and $T'$. But, in $F$, each of the elements of the chain that are internal in both $T$ and $T'$ is a singleton. Since there are at least three such elements, $w(F') < w(F)$; a contradiction.

Now say that $(L_i - A) \cap X'_1$ is empty. As $T|L_i$ and $T'|L_i$ have a common binary refinement, for any two elements in $L'_i$, the path in $T'$ from each of these elements to $\rho$ meets the path from
binary refinement, the label set containing \( a \) has the same parent in \( T \), and the label set containing \( a \) contains elements in \((X \cup \{\rho\}) - A\), then, as we are in case (A), \( p_T(a) \) and \( p_T(a) \) are ancestors of each of the elements in this label set. The same reasoning also shows that if \( a_n \) is external in \( T \) and not in \( L_i \), then its label set contains no elements in \((X \cup \{\rho\}) - A\). Furthermore, if \( a_j \) and \( a_k \) are internal elements of both \( T \) and \( T' \), then, as \( \mathcal{T}|\mathcal{L}_i \) and \( \mathcal{T}'|\mathcal{L}_i \) have a common binary refinement, the label set containing \( a_j \) is a subset of \( A \) if \( p_T(a_j) \neq p_T(a_i) \). Also, as no label sets in \( \mathcal{F} \) edge-overlap in \( T \), the elements \( a_j \) and \( a_k \) are in separate label sets in \( \mathcal{F} \) if \( p_T(a_j) \neq p_T(a_k) \). Thus there are two such subsets of \( A \) in \( \mathcal{F} \). Now let \( \mathcal{F}' \) be the partition of \( X \cup \{\rho\} \) obtained from \( \mathcal{F} \) by removing each label set \( L_j \) with \( j \in J \) and inserting the new label sets \( \bigcup_{j \in J} L_j - L'_i \) and \( L'_i \). It is clear that \( \mathcal{F}' \) is an agreement forest for \( T \) and \( T' \), and, by Lemma ??, that \( \mathcal{F}' \) satisfies (P). Moreover, it is easily checked that, as \( \mathcal{F} \) is acyclic, \( \mathcal{F}' \) is acyclic. But \( w(\mathcal{F}') < w(\mathcal{F}) \); a contradiction.

It now follows that we may assume that \( L_i \cap A = \{a_n\} \), where \( a_n \) is external in either \( T \) or \( T' \). By considering \( T \), it is easily seen that if \( a_j \) and \( a_k \) are internal elements in \( T \) and \( a_n \not\in \{a_j, a_k\} \), then the label set in \( \mathcal{F} \) containing \( a_j \) is a subset of \( A \), and \( a_j \) and \( a_k \) can only be in the same label set in \( \mathcal{F} \) if they have the same parent in \( T \). Now consider \( T' \). If \( p_{T'}(a_1) \) is an ancestor of an element in \( L_i \), then \( \mathcal{F} \) satisfies (ii) in the statement of the lemma. Therefore, assume that \( p_{T'}(a_1) \) is not an ancestor of any element in \( L_i \), that is \( X'_1 \) is empty. Now \( \mathcal{L}_i' \) contains an element of \( A \) and \( \mathcal{T}'(\mathcal{L}_i') \) contains a non-pendant edge of \((a_1, a_2, \ldots, a_n) \). If \( a_1 \in \mathcal{L}_i' \) and \( \mathcal{L}_i' \) contains an element in \((X \cup \{\rho\}) - A \) that is not a descendant of \( p_{T'}(a_1) \) in \( T' \), then again \( \mathcal{F} \) satisfies (ii) in the lemma. Noting that the label set containing \( a_1 \) can only contain another element of \( A \) if \( a_1 \) is internal in \( T \), it is now easily checked that, as \( \mathcal{F} \) is a legitimate-agreement forest for \( T \) and \( T' \) of minimum weight, then \( \mathcal{F} \) satisfies (iii) in the statement of the lemma with \( T \) as the distinguished tree unless \( a_n \) is internal in \( T \). But then a similar argument to that in the previous paragraph shows that the partition \( \mathcal{F}' \) of \( X \cup \{\rho\} \) obtained from \( \mathcal{F} \) by removing each label set \( L_j \) with \( j \in J \) and inserting the new label sets \( \bigcup_{j \in J} L_j - L'_i \) and \( L'_i \) is a legitimate-agreement forest of smaller weight than \( \mathcal{F} \); a contradiction. This completes the analysis of the second part, and therefore (I).

**Subcase (II).** We may assume that for one of the trees, say \( T \), whenever a label set \( L_r \) in \( \mathcal{F} \) contains an element in \( A \), then, unless this element is external, \( L_r \subseteq A \) and all elements in \( L_r \) have the same parent in \( T \). If \( \mathcal{F} \) satisfies (ii) in the statement of the lemma, then we are done; so
assume that this is not the case. Then there is a label set, \( L_i \) say, in \( F \) that contains at least two elements in \( A \). In \( T' \), these elements have different parents. Since \( F \) is a legitimate-agreement forest for \( T \) and \( T' \) of minimum weight, it is now easily checked that \( F \) satisfies (iii) in the statement of the lemma. This completes the analysis of (II) and, therefore, (A).

