A STRUCTURE THEOREM FOR TREE-BASED PHYLOGENETIC NETWORKS

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ABSTRACT. Attempting to recognize a tree inside a phylogenetic network is a fundamental undertaking in evolutionary analysis. Therefore, the concept of “tree-based” phylogenetic networks, which was introduced by Francis and Steel, has attracted much attention of theoretical biologists in the last few years. In this context, spanning trees of a certain kind called “subdivision trees” play an essential role and there are many important computational problems about them, whose time complexity is still unclear. Against this backdrop, the present paper aims to provide a graph theoretical framework for solving different problems on subdivision trees in a simple and unified manner. To this end, we focus on a structure called the maximal zig-zag trail decomposition that is inherent in any rooted binary phylogenetic network $N$ and prove a structure theorem that characterizes the collection of all subdivision trees of $N$. Our theorem does not only imply and unify various results in the literature but also yield linear time (for enumeration, linear delay) algorithms for the following problems: given a rooted binary phylogenetic network $N$, 1) determine whether or not $N$ has a subdivision tree and find one if there exists any (decision/search problem); 2) compute the number of subdivision trees of $N$ (counting problem); 3) list all subdivision trees of $N$ (enumeration problem); and 4) find a subdivision tree to maximize or minimize a prescribed objective function (optimization problem). Importantly, the results and algorithms in this paper still hold true for some non-binary phylogenetic networks, and this generalization gives a partial answer to an open question from Pons, Semple, and Steel. We also mention some statistical applications and further research directions.

1. INTRODUCTION

Although phylogenetic networks are widely used to describe non-tree-like evolution or to represent conflicts in data or uncertainty in evolutionary histories (e.g., [2, 3, 8, 15]), phylogenetic trees are still regarded as a fundamental model of evolution for their ultimate simplicity. Therefore, it is an essential undertaking to try to recognize a tree within a phylogenetic network (e.g., [12, 17]), which gives a possible explanation for Francis and Steel’s philosophy behind their definition of “tree-based” phylogenetic networks [5] (see also [15]).

Intuitively, tree-based phylogenetic networks can be seen as a natural generalization of phylogenetic trees since they are merely trees with additional arcs [5]. In the last few years, tree-based networks have attracted much attention of theoretical biologists and their mathematical and computational aspects have been actively studied (e.g., [1, 7, 10, 13, 18]). In this context, although we will provide formal definitions later, the notion of “subdivision trees” plays an essential role because tree-based networks can be defined as those having at least one subdivision trees.

In the theory of computational complexity, the most fundamental type of questions is concerning the time complexity of a decision/search problem, such as the problem of determining whether or not a given phylogenetic network $N$ is tree-based and finding a subdivision tree of $N$ if there exists any. In [5], Francis and Steel proved that this problem can be formulated as the 2-satisfiability (2-SAT) problem and provided a linear time algorithm for solving it. Then, in view of the fact that computing the number of satisfying solutions of 2-SAT is #P-complete [16], they conjectured that the problem of counting all subdivision trees of $N$ might also be hard [5].

2010 Mathematics Subject Classification. 05C75 (Primary), 05C30, 05C20, 05C05, 05C85, 05C90, 92D15.

Key words and phrases. phylogenetic tree, tree-based phylogenetic network, subdivision tree, counting, enumeration, optimization, quantifying the complexity of phylogenetic networks.

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Including the above counting problem, below we pose a series of computational problems surrounding subdivision trees, with the overarching aim to explore new applications of tree-based phylogenetic networks.

- **Counting problem**: given a rooted binary phylogenetic network $N$, count the number $\alpha(N)$ of subdivision trees of $N$. In contrast to a similar tree-counting problem that is #P-complete \[12\], this problem can be solved in polynomial time as indicated by the formulae for $\alpha(N)$ that were obtained in \[10, 13\]. This counting problem has an interesting connection to the data analysis for quantifying the complexity of phylogenetic networks because networks having many spanning trees tend to be more complex than those with only a few. Thus, it is meaningful to analyze the time complexity of this problem in more details and to develop a fast algorithm for counting $\alpha(N)$.

- **Enumeration problem**: given a rooted binary phylogenetic network $N$, list all subdivision trees $T_1, \ldots, T_{\alpha(N)}$ of $N$. It is obvious that the time complexity of this problem is exponential in the size of $N$ \[5\], but this does not deny the existence of a fast algorithm. Indeed, we need a fuller complexity analysis because in the usual context of algorithm theory, the time complexity of enumeration problems is evaluated in terms of the size of both input and output. It is also important to consider a fast enumeration algorithm because listing a designated number of solutions, rather than all, enables statistical applications such as generating subdivision trees of $N$ uniformly at random.

- **Optimization problem**: given a rooted binary phylogenetic network $N$ together with a non-negative weighting $w$ on the arcs of $N$, find a subdivision tree $T$ of $N$ to maximize (or minimize) the value of a prescribed objective function $f(T)$. From a statistical perspective, this problem can be viewed as modeling the situation where a phylogenetic network $N$ and the probability $w$ of the arcs of $N$ are given and we wish to estimate the best-fit tree $T$ inside $N$ to maximize the likelihood or log-likelihood $f(T)$. An obvious algorithm computes the values $f(T_1), \ldots, f(T_{\alpha(N)})$ of the objective function, which requires exponential time in the size of $N$. The question is whether it is possible or not to obtain an optimal solution without doing such an exhaustive search.

