Planar Rooted Phylogenetic Networks

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Abstract—A rooted phylogenetic network is a directed acyclic graph with a single root, whose sinks correspond to a set of species. As such networks are useful for representing the evolution of species that have undergone reticulate evolution, there has been great interest in developing the theory behind and algorithms for constructing them. However, unlike evolutionary trees, these networks can be highly non-planar, which can make them difficult to visualise and interpret. Here we investigate properties of planar rooted phylogenetic networks and algorithms for deciding whether or not rooted networks have certain special planarity properties. In particular, we introduce three natural subclasses of planar rooted phylogenetic networks and show that they form a hierarchy. In addition, for the well-known level-\(k\) networks, we show that level-1, -2, -3 networks are always outer, terminal, and upward planar, respectively, and that level-4 networks are not necessarily planar. Finally, we show that a regular network is terminal planar if and only if it is pyramidal. Our results make use of the highly developed field of planar digraphs, and we believe that the link between phylogenetic networks and planar graphs should prove useful in future for developing new approaches to both construct and visualise phylogenetic networks.

Index Terms—Phylogenetic network, planar digraph, upward planar, level-\(k\) network, pyramid, regular network

1 \hspace{1em} INTRODUCTION

PHYLOGENETIC networks are a generalization of evolutionary trees that are commonly used to study species whose evolution have involved recombination processes such as recombination, hybridization and lateral gene transfer. These networks have been used to analyze the evolution of organisms such as viruses, plants, bacteria, as well as animals (see e.g., [1]). In general, phylogenetic networks come in two main types: Those that aim to represent evolutionary patterns in the data, and those that try to represent the actual evolutionary history (sometimes called implicit and explicit networks, respectively; see e.g., [2]). Note that for the special case of evolutionary trees, implicit and explicit networks can be thought of as corresponding to unrooted and rooted trees, respectively. More generally, implicit networks tend to be undirected graphs whereas explicit ones are directed.

Although the concept of a phylogenetic network has been considered in the literature for quite some time, the first algorithmic approaches to produce such networks mainly focused on generating implicit networks. In particular, one of the archetypical types of implicit networks are the so-called split networks that were first introduced in [3]. For example, in the left panel of Fig. 1 we present an example of a split network generated for collection of HIV virus sequences described in [4, Chapter 21] that was generated by the SplitsTree program [5] using the NeighborNet algorithm [6]. In general, split networks are isometric subgraphs of hypercubes [3], and which means that they can be potentially highly non-planar (i.e., it is not possible to draw them in the plane without some edges crossing one another). Even so, split networks have proven to be very popular, one of the main reasons probably being that algorithms such as the NeighborNet algorithm are designed to generate split networks that are planar which greatly facilitates their visualisation (see e.g., [7], [8], [9]) and subsequent biological interpretation.

More recently, the focus of the phylogenetic networks literature has shifted more towards explicit networks, and especially rooted networks. Essentially, a rooted phylogenetic network (which from now on we will just call a phylogenetic network) is a directed acyclic graph with a single source called the root, whose sinks (which are usually called the leaves of the network) correspond to the set of species. For example, in the right panel of Fig. 1 we present a network generated using the Trilopnet program [10]. There are several types of phylogenetic networks (see e.g., [11, Chapter 10] for a recent review), and various programs are available for their generation (e.g., [12], [13], [14] and [15] for a recent comparison of some of these programs). Even so, although some of these types of networks (such as so-called level-1 networks) are always planar, just as with split networks this is not true in general. Thus, it is interesting to study planarity of phylogenetic networks, with the view to developing new approaches and algorithms for generating phylogenetic networks that can be more readily visualized.

In this paper we shall present some new concepts and results concerning planar phylogenetic networks, which we now brefly summarize. To help prove our results we shall use the highly developed theory of planar directed graphs and posets, some of which we shall review in the next section. In Section 3, we then consider planar phylogenetic networks and introduce and compare three subclasses of such networks: upward planar, terminal planar, and outer planar networks. Upward and outer planar phylogenetic networks are special examples planar digraphs with the same name, whereas terminal planar networks are networks where the...
source and sinks (i.e., the root and leaves) must all lie in the so-called outer face of some planar drawing of the network. We present a characterisation of terminal planar networks in Theorem 3.1, and use this result to show that the four types of planar networks form a hierarchy (Theorem 3.2). As a consequence we also show that there are polynomial time algorithms for deciding whether or not a phylogenetic network is contained in each one of these classes or not (Theorem 3.3).