**Case (B).** First note that, since \( T|L_i \) and \( T'|L_i \) have a common binary refinement, \( p_{T'}(a_1) \) is not an ancestor of any element in \( L_i - A \) in \( T' \) unless \( L_i \cap A = \{a_1\} \) and \( a_1 \) is external in \( T \) or \( L_i \cap A = \{a_n\} \) and \( a_n \) is external in \( T' \). The analysis of this case is separated into two subcases:

(I) \( L_i \cap A \) contains an element that is internal in both \( T \) and \( T' \).

(II) \( L_i \cap A \) contains no element that is internal in both \( T \) and \( T' \).

**Subcase (I).** Let \( a_i \) be an element of \( L_i \cap A \) that is internal in both \( T \) and \( T' \). Let \( a_j \) be an element of \( A \) that is internal in both \( T \) and \( T' \). If \( p_T(a_j) \neq p_T(a_i) \), then using the facts that no label sets in \( F \) edge-overlap in \( T \) or \( T' \), that \( T|L_i \) and \( T'|L_i \) have a common binary refinement, and that \( F \) is acyclic, it is easily checked that \( a_j \) is in a label set of \( F \) containing only elements of \( A \) and all of the elements in this set have the same parent in \( T \). Because of the requirement on internal parents in (iii) in the definition of the long-chain reduction, there are at least two such label sets. Also, if \( p_T(a_j) = p_T(a_i) \) for some \( j \neq i \) and \( a_j \notin L_i \), then, because \( F \) is acyclic and no label sets in \( F \) edge-overlap in \( T \), \( a_j \) is in a label set of \( F \) containing only elements of \( A \) and all of the elements in this set have the same parent. Furthermore, since \( T|L_i \) and \( T'|L_i \) have a common binary refinement, any two distinct elements in \( L_i - A \) intersect the path from \( a_n \) to \( p \) in \( T' \) in exactly one place.

We next consider \( a_1 \) if \( a_1 \) is external in either \( T \) or \( T' \), and \( a_n \) if \( a_n \) is external in either \( T \) or \( T' \). If \( a_1 \) is external in \( T \), then, as \( T|L_i \) and \( T'|L_i \) have a common binary refinement, \( a_1 \notin L_i \). Furthermore, \( a_1 \) is in a label set of \( F \) that contains no other elements of \( A \) and, moreover, both \( p_T(a_1) \) and \( p_{T'}(a_1) \) are ancestors of all elements in this label set. If \( a_1 \) is external in \( T' \), then it easily checked that \( a_1 \) behaves in the same way as elements in \( A \) that are internal in both \( T \) and \( T' \). Now consider \( a_n \). If \( a_n \) is external in \( T \), then, as \( T|L_i \) and \( T'|L_i \) have a common binary refinement, \( a_n \notin L_i \). Also, as \( F \) is acyclic, \( a_n \) is in a label set of \( F \) that contains no other elements of \( A \) and, moreover, \( p_T(a_n) \) is an ancestor of all elements in this label set, but \( p_{T'}(a_1) \) is an ancestor of none. Furthermore, except for \( a_n \), the vertex \( p_{T'}(a_1) \) is an ancestor of all elements in this set. Now assume that \( a_n \) is external in \( T' \). If \( a_n \notin L_i \), then, as no label sets in \( F \) edge-overlap in \( T' \), the element \( a_n \) is the only element of \( A \) in its label set and, if this
label set contains elements in \((X \cup \{\rho\}) - A\), then \(p_{T'}(a_i)\) is not an ancestor of any of these elements and all elements in \(L_i\) are descendants of \(p_{T'}(a_n)\).

With the above conclusions in hand and noting that it is possible for \(a_n\) to be external in \(T'\) and \(a_n \in L_i\), let \(J\) index the label sets of \(F\) that contain elements of the chain. Let \(F'\) be the forest obtained from \(F\) by removing each label set \(L_j\) with \(j \in J\) and inserting the new label sets

\[
\bigcup_{j \in J} L_j - (L_i - A) - (L_n - \{a_n\})
\]

\(L'_i = L_i - A\), and \(L'_n = L_n - A\) if \(a_n\) is external in \(T\), where \(L_n\) is the label set in \(F\) containing \(a_n\), and

\[
\bigcup_{j \in J} L_j - (L_i - A)
\]

and \(L'_i = L_i - A\) if \(a_n\) is external in \(T'\). Note that \(F'\) is a partition of \(X \cup \{\rho\}\). By considering the possibilities for \(a_i\) and \(a_n\), and noting that \(p_{T'}(a_i)\) is not an ancestor of any element in \(L_i - A\), it is clear that \(F'\) is an agreement forest for \(T\) and \(T'\). Using arguments similar to that used in (A), a straightforward check shows that, as \(F\) is acyclic, \(F'\) is acyclic. Since \(F\) satisfies (P), it follows by Lemma 1\# that \(F'\) satisfies (P). Therefore, \(F'\) is a legitimate-agreement forest for \(T\) and \(T'\). But, as there are at least two label sets in \(F\) containing just elements of \(A\), we have \(w(F') < w(F)\); contradicting the minimality of \(F\). Thus subcase (I) does not arise.