The main goal of this paper is to provide a graph theoretical framework for solving many different problems on subdivision trees, including the above-mentioned ones, in a simple and unified manner. To this end, we prove a “structure theorem for tree-based phylogenetic networks” (Theorem 4.4) that characterizes the (possibly empty) collection $\mathcal{F} = \{T_1, \ldots, T_{\alpha(N)}\}$ of all subdivision trees of a given rooted binary phylogenetic network $N$. Our theorem furnishes linear time (for enumeration, linear delay) algorithms for the above problems.

Furthermore, we must stress that the results and algorithms in this paper still hold true for some non-binary phylogenetic networks. Hence, we can obtain a partial answer to the question from Pons, Semple, and Steel \[13\] as to what the number $\alpha(N)$ is when $N$ is not necessarily binary. This is an interesting byproduct that illustrates an advantage of our structural approach compared to earlier work exploiting existing tools such as 2-SAT algorithms \[5\] and Hall’s marriage theorem \[9\] \[10\] \[13\] \[18\].

The remainder of this paper is organized as follows. We set up basic definitions and notation in Section 2 and give a more detailed description of the above motivating problems in Section 3. In Section 4, we introduce a structure called the “maximal zig-zag trail decomposition” that is inherent in each rooted binary phylogenetic network (Lemma 4.2). Using this key lemma along with a structural version of Francis and Steel’s theorem (Lemma 4.3), we state and prove our main result as in Theorem 4.4. Section 5 is about the algorithmic implications of the theorem; we describe a series of algorithms for the problems posed in Section 3 and give a numerical
example where appropriate. Section 6 contains a brief summary of relevant research with the intention to show that our theorem implies and unifies various results in the literature. Finally, we conclude the paper by suggesting two possible directions for further research in Section 7, where we provide a conjecture on a related open problem raised in [5] and also derive a partial solution to the aforementioned problem posed by Pons et al. [13].

2. Preliminaries

Throughout this paper, $X$ denotes a non-empty finite set, and the terms “graph” and “network” all refer to finite, simple, acyclic digraphs (directed graphs), which we now define. A digraph is an ordered pair $(V, A)$ of a set $V$ of vertices and a set $A$ of arcs (i.e., directed edges). Given a digraph $G$, we write $V(G)$ and $A(G)$ to represent the sets of vertices and arcs of $G$, respectively. If $V(G)$ and $A(G)$ are finite sets, then $G$ is said to be finite. We use the notation $(u, v)$ for an arc $a$ oriented from a vertex $u$ to a vertex $v$, and also write $\text{head}(a)$ and $\text{tail}(a)$ to mean $u$ and $v$, respectively. A digraph $G$ is said to be simple if $\text{head}(a) \neq \text{tail}(a)$ holds for any $a \in A(G)$ and $(\text{head}(a), \text{tail}(a)) \neq (\text{head}(a'), \text{tail}(a'))$ holds for any $a, a' \in A(G)$ with $a \neq a'$. A simple digraph $G$ is said to be acyclic if $G$ has no cycle, namely, there is no sequence $(a_0, a_1, \ldots, a_k)$ of three or more elements of $A(G)$ such that $\text{head}(a_{i-1}) = \text{tail}(a_i)$ holds for each $i \in [1, k]$, with indices taken mod $k$.

For graphs $G$ and $H$, $G$ is called a subgraph of $H$ if both $V(G) \subseteq V(H)$ and $A(G) \subseteq A(H)$ hold, in which case we write $G \subseteq H$. A subgraph $G \subseteq H$ is said to be proper if we have either $V(G) \neq V(H)$ or $A(G) \neq A(H)$. A subgraph $G \subseteq H$ is said to be spanning if $V(G) = V(H)$ holds. Given a graph $G$ and a subset $A' \subseteq A(G)$, $A'$ is said to induce the subgraph $G[A'] := (V(A'), A')$ of $G$, where $V(A')$ denotes a set of the heads and tails of all arcs in $A'$. Besides, given a graph $G$ with $|A(G)| \geq 1$ and a partition $\{A_1, \ldots, A_\ell\}$ of $A(G)$, the collection $\{G[A_1], \ldots, G[A_\ell]\}$ is called a decomposition of $G$, where a partition of a set $S$ is defined to be a collection of non-empty disjoint subsets of $S$ whose union is $S$.

For a vertex $v$ of a digraph $N$, the in-degree and out-degree of $v$ in $N$, denoted by $\text{deg}_N^-(v)$ and $\text{deg}_N^+(v)$, are defined to be the cardinalities of the sets $\{a \in A(N) \mid \text{head}(a) = v\}$ and $\{a \in A(N) \mid \text{head}(a) = v\}$, respectively. Given an acyclic digraph $N$, a vertex $v \in V(N)$ is called a leaf of $N$ if $(\text{deg}_N^-(v), \text{deg}_N^+(v)) = (1, 0)$ holds.

**Definition 2.1.** Given a finite set $X$, a rooted binary phylogenetic $X$-network is defined to be any finite simple acyclic digraph $N$ that has the following properties:

1. there exists a unique vertex $\rho$ of $V(N)$ with $\text{deg}_N^-(\rho) = 0$ and $\text{deg}_N^+(\rho) \in \{1, 2\}$;
2. $X$ is the set of leaves of $N$;
3. each vertex $v \in V(N) \setminus (X \cup \{\rho\})$ satisfies $\{\text{deg}_N^-(v), \text{deg}_N^+(v)\} = \{1, 2\}$.

