ON THE EXISTENCE OF INFINITELY MANY UNIVERSAL TREE-BASED NETWORKS

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Abstract. A tree-based network on a set $X$ of $n$ leaves is said to be universal if any rooted binary phylogenetic tree on $X$ can be its base tree. Francis and Steel showed that there is a universal tree-based network on $X$ in the case of $n = 3$, and asked whether such a network exists in general. We settle this problem by proving that there are infinitely many universal tree-based networks for any $n > 1$.

1. Introduction

Throughout this paper, $n$ denotes a natural number that is greater than 1 and $X$ represents the set $\{1, 2, \ldots, n\}$. All graphs considered here are directed acyclic graphs. A graph $G'$ is said to be a subdivision of a graph $G$ if $G'$ can be obtained from $G$ by inserting vertices into arcs of $G$ zero or more times. Given a vertex $v$ of a graph with \text{indeg}(v) = \text{outdeg}(v) = 1$, smoothing (or suppressing) $v$ refers to removing $v$ and then adding an arc from the parent to the child of $v$. Two graphs are said to be homeomorphic if they become isomorphic after smoothing all vertices of in-degree one and out-degree one.

For the reader’s convenience, we briefly recall the relevant background from [1] (see [4] for the terminology in phylogenetics).

Definition 1.1. A rooted binary phylogenetic network on $X$ is defined to be a directed acyclic graph $(V, A)$ with the following properties:

- $X = \{v \in V | \text{indeg}(v) = 1, \text{outdeg}(v) = 0\}$;
- there is a unique vertex $\rho \in V$ with $\text{indeg}(\rho) = 0$ and $\text{outdeg}(\rho) \in \{1, 2\}$;
- for all $v \in V \setminus \{X \cup \{\rho\}\}$, $\{\text{indeg}(v), \text{outdeg}(v)\} = \{1, 2\}$.

The vertices in $X$ are called leaves, and the vertex $\rho$ is called the root.

Definition 1.2. Suppose $T = (V, A)$ is a rooted binary phylogenetic tree on $X$. A rooted binary phylogenetic network $N$ on $X$ is said to be a tree-based network on $X$ with base tree $T$ if there are a subdivision $T' = (V', A')$ of $T$ and a set $I$ of mutually vertex-disjoint arcs between vertices in $V' \setminus V$ such that $(V', A' \cup I)$ is acyclic and is homeomorphic to $N$. The vertices in $V' \setminus V$ are called attachment points, and the arcs in $I$ are called linking arcs.

Tree-based networks can have an important role to play in modern phylogenetic inference as they can represent more intricate or realistic relationships among taxa.

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than phylogenetic trees without compromising the concept of ‘underlying trees’ (cf., [1, 3]).

In order to state the problem formally, we now introduce the notion of universal tree-based networks. A tree-based network on \( X \) is said to be \emph{universal} if any binary phylogenetic tree on \( X \) can be a base tree. We can define universal tree-based networks in a more concrete manner with the number \((2n - 3)!!\) of binary phylogenetic trees on \( X \) as follows.

**Definition 1.3.** A tree-based network \( \mathcal{N} = (V, A) \) on \( X \) is said to be \emph{universal} if any binary phylogenetic tree \( T^{(i)} \) on \( X \) \((i \in \{1, 2, \cdots , (2n - 3)!!\})\), there is a set \( I^{(i)} \subset A \) of linking arcs such that \((V, A \setminus I^{(i)})\) is homeomorphic to \( T^{(i)} \).

**Problem 1.4 ([1]).** Does a universal tree-based network on a set \( X \) of \( n \) leaves exist for all \( n \)?

This problem is fundamental because it explores whether a phylogenetic tree on \( X \) is always reconstructable from a tree-based network on \( X \). In [1], Francis and Steel pointed out that the answer is ‘yes’ for \( n = 3 \). In this paper, we will completely settle their question in the affirmative and provide further insights into universal tree-based networks (Theorem 3.1).

2. Preliminaries

Here, we slightly generalise the concept of tree shapes. Given a tree-based network \( \mathcal{N} \) on \( X \), ignoring the labels on the leaves of \( \mathcal{N} \) results in an unlabelled tree-based network \( \mathcal{N} \) with \( n \) leaves. We use the two different types of symbols, such as \( N \) and \( N' \), to mean unlabelled and labelled tree-based networks, respectively. Two tree-based networks \( \mathcal{N} \) and \( \mathcal{N}' \) on \( X \) are said to be \emph{shape equivalent} if \( N \) and \( N' \) are isomorphic. This equivalence relation partitions a set of the tree-based networks on \( X \) into equivalence classes called \emph{tree-based network shapes with} \( n \) \emph{leaves}.

**Definition 2.1.** A tree-based network shape \( N \) with \( n \) leaves is said to be \emph{universal} if for any rooted binary phylogenetic tree shape \( T^{(i)} \) with \( n \) leaves \((i \in \{1, 2, \cdots , r_n\})\), there is a set \( I^{(i)} \) of linking arcs such that \((V, A \setminus I^{(i)})\) is homeomorphic to \( T^{(i)} \). Here, \( r_n \) denotes the number of rooted binary phylogenetic tree shapes with \( n \) leaves.

The following proposition is not directly relevant to this paper, but ideas behind it, which are summarised in Remark 2.3, will be useful in the proof of Theorem 3.1.