**Subcase (II).** First observe that \(L_i \cap A\) is a non-empty subset of \(\{a_1, a_n\}\) and each of the elements in \(L_i \cap A\) is external in either \(T\) or \(T'\). Let \(a_j, a_k \in A\) such that neither \(a_j\) nor \(a_k\) is \(a_i\) if \(a_i\) is external in either \(T\) or \(T'\) and neither \(a_j\) nor \(a_k\) is \(a_i\) if \(a_i\) is external in either \(T\) or \(T'\). Assume first that \(a_1 \in L_i\). Since \(F\) is acyclic and no label sets in \(F\) edge-overlap in \(T\) or \(T'\), it is easily checked that \(a_j\) and \(a_k\) are in separate label sets in \(F\) and none of these label sets contain elements in \((X \cup \{\rho\}) - A\). Arguing similarly, if \(a_n\) is external in \(T\), and therefore internal in \(T'\), then \(\{a_n\}\) is a label set in \(F\). It now follows that if \(a_n\) is not external in \(T'\), then \(F\) satisfies (ii) in the statement of the lemma. Therefore, assume that \(a_n\) is external in \(T'\).

If \(a_n \notin L_i\), then, as no label sets in \(F\) edge-overlap in \(T'\), the elements \(a_j\) and \(a_n\) are not in the same label set in \(F\) for all \(j\). Thus \(F\) again satisfies (ii) in the statement of the lemma, so assume that \(a_n \in L_i\). Since \(T|L_i\) and \(T'|L_i\) have a common binary refinement, \(p_{T'}(a_n)\) is an ancestor of all elements in \(L_i\). Let \(F'\) be the partition of \(X \cup \{\rho\}\) that is obtained from \(F\) by replacing \(L_i\) and all other label sets containing elements of \(A\) with the three sets \(L'_i, L''_i, \) and
A, where $L_i''$ contains precisely the elements in $L_i - A$ that are descendants of $p_{T'}(a_1)$ in $T'$ and $L_i' = L_i - (A \cup L_i'')$. Clearly, $F'$ is an agreement forest for $T$ and $T'$. Furthermore, using arguments similar to that used in (A), it is easily checked that, as $F$ is acyclic, $F'$ is acyclic.

By Lemma ??, $F'$ satisfies (P) as $F$ satisfies (P), and so $F'$ is a legitimate-agreement forest for $T$ and $T'$. But $F$ has the property that $\{a_j\} \in F$ for all $a_j \in A - \{a_1, a_n\}$. Since $|A| \geq 5$, this implies that $w(F') < w(F)$; a contradiction.

We may now assume that $a_n \in L_i$ and $a_1 \notin L_i$. First note that if $p_{T'}(a_1)$ is an ancestor of an element in $L_i$, then, as the label sets in $F$ are edge-disjoint in $T'$, $F$ satisfies (ii) in the statement of the lemma. Thus we may also assume that $p_{T'}(a_1)$ is not an ancestor of any element in $L_i$. Since no label sets in $F$ edge-overlap in $T$, it follows that if $p_T(a_1) \neq p_T(a_k)$ or $p_T(a_1) \neq p_T(a_j)$, then $a_j$ and $a_k$, and $a_1$ and $a_j$ are in separate label sets in $F$, respectively. Furthermore, unless $p_T(a_1) = p_T(a_n)$ and $a_n$ is external in $T'$, the label set containing $a_j$ does not contain an element of $(X \cup \{\rho\}) - A$. Also, if $a_1$ is internal in $T$, then its label set does not contain an element of $(X \cup \{\rho\}) - A$. It is now easily checked that if $a_n$ is external in $T$, then, as $a_n$ is internal in $T'$ and $F$ is a legitimate-agreement forest of minimum weight, $F$ satisfies (iii) in the statement of the lemma with $T$ as the distinguished tree. Therefore, assume that $a_n$ is external in $T'$.

If $a_1$ is external in $T$ and its label set contains an element in $(X \cup \{\rho\}) - A$ that is not an ancestor of $p_T(a_1)$, then $F$ satisfies (ii) in the lemma. Thus if the label set containing $a_1$ contains an element in $(X \cup \{\rho\}) - A$, we may assume that it is a descendant of $p_T(a_1)$.

Now, apart from $L_i$ and the label set containing $a_1$, if $a_1$ is external in $T$, the only other possible label set, $L_k$ say, in $F$ that has a non-empty intersection with $A$ and $(X \cup \{\rho\}) - A$ has the property that if $a_k \in L_k \cap A$, then $p_T(a_k) = p_T(a_n)$. If no label set in $F$ contains at least two elements of $A$ each having a different parent in $T'$ and there exists no such label set $L_k$, then $F$ satisfies (ii) in the statement of the lemma. Therefore, suppose that one of these two possibilities occur. Let $F'$ be the partition of $X \cup \{\rho\}$ obtained from $F$ by replacing $L_i$, $L_k$ if such a label set exists, and all other label sets containing elements in $A$ with the sets $L_i'$, $A \cup L_1 \cup L_k'$ and $L_k''$, where $L_i' = L_i - \{a_n\}$, $L_1$ is the label set of $F$ containing $a_1$ if $a_1$ is external in $T$, $L_k'$ contains precisely the elements in $L_k - A$ that are descendants of $p_{T'}(a_1)$, and $L_k'' = L_k - L_k'$. Note that, as no label sets in $F$ edge-overlap in $T$ or $T'$, either $L_1 - \{a_1\}$ or $L_k'$ is empty. Clearly, $F'$ is an agreement forest for $T$ and $T'$. Furthermore, using the fact
that one of the two above possibilities occurs, it is easily checked that, as \( F \) is acyclic, \( F' \) is acyclic. Moreover, as \( F \) satisfies (P), it follows by Lemma ?? that \( F' \) satisfies (P), and so \( F' \) is a legitimate-agreement forest for \( T \) and \( T' \). But \( w(F') < w(F) \) as \( T \) has at least three internal parents. This contradiction completes the proof of (B) and hence the lemma.