In Definition [2.1], the vertex $\rho$ is called the root of $N$, which can be interpreted as the origin of all species that are signified by the leaves of $N$. In addition, we call $v \in V(N) \setminus (X \cup \{\rho\})$ a tree vertex of $N$ if $(\text{deg}_N^-(v), \text{deg}_N^+(v)) = (1, 2)$ holds, and a reticulation vertex of $N$ otherwise. In the case when $N$ has no reticulation vertex, $N$ is called a rooted binary phylogenetic $X$-tree.

**Definition 2.2** ([5]; see also [13]). For any rooted binary phylogenetic $X$-network $N$, a subdivision tree of $N$ is defined to be a spanning tree $T$ of $N$ that can be obtained from a rooted binary phylogenetic $X$-tree $\tilde{T}$ by inserting zero or more vertices into each arc of $\tilde{T}$.

**Definition 2.3** ([5]). Suppose $N$ is a subgraph of a rooted binary phylogenetic $X$-network. We say that a subset $S$ of $A(N)$ is admissible if $S$ satisfies the following conditions:

- **C0:** $S$ contains all $(u, v) \in A(N)$ with $\text{deg}_N^-(v) = 1$ or $\text{deg}_N^+(u) = 1$. 

C1: for any \( a_1, a_2 \in A(N) \) with \( \text{head}(a_1) = \text{head}(a_2) \), exactly one of \( \{a_1, a_2\} \) is in \( S \).

C2: for any \( a_1, a_2 \in A(N) \) with \( \text{tail}(a_1) = \text{tail}(a_2) \), at least one of \( \{a_1, a_2\} \) is in \( S \).

### 3. Motivating problems

Here, we provide the relevant background on “tree-based” phylogenetic networks in order to describe the problems to be addressed in this paper. We say that a rooted binary phylogenetic \( X \)-network \( N \) is a tree-based phylogenetic network (on \( X \)) if \( N \) has at least one subdivision tree (see [5] for the original definition). Intuitively, tree-based networks can be viewed as a natural extension of rooted binary phylogenetic \( X \)-trees because they are merely trees with additional arcs. In [5], Francis and Steel gave an algorithmic characterization of this class of networks. More precisely, they proved that the following decision/search problem can be formulated as the 2-SAT problem and described a linear time algorithm for finding a subdivision tree of \( N \) if there exists any as a consequence of Theorem 3.1. Thus, they have shown that the following decision/search problems can be solved in linear time.

**Problem 1 ([5]).** Given a rooted binary phylogenetic \( X \)-network \( N \), determine whether or not \( N \) is a tree-based network on \( X \) and find a subdivision tree of \( N \) if there exists any.

**Theorem 3.1 ([5]).** Given a rooted binary phylogenetic \( X \)-network \( N \), any subdivision tree of \( N \) is a subgraph \( N[S] \) of \( N \) induced by an admissible subset \( S \) of \( A(N) \). Moreover, there exists a bijection between the families of admissible subsets \( S \) of \( A(N) \) and of arc-sets of subdivision trees of \( N \).

Then, the question arises: what is the time complexity of the following counting problem? Francis and Steel [5] noted that counting the number \( \alpha(N) \) of subdivision trees of a tree-based phylogenetic network \( N \) might also be \#P-complete as counting the number of satisfying solutions of 2-SAT is known to be \#P-complete [16]. Contrary to this conjecture, Jetten [9] and Pons et al. [13] derived equivalent formulae for \( \alpha(N) \) that indicate the existence of a polynomial time algorithm for it. However, a more detailed time complexity analysis has not been provided to date.

**Problem 2 ([5]).** Given a rooted binary phylogenetic \( X \)-network \( N \), count the number \( \alpha(N) \) of subdivision trees of \( N \).

In addition to the above two, let us describe some associated problems. The first question is whether there exists an efficient algorithm for the following enumeration problem.

**Problem 3.** Given a rooted binary phylogenetic \( X \)-network \( N \), list all subdivision trees \( T_1, \ldots, T_{\alpha(N)} \) of \( N \).

In general, the number of solutions of enumeration problems can be exponential in the size of input or even infinite. In the usual context of algorithm theory, therefore, the time complexity of listing combinatorial structures has been analyzed in terms of both input size and output size. In particular, polynomial delay algorithms [11], which generate all solutions one after another such that the time between the output of any two consecutive solutions is bounded by a polynomial function in the input size, is considered as one of the most efficient classes of enumeration algorithms [6]. Those algorithms are fast indeed as their running time is linear with respect to the size of the output. Hence, even though the number of solutions of Problem 3 is exponential in the size of \( N \) [5], if there exists a polynomial delay algorithm for it, then the problem turns out to be tractable, leading to statistical applications such as generating a subdivision tree of \( N \) uniformly at random.

The next question is whether the following optimization problem can be solved in polynomial time in the size of \( N \). Note that we can convert Problem 4 into a minimization problem by
changing the sign or use the objective function $f(T) = \prod_{a \in A(T)} w(a)$ by taking the exponential. Applications of this problem include the setting where, given a phylogenetic network $N$ and the probability $w$ of the arcs of $N$, we wish to estimate a subdivision tree $T$ of $N$ to maximize the likelihood or log-likelihood $f(T)$.

**Problem 4.** Given a rooted binary phylogenetic $X$-network $N$ and an associated weighting function $w : A(N) \to \mathbb{R}_{\geq 0}$, find a subdivision tree $T$ of $N$ to maximize the value of the objective function $f(T) = \sum_{a \in A(T)} w(a)$.