**Proposition 2.2 ([2]).** Let \( r_1 := 1 \) and \( k \in \mathbb{N} \) with \( k > 1 \). Then, we have the following recurrence equation:

\[
 r_n = \begin{cases} 
 1 & \text{if } n = 2; \\
 \sum_{i=1}^{k-1} r_i r_{n-i} & \text{if } n = 2k - 1; \\
 \frac{r_n(r_n+1)}{2} + \sum_{i=1}^{k-1} r_i r_{n-i} & \text{if } n = 2k. 
\end{cases}
\]

**Remark 2.3.** We assume that \( T_1 \) represents a rooted chain shape. Any rooted binary phylogenetic tree shape \( T_n \) with \( n \) leaves can be decomposed into two first-order subshapes \( T_m \) and \( T_{n-m} \) with \( m \in \mathbb{N} \). In other words, using Harding’s notation [2], we can write \( T_n = T_m + T_{n-m} \).
Theorem 3.1. For any natural number \( n > 1 \), there are infinitely many universal tree-based networks on a set \( X \) of \( n \) leaves.

Proof. First, we will show that there is a universal tree-based network shape with \( n \) leaves. Let \( U_n \) be a rooted binary phylogenetic network shape with \( n \) leaves as illustrated in the left panel of Figure 1, which can be obtained by adding \((n-1)(n-2)/2\) linking arcs and \((n-1)(n-2)\) attachment points to a rooted caterpillar tree shape with \( n \) leaves. By definition, \( U_n \) is a tree-based network shape with \( n \) leaves.

We will prove that \( U_n \) is universal by induction. (i) It is easy to see that \( U_2 \) and \( U_3 \) are universal. (ii) Assuming \( U_k \) is universal for any \( k \in \mathbb{N} \) (\( 2 \leq k \leq n \)), we will show that \( U_{n+1} \) is universal. We claim that any binary phylogenetic tree shape \( T_{n+1} \) with \( T_{n+1} = T_n + T_1 \) can be a base tree shape of \( U_{n+1} \). Indeed, \( U_{n+1} \) contains mutually vertex-disjoint arcs whose removal turns \( U_{n+1} \) into the union of two subgraphs that are homeomorphic to \( U_n \) and \( T_1 \), respectively (see the middle panel of Figure 1).

Because \( U_n \) is universal, our claim holds true. We next claim that any binary phylogenetic tree shape \( T_{n+1} \) with \( T_{n+1} = T_k + T_{n-k+1} \) can be a base tree of \( U_{n+1} \). The right panel of Figure 1 indicates that \( U_{n+1} \) contains two distinct subsets of mutually vertex-disjoint arcs, one of which delineates \( U_{n-k+1} \) (shown in thick gray line) and the other distinguishes \( U_k \) from the remainder. Because both \( U_{n-k+1} \) and \( U_k \) are universal, our claim holds true. Therefore, \( U_{n+1} \) is universal. Hence, \( U_n \) is universal for all \( n \).

Next, we will provide a method to create infinitely many universal tree-based networks on \( X \) from \( U_n \). Let \( E_n \) be a tree-based network on \( X \) obtained from \( U_n \) by specifying a permutation \( \pi_0 \) of \( X \). In what follows, we use the same notation \( i \) both for a leaf labelled \( i \) and for the terminal arc incident with \( i \). A crossover \( \sigma_{ij} \) refers to a pair of crossed additional arcs between two distinct terminal arcs \( i \) and \( j \) as described in Figure 2.

Note that \( \sigma_{ij} \) can be viewed as representing the transposition \((i, j)\) of the labels. For any permutation \( \pi_1 \neq \pi_0 \) of \( X \), there is a series of adjacent crossovers that converts \( \pi_0 \) into \( \pi_1 \) and then vice versa (note that any permutation can be expressed as a product of transpositions and that the symmetric group \( S_n \) is generated by the adjacent transpositions). Then, by sequentially adding \( n!-1 \) series of crossovers, we can construct a universal tree-based network \( U_\pi \) on \( X \) from \( E_n \). Moreover, it is possible to create infinitely many universal tree-based networks on \( X \) because we may add an arbitrary number of redundant crossovers among the terminal arcs of \( U_\pi \). This completes the proof. \( \square \)

We note that the construction described in the proof of Theorem 3.1 adds more arcs than necessary (cf. Figure 1 in [1]). It would be interesting to consider how to construct universal tree-based networks on \( X \) with the smallest number of arcs.

Comments

We studied Problem 1.4 independently from Louxin Zhang [5].

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Figure 1. The first part of the proof of Theorem 3.1. The left panel is an illustration of $U_n$ for $n = 8$. The other panels show examples of $T_{n+1}$ in $U_{n+1}$ for $n + 1 = 8$, and the right panel describes the case of $T_{n+1} = T_k + T_{n-k+1}$ with $k = 3$.

Figure 2. The second part of the proof of Theorem 3.1. Left: A crossover $\sigma_{ij}$ is defined to be a pair of crossed additional arcs placed between arcs $i$ and $j$ ($i \neq j$) after subdividing both arcs twice. Right: When the two arcs in $\sigma_{ij}$ are selected as tree arcs, $\sigma_{ij}$ represents the transposition $(i \, j)$.

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