**Lemma 5.5:** Let \( T \) and \( T' \) be a pair of weighted rooted phylogenetic \( X \)-trees. Let \((a_1, a_2, \ldots, a_n)\) be a maximal chain of both \( T \) and \( T' \) that does not cross \( P \) and has the property that in one of the trees, say \( T \), this chain has exactly one parent, while in the other tree \( T' \) this chain has at least three internal parents. Then, for every legitimate-agreement forest \( F \) for \( T \) and \( T' \) of minimum weight, exactly one of the following holds:

(i) \( \{a_1, a_2, \ldots, a_n\} \) is a subset of a label set in \( F \), or

(ii) no label set in \( F \) contains at least two elements of the chain and, if \( a_i \) is an internal element of \( \{a_1, a_2, \ldots, a_n\} \) in \( T' \), then \( \{a_i\} \) is a singleton in \( F \).

**Proof:** Let \( F = \{L_0, L_1, L_2, \ldots, L_k\} \) be a legitimate-agreement forest for \( T \) and \( T' \) of minimum weight, and let \( A = \{a_1, a_2, \ldots, a_n\} \). Let \( J \) index the label sets of \( F \) that contain elements of \( A \), and let \( L_a = \bigcup_{j \in J} L_j \). Suppose that neither (i) nor (ii) holds for \( F \). If no label set in \( F \) contains at least two elements of \( A \), then, relative to \( T' \), there is a label set in \( F \) that contains an internal element of the chain as well as an element of \( (X \cup \{\rho\}) - A \). By considering the structure of \( (a_1, a_2, \ldots, a_n) \) in \( T' \), it is easily seen that, as \( (a_1, a_2, \ldots, a_n) \) has at least three internal elements relative to \( T' \), at least one of these internal elements is a singleton in \( F \). A routine check shows that, apart from one exceptional case, we can replace such a singleton and a label set in \( F \) that contains an internal element of the chain in \( T' \) as well as an element of \( (X \cup \{\rho\}) - A \) with the union of these two sets to obtain a legitimate-agreement forest of \( T \) and \( T' \) that has smaller weight than \( F \); a contradiction. In the exceptional case, there is exactly one label set, \( L_i \) say, in \( F \) that contains an internal element of the chain in \( T' \) and an element in \( (X \cup \{\rho\}) - A \), and this set has the properties that \( |L_i \cap A| = 1 \), and \( p_{T'}(a_1) \) is an ancestor of all the elements in \( L_i - A \), but \( p_T(a_1) \) is not an ancestor of all the elements in \( L_i \). Since \( F \) is acyclic, it follows that each of the remaining internal elements of the chain in \( T' \) are singletons in \( F \). A straightforward check now shows that

\[
\{L - A : L \in F\} \cup \{A\}
\]

is a legitimate-agreement forest for \( T \) and \( T' \), but with smaller weight than \( F \). This contradiction
implies that there is a label set in \( F \) containing at least two elements of \( A \). Without loss of generality, we may assume that this set is \( L_i \) and that \( a_i \in L_i \cap A \), where \( i > i' \) for all \( a_{i'} \in L_i \cap A \).

Suppose that there exists an \( L_h \in F - \{ L_i \} \) such that \(|L_h \cap A| \geq 1\), \(|L_h \cap ((X \cup \{ \rho \}) - A)| \geq 1\), and let \( a_h \in (L_h \cap A) \). If \( p_T(a_h) \) is a descendant of \( p_T(a_i) \), then, as \(|L_i| \geq 2\) and no label sets in \( F \) edge-overlap in \( T' \), the vertex \( p_T(a_h) \) in \( T' \) is an ancestor of all elements in \( L_h \cap ((X \cup \{ \rho \}) - A) \). Because \( F \) is acyclic, it follows that the vertex \( p_T(a_h) \) in \( T \) is an ancestor of all elements in \( L_h \cap ((X \cup \{ \rho \}) - A) \); otherwise \( G_F \) contains a directed 2-cycle. Now assume that \( p_T(a_h) \) is an ancestor of \( p_T(a_i) \). If \( L_i \) contains an element \( z \) that is not a descendant of \( p_T(a_n) \) in \( T' \), then, as \( G_F \) is acyclic, \( p_T(a_n) \) is an ancestor of all elements in \( L_h \) in \( T \). Similarly, if \( L_h \) contains an element \( z \) that is not a descendant of \( p_T(a_n) \) in \( T' \), then, as \( G_F \) is acyclic, \( p_T(a_n) \) is an ancestor of all elements in \( L_i \) in \( T \). Now let \( F' \) be the forest obtained from \( F \) by removing each label set \( L_j \) with \( j \in J \) and inserting the new label set \( L_a \). Using the outcomes of the above two possibilities, it is easy seen that \( F' \) is an agreement forest for \( T \) and \( T' \). Furthermore, as \( F \) satisfies (P), it follows by Lemma 3.16 that \( F' \) satisfies (P). Using the facts that \( F \) is acyclic and at least one of the label sets in \( F \) contains at least two elements of \( A \), it is straightforward to show that \( F' \) is acyclic. But then \( w(F') < w(F) \); a contradiction to the minimality of \( F \). Thus \( F \) satisfies either (i) or (ii).