### 4. Structure theorem for tree-based phylogenetic networks

For a rooted binary phylogenetic $X$-network $N$, we define a zig-zag trail in $N$ as a connected subgraph $Z$ of $N$ with $|A(Z)| \geq 1$ such that there exists a permutation $(a_1, \ldots, a_m)$ of $A(Z)$ where either $\text{head}(a_1) = \text{head}(a_{i+1})$ or $\text{tail}(a_1) = \text{tail}(a_{i+1})$ holds for each $i \in [1, m - 1]$. Any zig-zag trail $Z$ in $N$ can be expressed by an alternating sequence of (not necessarily distinct) vertices and distinct arcs, such as $(v_0, (v_0, v_1), v_1, (v_2, v_3), v_2, (v_2, v_3), \ldots, (v_m, v_{m-1}), v_m)$; however, we will more concisely represent above $Z$ by writing $v_0 > v_1 < v_2 > v_3 < \cdots > v_{m-1} < v_m$ or in reverse order. The notation $(a_1, \ldots, a_m)$ may be also used when no confusion arises.

A zig-zag trail $Z$ in $N$ is said to be maximal if $N$ contains no zig-zag trail $Z'$ such that $Z$ is a proper subgraph of $Z'$. Any maximal zig-zag trail $Z$ in $N$ falls into one of the four types, which are defined as follows (see also Figure 1). A maximal zig-zag trail $Z$ in $N$ with even $m := |A(Z)| \geq 4$ is called a crown if $Z$ can be written in the form $v_0 < v_1 < v_2 > v_3 < \cdots > v_{m-2} < v_{m-1} > v_m = v_0$; otherwise, it is called a fence. Furthermore, a fence $Z$ with odd $m := |A(Z)| \geq 1$ is called an $N$-fence, which can be expressed as $Z : v_0 > v_1 < v_2 > v_3 < \cdots > v_{m-2} < v_{m-1} > v_m$. Also, a fence $Z$ with even $m \geq 2$ is called a $W$-fence if it can be written as $Z : v_0 > v_1 < v_2 > v_3 < \cdots < v_{m-2} > v_{m-1} < v_m$ while it is called an $M$-fence if it can be written as $Z : v_0 < v_1 > v_2 < v_3 > \cdots > v_{m-2} < v_{m-1} > v_m$. For any fence $Z$, its vertices $v_0$ and $v_m$ on both ends are called the endpoints of $Z$.

**Remark 4.1.** Although the terms fence and crown in the theory of partially ordered sets usually refer to those that can be represented using bipartite graphs as in Figure 1 (the interested reader is referred to [14]), in our terminology, such an atypical $M$-fence as in Figure 2 is also allowed.

![Figure 1](image1.png)

**Figure 1.** An illustration of the four cases of maximal zig-zag trails $Z$ in $N$. Top left is a crown. Bottom left shows an $N$-fence. On the right are a $W$-fence (top) and an $M$-fence (bottom).

The following lemma is essential to state our subsequent structural results as it describes a structure inherent in each rooted binary phylogenetic $X$-network.
Lemma 4.2. For any rooted binary phylogenetic $X$-network $N$, there exists a unique decomposition $\mathcal{Z} = \{Z_1, \ldots, Z_\ell\}$ of $N$ such that each $Z_i \in \mathcal{Z}$ is a maximal zig-zag trail in $N$.

Proof. The proof is divided into two parts. We first claim that $A(Z_i) \cap A(Z_j) = \emptyset$ holds for any $i, j \in [1, \ell]$ with $i \neq j$. Indeed, any zig-zag trails $Z$ and $Z'$ in $N$ have a common arc if and only if either $Z \subseteq Z'$ or $Z \supseteq Z'$ holds because $N$ would contain a vertex of in-degree or out-degree $\geq 3$ otherwise. Then, the claim follows from the maximality of $Z_i$ and $Z_j$. Next, we will prove that for any $a \in A(N)$, there exists a unique element $Z_i$ of $\mathcal{Z}$ with $a \in A(Z_i)$. For any $a \in A(N)$, there exists an obvious zig-zag trail $Z$ in $N$, that is, $Z : \text{tail}(a) > \text{head}(a)$. Then, because $N$ is finite, there exists maximal one $Z_i \in \mathcal{Z}$ with $Z \subseteq Z_i$. By using the first claim, we can conclude that such $Z_i$ is uniquely determined by $a$. This completes the proof. \hfill \Box

Figure 2. An illustrative example mentioned in Remark 4.1. The above shows a possible maximal M-fence in $N$ that can be written in the form $v_0 < v_1 > v_2 < v_3 > v_4$.

Figure 3. Examples of maximal zig-zag trail decomposition as in Lemma 4.2 where different types of lines are used to highlight distinct maximal zig-zag trails in each rooted binary $X$-phylogenetic network with $X = \{x_1, x_2, x_3\}$. The network on the left is decomposed into 3 maximal M-fences, 2 maximal N-fences, and 1 maximal W-fence. On the right is the maximal zig-zag trail decomposition of a network discussed in [5], where the M-fence isomorphic to the one in Figure 2 is shown in bold solid arrows.

Using the idea of maximal zig-zag trail decomposition, we can state a structural version of Theorem 3.1 as follows.