VI. HYBRIDIZATION NUMBER IS FIXED-PARAMETER TRACTABLE

In this section, we prove Theorem 3.2. We begin by showing that each of the three reductions described in the last section preserves the minimum weight of a legitimate-agreement forest. For a chain \( (a_1, a_2, \ldots, a_n) \) of \( T \), the partition of \( \{a_1, a_2, \ldots, a_n\} \) defined by putting \( a_i \) and \( a_j \) in the same part precisely if \( p_T(a_i) = p_T(a_j) \) is called the parent partition of \( (a_1, a_2, \ldots, a_n) \) induced by \( T \).

**Proposition 6.1:** Let \( T \) and \( T' \) be a pair of weighted rooted phylogenetic \( X \)-trees. Let \( S \) and \( S' \) be the pair of weighted rooted phylogenetic \( X' \)-trees obtained from \( T \) and \( T' \), respectively, by applying the subtree, long-chain, or short-chain reduction. Then \( f(T, T') = f(S, S') \).

**Proof:** It is an immediate consequence of Lemma 3.16 that if \( S \) and \( S' \) have been obtained from \( T \) and \( T' \) by an application of the subtree reduction, then the proposition holds. We next prove the result for when \( S \) and \( S' \) have been obtained from \( T \) and \( T' \) by applying the long-chain
reduction. The proof of the result for the short-chain reduction is similar and omitted.

Suppose that \((a_1, a_2, \ldots, a_n)\) is the common chain of \(\mathcal{T}\) and \(\mathcal{T}'\) used in this application of the long-chain reduction. Now let \(\mathcal{F}_T\) be a legitimate-agreement forest for \(\mathcal{T}\) and \(\mathcal{T}'\) of minimum weight. Then, by Lemma ?? one of the following holds:

(i) \(\{a_1, a_2, \ldots, a_n\}\) is a subset of a label set of \(\mathcal{F}_T\),

(ii) no label set in \(\mathcal{F}_T\) contains at least two elements of the chain and, if \(a_i\) is an internal element of both \(\mathcal{T}\) and \(\mathcal{T}'\), then \(\{a_i\}\) is a singleton in \(\mathcal{F}_T\), or

(iii) for either \(\mathcal{T}\) or \(\mathcal{T}'\), say \(\mathcal{T}\), two elements of the chain are in the same label set precisely if they have the same parent and, moreover, if that parent is internal in \(\mathcal{T}\), then the corresponding set contains no other elements of \(X \cup \{\rho\}\).

Let \(\mathcal{F}_S\) be the forest obtained from \(\mathcal{F}_T\) by replacing \(a_1\) and \(a_n\) with \(e_1\) and \(e_2\), respectively, if \(a_1\) or \(a_n\) is external in either \(\mathcal{T}\) or \(\mathcal{T}'\), and then, depending on which of (i), (ii), or (iii) holds, respectively replace the remaining elements of \(A\) as follows: replace \(a_1, a_2, \ldots, a_n\) with \(a, b,\) and \(c\); collectively replace the label sets of the form \(\{a_i\}\) with \(\{a\}\), \(\{b\}\), and \(\{c\}\); or collectively replace the label sets of the form \(\{a_i, a_{i+1}, \ldots, a_j\}\) with \(\{a_i\}\), \(\{b\}\), \(\{c\}\) and, if there is a label set of the form \(\{e_1, a_2, \ldots, a_{j'}\}\) or \(\{a_j', a_{j'+1}, \ldots, e_2\}\), replace it with \(\{e_1\}\) or \(\{e_2\}\), respectively. Since \(\mathcal{F}_T\) is a legitimate-agreement forest for \(\mathcal{T}\) and \(\mathcal{T}'\), it is easily checked that \(\mathcal{F}_S\) is a legitimate-agreement forest for \(S\) and \(S'\). In the case that (ii) holds, the contribution of the singletons containing elements that are internal in both \(\mathcal{T}\) and \(\mathcal{T}'\) to \(w(\mathcal{F}_T)\) is exactly the same as the contribution of \(\{a\}\), \(\{b\}\), and \(\{c\}\) to \(w(\mathcal{F}_S)\). Furthermore, in the case that (iii) holds, the contribution of the label sets containing just internal elements of \(A\) in \(\mathcal{T}\) to \(w(\mathcal{F}_T)\) is equal to the contribution of \(\{a, b\}\), \(\{c\}\), and \(\{e_1\}\) and \(\{e_2\}\) if either \(e_1\) or \(e_2\) are internal elements of the reduced chain in \(\mathcal{F}_S\) respectively, to \(w(\mathcal{F}_S)\). Thus \(w(\mathcal{F}_S) = w(\mathcal{F}_T)\), and so \(f(S, S') \leq f(\mathcal{T}, \mathcal{T}')\).