Lemma 4.3. Let $N$ be a rooted binary phylogenetic $X$-network and $\mathcal{Z} = \{Z_1, \ldots, Z_\ell\}$ be the maximal zig-zag trail decomposition of $N$. Then, $S \subseteq A(N)$ is an admissible subset of $A(N)$ if and only if $S_i := S \cap A(Z_i)$ is an admissible subset of $A(Z_i)$ for each $i \in [1, \ell]$. 
Proof. Our goal is to prove that $S$ satisfies the conditions $C0$, $C1$, and $C2$ in Definition \[2.3\] if and only if for each $i \in \{1, \ell\}$, the following $C0'$, $C1'$, and $C2'$ hold:

$C0'$: $S_i$ contains all $(u, v) \in A(Z_i)$ with $\deg^-_{Z_i}(v) = 1$ or $\deg^+_Z(u) = 1$;

$C1'$: for any $a_1, a_2 \in A(Z_i)$ with $\head(a_1) = \head(a_2)$, exactly one of $\{a_1, a_2\}$ is in $S_i$;

$C2'$: for any $a_1, a_2 \in A(Z_i)$ with $\tail(a_1) = \tail(a_2)$, at least one of $\{a_1, a_2\}$ is in $S_i$.

If $(u, v) \in A(N)$ satisfies $\deg^-_{N}(v) = 1$ (or $\deg^+_N(u) = 1$), then there exists a unique element $Z_i$ of $\mathcal{Z}$ with $(u, v) \in A(Z_i)$ and $\deg^-_{Z_i}(v) = 1$ (or $\deg^+_Z(u) = 1$) by Lemma \[4.2\]. The converse also holds as $Z_i$ would not be maximal otherwise. Lemma \[4.2\] also implies that $S$ is partitioned into $S_1,\ldots,S_\ell$ (note that no element of $S$ is empty). Thus, we can assert that $S$ satisfies $C0$ if and only if $C0'$ holds for each $i \in \{1, \ell\}$. By similar reasoning, we can deduce that $\{a_1, a_2\} \subseteq A(N)$ satisfies $\head(a_1) = \head(a_2)$ if and only if there exists a unique element $Z_i$ of $\mathcal{Z}$ such that $\{a_1, a_2\} \subseteq A(Z_i)$ has the same property. Recalling that $\{S_1,\ldots,S_\ell\}$ is a partition of $S$, we have $S \cap \{a_1, a_2\} = S_i \cap \{a_1, a_2\}$ for any $i \in \{1, \ell\}$ and any $a_1, a_2 \in A(Z_i)$ with $\head(a_1) = \head(a_2)$.

Hence, $S$ satisfies $C1$ if and only if $C1'$ holds for each $i \in \{1, \ell\}$. The same arguments derive the desired conclusion regarding $C2$ and $C2'$.

This completes the proof.

From now on, we consider an ordered set $(Z_1, \ldots, Z_\ell)$ of maximal zig-zag trails in $N$ so that we can identify a subgraph $G$ of $N$ with a direct product $\prod_{i \in \{1, \ell\}} A(G) \cap A(Z_i)$. In addition, for each $i \in \{1, \ell\}$, we represent the set $A(Z_i)$ using a sequence $(a_1,\ldots,a_m)$ of the elements of $A(Z_i)$ that form the zig-zag trail in this order, where $m_i := |A(Z_i)|$. This allows us to encode arbitrary subset of $A(Z_i)$ using a 0-1 sequence of length $m_i$. For example, given $A(Z_i) = (a_1, a_2, a_3, a_4, a_5)$, we can specify the subset $(a_2, a_4, a_5) \subseteq A(Z_i)$ by the sequence $(01011) = (01)^2$. Using this notation, for each $i \in \{1, \ell\}$, we define a family $\mathcal{F}(Z_i)$ of subsets of $A(Z_i)$ as follows.

$$\mathcal{F}(Z_i) := \begin{cases} \{(10)^{m_i/2}\}, \{(01)^{m_i/2}\} & \text{if } Z_i \text{ is a crown;} \\ \{(10)^{m_i-1/2}\} & \text{if } Z_i \text{ is an N-fence;} \\ \{(01)^p(10)^q\} & \text{if } Z_i \text{ is an M-fence.} \\
\end{cases} \quad (1)$$

Note that the above sequence representation of the subsets in $\mathcal{F}(Z_i)$ does not depend on the ordering $(a_1,\ldots,a_m)$ of the arcs of $Z_i$ by virtue of the symmetric structure. For example, when $Z_i$ is an N-fence, the sequence $(10)^{m_i-1/2}$ and its reverse ordering are identical.

**Theorem 4.4 (Structure theorem for tree-based phylogenetic networks).** Let $N$ be a rooted binary phylogenetic $X$-network and $\mathcal{Z} = \{Z_1, \ldots, Z_\ell\}$ be a decomposition of $N$ where each $Z_i \in \mathcal{Z}$ is a maximal zig-zag trail in $N$. Then, $N$ is a tree-based network on $X$ if and only if no element $Z_i \in \mathcal{Z}$ is a W-fence. In this case, the collection $\mathcal{F}$ of subdivision trees of $N$ are characterized by

$$\mathcal{F} = \prod_{i \in \{1, \ell\}} \mathcal{F}(Z_i), \quad (2)$$

where $\mathcal{F}(Z_i)$ is defined in \[1\].