Now suppose that \(\mathcal{F}_S\) is a legitimate-agreement forest for \(S\) and \(S'\) of minimum weight. As \(\mathcal{F}_S\) is legitimate, one of the following holds, where \(e_1\) and \(e_2\) may or may not exist depending on whether \(a_1\) or \(a_n\) is external in either \(\mathcal{T}\) or \(\mathcal{T}'\):

(i) \(\{e_1, a, b, c, e_2\}\) is contained in a label set, \(\mathcal{L}\), say, in \(\mathcal{F}_S\),

(ii) \(\{a\}\), \(\{b\}\), and \(\{c\}\) are label sets in \(\mathcal{F}_S\), and \(e_1\) and \(e_2\) are in separate label sets in \(\mathcal{F}_S\),

(iii) \(\{a, b\}\) and \(\{c\}\) are label sets in \(\mathcal{F}_S\), and \(e_1\) and \(e_2\) are in separate label sets in \(\mathcal{F}_S\) and, relative to \((e_1, a, b, c, e_2)\), if \(e_1\) or \(e_2\) is internal in \(\mathcal{T}\), then \(\{e_1\}\) or \(\{e_2\}\) is a label set in \(\mathcal{F}_S\).
respectively, or

(iv) \( \{a\} \) and \( \{b, c\} \) are label sets in \( F_S \), and \( e_1 \) and \( e_2 \) are in separate label sets in \( F_S \) and, relative to \( (e_1, a, b, c, e_2) \), if \( e_1 \) or \( e_2 \) is internal in \( T' \), then \( \{e_1\} \) or \( \{e_2\} \) is a label set in \( F_S \), respectively.

Let \( F_T \) be the forest obtained from \( F_S \) by replacing \( e_1 \) and \( e_2 \) with \( a_1 \) and \( a_n \), respectively, if \( a_1 \) or \( a_n \) is external in either \( T \) or \( T' \), and then, depending on which of (i) to (iv) holds, make one of the following replacements for \( a, b, \) and \( c \):

(i) \( \mathcal{L} \) with \( (\mathcal{L} \setminus \{a, b, c\}) \cup A \),

(ii) \( \{a\}, \{b\}, \) and \( \{c\} \) with the sets \( \{a_i\} \), where \( a_i \) is an internal element in both \( T \) and \( T' \),

(iii) \( \{a, b\} \) and \( \{c\} \) with the parts of the parent partition of \( (a_1, a_2, \ldots, a_n) \) induced by \( T \) whose corresponding parents are internal in \( T \), and deleting \( \{a_1\} \) or \( \{a_n\} \) if \( e_1 \) or \( e_2 \) is internal in \( S \), or

(iv) \( \{a\} \) and \( \{b, c\} \) with the parts of the parent partition of \( (a_1, a_2, \ldots, a_n) \) induced by \( T' \) whose corresponding parents are internal in \( T' \), and deleting \( \{a_1\} \) or \( \{a_n\} \) if \( e_1 \) or \( e_2 \) is internal in \( S' \).

A routine check shows that, as \( F_S \) is a legitimate-agreement forest for \( S \) and \( S' \), the collection \( F_T \) of sets is a legitimate-agreement forest for \( T \) and \( T' \). In (ii), the contribution of the singletons \( \{a\}, \{b\}, \) and \( \{c\} \) to \( w(F_S) \) is the same as the contribution of the sets \( \{a_i\} \) to \( w(F_T) \), where \( a_i \) is an internal element of both \( T \) and \( T' \). Furthermore, in (iii), and analogously in (iv), the contribution of \( \{a, b\} \) and \( \{c\} \), and \( \{e_1\} \) and \( \{e_2\} \) if \( e_1 \) or \( e_2 \), respectively, are internal in \( S \) to \( w(F_S) \) is equal to the contribution of the label sets in \( F_T \) which exclusively contain internal elements of \( A \) in \( T \) to \( w(F_T) \). Thus \( w(F_T) = w(F_S) \), and so \( f(T, T') \leq f(S, S') \). Hence \( f(T, T') = f(S, S') \), completing the proof of the proposition.

Lemma 6.2: Let \( T \) and \( T' \) be a pair of weighted rooted phylogenetic X-trees, and let \( (a_1, a_2, \ldots, a_n) \) be a maximal chain of \( T \) and \( T' \) that does not cross \( P \). Then, by a sequence of long- and short-chain reductions applied to this chain, the length of the resulting chain is at most 17.

Proof: Suppose first that there is an element of the chain that is internal in both \( T \) and \( T' \). With \( i \leq j \), choose \( a_i \) and \( a_j \) as follows:

(a) If \( a_1 \) is internal in both \( T \) and \( T' \), choose \( a_i \) to be \( a_1 \). If \( a_1 \) is external in both \( T \) and \( T' \), but \( a_2 \) is internal in both \( T \) and \( T' \), choose \( a_i \) to be \( a_2 \). Otherwise, for some \( R \in \{T, T'\} \),
$a_1$ and $a_2$ are external in $R$. In this case, choose $a_i$ to be the element of the chain that is external in $R$ and has maximum index with $a_1, a_2, \ldots, a_i$ all external in $R$.