**Proof.** We first recall Theorem \[3.1\]. By Lemma \[4.2\] and Lemma \[4.3\] one can produce every admissible subset $S$ of $A(N)$ by choosing each $S_i := S \cap A(Z_i)$ independently. In what follows, we consider a maximal zig-zag trail $Z \in \mathcal{Z}$ with $A(Z) = (a_1,\ldots,a_m)$. We enumerate all 0-1 sequences $(x_1 \ldots x_m)$ corresponding to the admissible subsets of $A(Z)$ in each of the following four cases (see also Figure 3).
- When $Z$ is a crown $v_0 > v_1 < v_2 > v_3 \ldots < v_{m-2} > v_{m-1} < v_m = v_0$, the condition $C0'$ does not apply. Repeated application of the conditions $C1'$ and $C2'$ derives the only solution $(1010\ldots10)$ from $x_1 = 1$. Similarly, $x_1 = 0$ implies $(0101\ldots01)$. This proves that a family of all admissible subsets of $A(Z)$ is given by $\mathcal{F}(Z) = \{(10)^{m/2}, (01)^{m/2}\}$.

- When $Z$ is an N-fence $v_0 > v_1 < v_2 > v_3 \ldots < v_{m-2} < v_{m-1} > v_m$, one of its endpoints $v_0$ is a reticulation vertex of $N$. Then, the condition $C0'$ gives $x_1 = 1$, which implies $(1010\ldots01)$ as in the previous case. This proves that $(01(1)^{(m-1)/2})$ is the only admissible subset of $A(Z)$.

- When $Z$ is a W-fence $v_0 > v_1 < v_2 > v_3 \ldots < v_{m-2} > v_{m-1} < v_m$, both $v_0$ and $v_m$ are reticulation vertices of $N$, so the constraint $C0'$ gives $x_1 = 1$ and $x_m = 1$ again. Similarly to the above, $x_1 = 1$ implies $(1010\ldots)$ while $x_m = 1$ implies $(\ldots0101)$ according to $C1'$ and $C2'$. However, this means that no admissible subset of $A(Z)$ exists because $m$ is even.

- When $Z$ is an M-fence $v_0 < v_1 > v_2 < v_3 \ldots < v_{m-2} < v_{m-1} > v_m$, we have $x_1 = 1$ and $x_m = 1$ again but the other values $x_2, \ldots, x_{m-2}$ are left undetermined. We claim that a family of all admissible subsets of $A(Z)$ with $|A(Z)| = m \geq 2$ is given by $\mathcal{F}(Z) = \{(10)^{m/2}(10)^q1 \mid p, q \in \mathbb{Z}_{\geq 0}, p + q = (m - 2)/2\}$. The proof is by induction on the length $m$ (recall that $m$ is even). The assertion is trivial for $m = 2$. We consider the two cases according to the value of $x_{m+1}$ in the sequence $(x_2 \ldots x_{m+1}1)$ of length $m + 2$. When $x_{m+1} = 1$ holds, $(10)^{m/2}1 = (10)^{m/2}(10)^q1$ is the only admissible subset of $A(Z)$ having this form. When $x_{m+1} = 0$ holds, this only implies $(1x_2 \ldots x_{m-1}101)$. By the induction hypothesis, the family of admissible subsets having this form consists of the sequences $(10)^{m/2}(10)^q1$ with $p \in \mathbb{Z}_{\geq 0}, q \in \mathbb{N}$, and $p + q = m/2$. This proves the claim.

This completes the proof.

\section{Algorithmic Implications}

From Theorem 4.4 we can derive fast algorithms for the problems posed in Section 3. The next proposition is relevant to each problem because all algorithms presented here start by decomposing the input network into maximal zig-zag trails.

**Proposition 5.1.** For any rooted binary phylogenetic X-network $N$, one can obtain the maximal zig-zag trail decomposition $\mathcal{Z} = \{Z_1, \ldots, Z_\ell\}$ of $N$ in $O(|A(N)|)$ time.

**Proof.** As described in Algorithm 1, the above decomposition $\mathcal{Z}$ can be obtained by visiting each arc of $N$ exactly once, which requires $O(|A(N)|)$ time. This completes the proof.

\begin{algorithm}
\caption{Decompose a rooted binary phylogenetic X-network $N$ into $\ell \geq 1$ maximal zig-zag trails}
\textbf{Input:} A rooted binary phylogenetic X-network $N$
\textbf{Output:} The maximal zig-zag trail decomposition $\mathcal{Z} = \{Z_1, \ldots, Z_\ell\}$ of $N$
\begin{algorithmic}[1]
\STATE initialize $\mathcal{Z} := \emptyset, G := N$
\FORALL {$a \in A(G)$}
\STATE compute a (unique) maximal zig-zag trail $Z$ in $G$ that contains $a$
\STATE update $\mathcal{Z} := \mathcal{Z} \cup \{Z\}, G := G[A(G) \setminus A(Z)]$
\ENDFOR
\RETURN $\mathcal{Z}$
\end{algorithmic}
\end{algorithm}
Corollary 5.2. Let $N$ be a rooted binary phylogenetic $X$-network that has $\alpha(N) \in \mathbb{Z}_{\geq 0}$ subdivision trees and $\mathcal{Z} = \{Z_1, \ldots, Z_\ell\}$ be the maximal zig-zag trail decomposition of $N$. Then, $\alpha(N) = \prod_{i=1}^{\ell} \alpha(Z_i)$ holds, where

$$
\alpha(Z_i) = \begin{cases} 
0 & \text{if } Z_i \text{ is a W-fence;} \\
1 & \text{if } Z_i \text{ is an N-fence;} \\
2 & \text{if } Z_i \text{ is a crown;} \\
\lfloor |A(Z_i)|/2 \rfloor & \text{if } Z_i \text{ is an M-fence.}
\end{cases}
$$

(3)

Now, we are in a position to describe a linear time algorithm for solving Problem 1 and Problem 2 simultaneously. Given a rooted binary phylogenetic $X$-network $N$, the algorithm counts the number $\alpha(N)$ of subdivision trees of $N$ as follows: 1) compute the maximal zig-zag trail decomposition $\mathcal{Z} = \{Z_1, \ldots, Z_\ell\}$ of $N$; 2) determine $\alpha(Z_i)$ for each $Z_i \in \mathcal{Z}$ according to the equation (3); 3) return $\alpha(N) = \alpha(Z_1) \times \cdots \times \alpha(Z_\ell)$. In this procedure, the most expensive step is the first one, which requires $O(|A(N)|)$ time by Proposition 5.1.

As we now demonstrate, the number $\alpha(N)$ can give insights into the complexity of $N$. Given a tree-based phylogenetic network $N$ shown in Figure 5, our algorithm starts by decomposing $N$ into 21 maximal N-fences consisting of a single arc and 7 maximal M-fences, and so returns FIGURE 4. Illustrative examples for the proof of Theorem 4.4. The arcs of $Z$ labeled “0” are shown in dotted lines while solid lines indicate those labeled “1”. The vertices of $Z$ are colored in black if they are reticulation vertices of $N$ and in white otherwise. (A-1) and (A-2) describe the two admissible arc-sets of a crown with 8 arcs that are expressed as $\langle (10)^4 \rangle$ and $\langle (01)^4 \rangle$, respectively. (B) shows the only admissible arc-set of a maximal N-fence with 7 arcs, $\langle 1(01)^3 \rangle$. The other three are the solutions for a maximal M-fence with 6 arcs, that is, $\langle 1(01)^21 \rangle, \langle 1(10)^21 \rangle, \langle 1(01)^4(10)^11 \rangle$. 

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\[ \alpha(N) = 7! = 5040. \] Comparing this output with the trivial upper bound \( 2^r = 2^{21} = 2097152, \) where \( r \) denotes the number of reticulation vertices of \( N, \) we can see that it is meaningful to compute the exact value of \( \alpha(N). \) Although the number \( \alpha(N) = 5040 \) may seem huge, it is smaller than the number of rooted binary phylogenetic \( X \)-trees that is given by \( (2|X| - 3)! = 13 \times 11 \times \cdots \times 5 \times 3 \times 1 = 135135. \) In other words, \( N \) does not have adequate complexity in order to cover all rooted binary phylogenetic \( X \)-trees. Thus, the number \( \alpha(N) \) can be used as a quantitative measure for the complexity of \( N, \) which may have implications on model selection in evolutionary data analysis.

![Figure 5](image.png)

**Figure 5.** An example to demonstrate our counting algorithm. This network was previously considered in two independent studies [7, 18] in the context of constructing "universal" tree-based phylogenetic networks.

The next corollary states that the problem of generating all solutions (Problem 3) can be easily solved in the same manner.

**Corollary 5.3.** For any rooted binary phylogenetic \( X \)-network \( N, \) the number \( \alpha(N) \) of subdivision trees of \( N \) can be counted in \( O(|A(N)|) \) time. Moreover, it is possible to list all subdivision trees \( T_1, \ldots, T_{\alpha(N)} \) of \( N \) in linear delay.

**Proof.** What remains unclear is the second statement. We may assume that \( \alpha(N) \geq 1 \) holds. Consider the algorithm that first decomposes \( N \) into maximal zig-zag trails \( Z_1, \ldots, Z_\ell \) and then generate all elements in the solution set \( \mathcal{F} = \prod_{i \in [1, \ell]} \mathcal{F}(Z_i). \) By Theorem 4.4, the elements of \( \mathcal{F}(Z_i) \) can be generated in \( O(|A(Z_i)|) \) time if \( Z_i \in \mathcal{Z} \) is an M-fence, and in \( O(1) \) time otherwise. Then, each of the following steps requires \( O(|A(N)|) \) time: find a solution; check whether there exists another solution that has not been found yet; find the next solution if there exists any. This completes the proof. \[ \square \]

Recalling that the running time of polynomial-time algorithms is linear in the size of the output as mentioned in Section 3, we have the following corollary.

**Corollary 5.4.** For any rooted binary phylogenetic \( X \)-network \( N \) having \( \alpha(N) \) subdivision trees, it is possible to generate \( k \leq \alpha(N) \) subdivision trees in \( O(k|A(N)|) \) time.
As stated in the next corollary, the optimization problem (Problem 4) can be solved in the size of $N$. Note that we can turn it into a minimization problem or define an objective function in the product form as mentioned in Section 3.

**Corollary 5.5.** For any rooted binary phylogenetic $X$-network $N$ and any associated weighting function $w : A(N) \to \mathbb{R}_{\geq 0}$, a subdivision tree $T$ of $N$ that maximizes the value of the objective function $f(T) = \sum_{a \in A(T)} w(a)$ can be found in $O(|A(N)|)$ time.

**Proof.** Assume that we have computed the maximal zig-zag trail decomposition $\{Z_1, \ldots, Z_\ell\}$ of $N$. By virtue of the decomposable nature of $f$, we have $f(T) = f_1(T) + \cdots + f_\ell(T)$, where $f_i(T) := \sum_{a \in A(T) \cap A(Z_i)} w(a)$ for each $i \in [1, \ell]$. Then, by focusing on the maximization of each term $f_i(T)$, we can obtain a global maximum. Finding a local maximum requires $O(|A(Z_i)|)$ time for each $i \in [1, \ell]$. Overall, $O(|A(N)|)$ time suffices. This completes the proof.