(b) If $a_n$ is internal in both $T$ and $T'$, choose $a_j$ to be $a_n$. If $a_n$ is external in both $T$ and $T'$, but $a_{n-1}$ is internal in both $T$ and $T'$, choose $a_j$ to be $a_{n-1}$. Otherwise, for some $S \in \{T, T'\}$, $a_n$ and $a_{n-1}$ are external in $S$. In this case, choose $a_j$ to be the element of the chain that is external in $S$ and has minimum index with $a_j, a_{j+1}, \ldots, a_n$ all external in $S$.

Having picked $a_i$ and $a_j$, consider the chain $(a_i, a_{i+1}, \ldots, a_j)$. If this chain satisfies (i) and the condition on internal parents at the end of (iii) in the description of the long-chain reduction, then we can apply this reduction to get a chain with at most 5 elements. Furthermore, if $(a_1, a_2, \ldots, a_{i-1})$ is a chain with at least three internal elements in the tree in $\{T, T'\}$ that is not $R$, then we can apply the short-chain reduction to get a chain with at most 3 elements. Lastly, if $(a_j+1, a_{j+2}, \ldots, a_n)$ is a chain with at least three internal elements in the tree in $\{T, T'\}$ that is not $S$, then we can again apply the short-chain reduction to get a chain with at most 3 elements. Note that if we cannot apply the first or the second of these short-chain reductions, then $i - 1 \leq 3$ and $n - j \leq 3$, respectively. It now follows that after these three reductions, the resulting chain has length at most 11.

Now assume that $(a_i, a_{i+1}, \ldots, a_j)$ does not satisfy (i) or the condition on internal parents at the end of (iii) in the description of the long-chain reduction. Then, up to the possibility of an additional internal parent which only has $a_j$ as its only child in $\{a_i, a_{i+1}, \ldots, a_j\}$, this chain has at most two internal parents in either $T$ or $T'$. Except for the children of these two parents, all of the remaining elements of $\{a_1, \ldots, a_n\}$ are external in either $T$ or $T'$. In particular, $a_1, \ldots, a_{i-1}$ share the same parent in $R$, and $a_{j+1}, \ldots, a_n$ share the same parent in $S$. As $(a_1, a_2, \ldots, a_n)$ has an internal element in both $T$ and $T'$, these two shared parents are distinct. Applying at most four short-chain reductions, it is easily checked that the resulting chain has length at most 17.

Now suppose that no element of the chain is internal in both $T$ and $T'$, then each element of the chain is external in either $T$ or $T'$. In this case, either we apply a single application of the short-chain reduction to get a chain of length at most 4 or we apply two applications of the short-chain reduction to get a chain of length at most 8. This completes the proof of the lemma.

Proposition ?? showed that the weight function is preserved under each of the three reductions. Part (iii) of the next lemma shows that these reductions can be applied so that the size of the label
set of the resulting rooted phylogenetic trees is bounded by a linear function in the minimum hybridization number.

**Lemma 6.3:** Let $T$ and $T'$ be two rooted phylogenetic $X$-trees, and let $P$ initially be an empty collection of subsets of $X$. Let $S$ and $S'$ be two weighted rooted phylogenetic $X'$-trees obtained from $T$ and $T'$, respectively, by repeatedly applying the subtree reduction until no further reduction is possible, and then, for each maximal chain common to both resulting trees, repeatedly applying the long-chain and short-chain reductions. Then

(i) $S$ and $S'$ have no pendant subtrees with common label set $A$ such that $S|A$ and $S'|A$ have a common binary refinement and $|A| \geq 2$,

(ii) the length of any chain common to both $S$ and $S'$ is at most 17, and

(iii) $|X'| < 89h(T, T')$.

**Proof:** For the proof of (i) and (ii), let $T_1$ and $T'_1$ be the rooted phylogenetic trees obtained from $T$ and $T'$ after repeatedly applying the subtree reduction until no further reduction is possible. Furthermore, observe that if $P_1, P_2 \in P$, then $S(P_1)$ and $S(P_2)$ are edge-disjoint, and $S'(P_1)$ and $S'(P_2)$ are edge-disjoint. Suppose that (i) does not hold, and let $A$ be such a label set. Without loss of generality, we may assume that $A$ is maximal. Then, because of maximality, if $A$ intersects a set in $P$, then that set is a subset of $A$. Now let $A'$ be the set obtained from $A$ by replacing the elements belonging to a set in $P$ with their original counterparts. Using the above observation, it is easily seen that $A'$ is a pendant subtree of $T_1$ and $T'_1$. But, as $S|A$ and $S'|A$ have a common binary refinement, $T_1|A'$ and $T'_1|A'$ have a common binary refinement; a contradiction. Thus (i) holds.

For (ii), suppose that there exists a chain common to both $S$ and $S'$ that has at least 18 elements. Without loss of generality, we may assume that this chain is maximal. Let $A$ denote the label set of this common chain. Analogous to (i), because of maximality, if $A$ intersects a set in $P$, then that set is a subset of $A$. Now let $A'$ be the set obtained from $A$ by replacing the elements belonging to a set in $P$ with their original counterparts. Using the above observation, it is easily seen that $A'$ is a pendant subtree of $T_1$ and $T'_1$. But, as $S|A$ and $S'|A$ have a common binary refinement, $T_1|A'$ and $T'_1|A'$ have a common binary refinement; a contradiction. Thus (ii) holds.

Now consider (iii). Let $\mathcal{F} = \{L_\rho, L_1, L_2, \ldots, L_k\}$ be a legitimate-agreement forest for $S$ and $S'$ of minimum weight. Let $B$ and $B'$ be two binary refinements of $S$ and $S'$, respectively, so that $\mathcal{F}$ is an acyclic-agreement forest for $B$ and $B'$. By Lemma ??, such binary refinements exist.
If \( B \) and \( B' \) have a common pendant subtree with label set \( A \) and \(|A| \geq 2\), then this subtree is a common binary refinement of \( S|A \) and \( S'|A \), contradicting (i). Thus \( B \) and \( B' \) have no such pendant subtree. Furthermore, if \( B \) and \( B' \) have a common chain with label set \( A \) and \(|A| \geq 18\), then this implies that \( S \) and \( S' \) have such a chain, contradicting (ii). Hence any chain common to both \( B \) and \( B' \) has at most 17 elements. With these restrictions on \( B \) and \( B' \), we can now use the argument for the analogous result for binary trees in [?] to complete the proof of (iii).

The only modification necessary is to replace chains of size 2 with chains of size at most 17. Making this change and working through the straightforward algebra gives \( \sum_{i} |L_i| \leq 89k - 51 \).

By definition of \( f \) and Proposition ??, \( k \leq f(S, S') = f(T, T') \). Since \( P \) is initially empty, \( f(T, T') = h(T, T') \) and the result follows.

**Proof of Theorem ??:** Let \( T \) and \( T' \) be two rooted phylogenetic \( X \)-trees, and let \( P \) be an empty collection of subsets of \( X \). Let \( k \) be an integer. Let \( S \) and \( S' \) be the weighted rooted phylogenetic \( X' \)-trees obtained from \( T \) and \( T' \) by repeatedly applying the subtree reduction until no further reduction is possible, and then, for each maximal chain common to both resulting trees, repeatedly applying the long-chain and short-chain reductions. As \( P \) is empty, \( h(T, T') = f(T, T') \) and so, by Proposition ??,

\[
h(T, T') = f(T, T') = f(S, S').
\]

It is clear that \( S \) and \( S' \) can be found in time polynomial in \(|X|\), say \( p(|X|) \). By Lemma ??(iii), \(|X'| \leq 89h(T, T')\) and so, if \(|X'| > 89k\), we declare that \( h(T, T') > k \).

Now suppose that \(|X'| \leq 89k\). The time taken to check whether a partition of \( X' \cup \{\rho\} \) is a legitimate-agreement forest for \( S \) and \( S' \) takes time polynomial in \( k \). Note that for deciding if two rooted phylogenetic trees \( T_1 \) and \( T'_1 \) have a common binary refinement, one simply needs to check whether or not \( C(T_1) \cup C(T'_1) \) is a hierarchy, that is, for all (edge) clusters \( C_1, C_2 \in C(T_1) \cup C(T'_1) \), the set \( C_1 \cap C_2 \in \{\emptyset, C_1, C_2\} \). Furthermore, as \(|X'| \leq 89k\), the number of forests with at most \( k + 1 \) parts is bounded by a computable function in \( k \), say \( f(k) \). If one of these forests is a legitimate-agreement forest for \( S \) and \( S' \) with weight at most \( k \), then we declare \( h(T, T') \leq k \); otherwise, we declare \( h(T, T') > k \). Hence we can answer the *Hybridization Number* decision problem for \( T \) and \( T' \) in time \( O(f(k) + p(|X|)) \). Thus *Hybridization Number* is fixed-parameter tractable. $\blacksquare$
**Remark.** While one could explicitly give a function in $k$ that bounds the number of partitions to consider in the proof of Theorem ??, it is unlikely to be the best theoretically and we expect in practice much better methods.

**VII. CONCLUDING REMARKS**

We end the paper with some remarks.

1. In this paper, we reduced a chain using two types of chain reductions. However, we believe that it is possible to do this with a single type of chain reduction. The drawback of such a reduction is that the number of possibilities for a legitimate-agreement forest for $\mathcal{T}$ and $\mathcal{T}'$ increases. Since the goal of the paper is to show that HYBRIDIZATION NUMBER is fixed-parameter tractable, we decided to use the two types of reductions, thereby reducing the complexity and lengths of the proofs.

2. The subtree, long-chain, and short-chain reductions are enough to kernalize HYBRIDIZATION NUMBER and yield an algorithm that is fixed-parameter tractable. These reductions extend the two reductions used to kernalize HYBRIDIZATION NUMBER when the initial two trees are both binary [?]. However, there is another type of reduction for binary trees that turns out to be particularly useful. This additional reduction, called the *cluster reduction* [?], allows for an attractive divide-and-conquer approach that breaks the problem into a number of smaller and, therefore, more tractable subproblems. Details on how this reduction can easily be fitted into the framework of (arbitrary) rooted phylogenetic trees can be found in [?].

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