6. **Connection to some known results**

Before showing that our structure theorem implies and unifies various results in the literature, we briefly review relevant studies on tree-based phylogenetic networks. After Francis and Steel [5] provided a linear time algorithm for the decision/search problem by focusing on its connection to the 2-SAT problem, Problem 1 and Problem 2 have been studied by several different authors. For example, Zhang [18] proposed yet another linear time algorithm for the above decision problem by characterizing forbidden subgraphs of tree-based networks via an application of Hall’s marriage theorem. Independently from [18], Jetten and van Iersel [10] obtained the same graph theoretical characterization and further considered non-binary phylogenetic networks. Jetten [9] also derived a formula for the number $\alpha(N)$ of subdivision trees of a tree-based phylogenetic network $N$. More recently, Pons et al. [13] re-derived an equivalent formula and pointed out that their results mean that Problem 2 is solvable in polynomial time.

We can easily derive the above results from Theorem 4.4 as it provides a characterization of the collection $\mathcal{T}$ of all subdivision trees of $N$. Our structural approach makes it easy to see that maximal W-fences are the forbidden subgraphs of tree-based phylogenetic networks (cf. [10, 18]) and that the number of crowns in $N$ and the number and lengths of maximal M-fences in $N$ are the factors that contribute to $\alpha(N)$ when $N$ is tree-based (cf. [9, 13]). Thus, we can obtain the same conclusions in a straightforward way without needing existing results from matching theory (cf. [9, 10, 13, 18]). Also, as we have seen earlier, the theorem yields a linear time algorithm for solving Problem 1 and Problem 2 simultaneously, revealing a precise bound on the time complexity of Problem 2 that cannot be seen through the application of the 2-SAT problem (cf. [5]).

Furthermore, we can readily give a partial solution to the open question from Pons et al. [13] as to what the number $\alpha(N)$ is when $N$ is not necessarily binary. We will discuss this point in more details in Subsection 7.2.

7. **Further research directions**

In this paper, we have posed various important computational problems about tree-based phylogenetic networks, and provided efficient algorithms for the individual problems in a unified manner as a consequence of the structural theorem for tree-based phylogenetic networks. Our work does not only present an elegant approach for proving various results in the literature but also enable new statistical applications such as measuring the complexity of tree-based networks, uniform sampling of subdivision trees, and finding the maximum likelihood subdivision tree. We shall end the paper by suggesting two research directions that would be interesting to pursue.
7.1. **Time complexity of counting base trees.** Given a subdivision tree $T$ of a rooted binary phylogenetic $X$-network $N$, such a rooted binary phylogenetic $X$-tree $\tilde{T}$ as described in Definition 2.2 is called a base tree of $N$ [5]. It is still unknown whether the following problem can be solved in polynomial time.

**Problem 5** ([5]). Given a tree-based phylogenetic network $N$, count the number $\beta(N)$ of base trees of $N$.

The tree-based network shown in Figure 6 strikingly demonstrates the difference between Problem 2 and Problem 5. Given this network as input $N$, our counting algorithm returns $\alpha(N) = 2^2$ although $\beta(N) = 1$ holds as it virtually contains only one phylogenetic tree. We conjecture that Problem 5 is #P-complete in contrast to Problem 2 being solvable in linear time. Even if so, however, it would be meaningful to consider the relationship between $\alpha(N)$ and $\beta(N)$ towards the development of useful criteria for analyzing the complexity of phylogenetic networks.

![Figure 6. An example showing the difference between Problem 2 and Problem 5.](image)

7.2. **Generalization to non-binary phylogenetic networks.** Recently, several attempts have been made to extend the results on binary tree-based phylogenetic networks to non-binary ones (e.g., [4, 10, 13]). There are many challenges in this direction; for example, Pons et al. [13] posed the natural problem of determining the number $\alpha(N)$ of subdivision trees if $N$ is not necessarily binary.

Therefore, it would be helpful to comment on the extendability of the present results to some non-binary phylogenetic networks and to provide a partial answer to the above question raised in [13]. First, our definition of tree-based phylogenetic networks does not require $N$ be binary (cf. 5). Also, by virtue of our decomposition-based approach, we can readily see that the results and algorithms in this paper still hold true for any rooted phylogenetic $X$-network $N$ such that each vertex $v \in V(N)$ satisfies both $\deg_{\tilde{N}}^-(v) \leq 2$ and $\deg_{\tilde{N}}^+(v) \leq 2$. Hence, the previous results referred to in Section 6 including the formulae for $\alpha(N)$ are still valid if $N$ contains such vertices as shown in Figure 7.

It is worth considering whether one can obtain a similar structural result that is more biologically meaningful because this might open up a new avenue of research on phylogenetic networks other than those studied in [4, 10, 13].
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ACKNOWLEDGMENT

This study was supported by JST PRESTO Grant Number JPMJPR16EB and was conducted independently from [10, 13, 18]. Most results in this paper were announced in the author’s talk entitled “A linear time algorithm for counting the number of support trees in a tree-based network” on February 13th, 2018 at the Portobello 2018 Conference (The Interface of Mathematics and Biology, The 22nd Annual New Zealand Phylogenomics Meeting). The author thanks Kazuhisa Makino for improving an earlier version of this paper by suggesting Problem 4.
and by providing useful comments on Subsection 7.2. The author is also grateful to Andrew Francis, Leo van Iersel, and Louxin Zhang for providing information on related studies.

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