In Sections 4 and 5 we investigate planarity for two special classes of phlogenetic networks: level-\(k\) (\(k \geq 0\)) [16] and regular networks [17]. Loosely speaking, the level of a network is measure of how far the network is from being a tree, where level-0 networks are trees. For level-\(k\) networks we show that level-1, -2, -3 networks are always outer, terminal, and upward planar, respectively, and that level-4 networks are not necessarily planar (Theorem 4.1). We also characterise when level-2 networks are terminal planar (Theorem 4.2). A regular network can be thought of as being a Hasse diagram of some collection of clusters of a set of species. We show that a regular network is terminal planar if and only if the underlying set of clusters forms a pyramid [18] (Theorem 5.1). We conclude in Section 6 with a discussion and some open problems.

## 2 Preliminaries

In this paper we shall assume that \(X\) is a finite set with \(|X| \geq 2\). The set \(X\) usually corresponds to a collection of extant species.

### 2.1 Posets and Cluster Systems

A set \(Y\) with a partial order \(\preceq\) (i.e., a binary reflexive, antisymmetric, and transitive relation) is called a partially ordered set or poset, and denoted by \((Y, \preceq)\). A poset \((Y, \preceq)\) is a lattice if for each pair of elements \((y_1, y_2)\) in \(Y\), the set \(Y\) contains both a join \(y_1 \lor y_2\) (i.e., a least upper bound) and a meet \(y_1 \land y_2\) (i.e., a greatest lower bound) of \(y_1\) and \(y_2\). Note that in case either a join or a meet exists then it is necessarily unique. The partial order \(\preceq\) is referred to as a linear order if in addition, for each pair of distinct elements \(y_1\) and \(y_2\) in \(Y\), we have either \(y_1 \preceq y_2\) or \(y_2 \preceq y_1\) (but not both). Clearly, a linear order is necessarily a lattice. Given a poset \(P\), we let \(P^*\) be \(P\) if it has the bottom element (i.e., a least element), and \(P\) with an extra bottom element \(\emptyset\) added otherwise.

The Hasse diagram \(H(P)\) of a poset \(P = (Y, \preceq)\) is the digraph with vertex set \(Y\) and so that \((y_1, y_2)\) is a directed edge from \(y_1\) to \(y_2\) in \(H(P)\) if \(y_1\) covers \(y_2\), that is, \(y_2 \preceq y_1\) and there is no element \(y_3\) in \(Y - \{y_1, y_2\}\) with \(y_2 \preceq y_3 \preceq y_1\). Note that the direction of the edges in our definition of the Hasse diagram is chosen for the convenience later on, and is the opposite to the way commonly used in the poset literature. However, this difference will be immaterial for the results presented here. It is well-known in poset theory that each partial order \(\preceq\) on \(Y\) has a linear extension, that is, a linear order \(\leq\) on \(Y\) such that \(y_1 \preceq y_2\) in \(Y\) implies that \(y_1 \leq y_2\). Following [19], the (Dushnik and Miller) dimension of a poset \((Y, \preceq)\) is the smallest cardinal number \(m\) such that \(\preceq\) is the intersection of \(m\) linear extensions \(\preceq_1, \ldots, \preceq_m\) of \(\preceq\), that is, \(y_1 \preceq y_2\) if and only if \(y_1 \preceq_i y_2\) for each \(1 \leq i \leq m\).

A cluster system \(C\) (on \(X\)) is a collection of non-empty subsets of \(X\) that contains \(X\) and the subset \(\{x\}\) for each \(x \in X\), where each subset of \(X\) in the system is referred to as a cluster. Furthermore, \(C\) is closed under intersection if for each pair of sets \(A\) and \(B\) in \(C\), we have either \(A \cap B = \emptyset\) or \(A \cap B \in C\). Note that any cluster system \(C\) is a poset \(P(C) = (C, \subseteq)\) under the ordering induced by taking set-inclusion; we let \(P^*(C)\) be the poset obtained from \(P(C)\) by adding the empty-set \(\emptyset\) as the bottom element. We now make a simple observation that we will use later on. We include a proof for completeness.

**Lemma 2.1.** Suppose that \(C\) is a cluster system on \(X\) that is closed under intersection. Then the poset \(P^*(C)\) is a lattice.
Proof. Let $A$ and $B$ be two distinct elements in $C$. Let $A \land B$ be $\emptyset$ if $A$ and $B$ are disjoint, and $A \land B$ otherwise. Since $C$ is closed under intersection, it follows that $A \land B$ is contained in $P^0(C)$ and it is in fact the meet of $A$ and $B$.

Next, let $u(A, B)$ be the collection of subsets $C$ in $C$ such that $A \subseteq C$ and $B \subseteq C$. Then $u(A, B)$ is non-empty as it contains $X$. Now, for $C_1$ and $C_2$ in $u(A, B)$, we have $A \cup B \subseteq C_1 \cap C_2$, and hence $C_1 \cap C_2 \neq \emptyset$. Therefore, $C_1 \cap C_2 \in u(A, B)$. In other words, $u(A, B)$ has a minimum element $C_0$ such that $C_0 \subseteq C$ for all $C \in u(A, B)$. Clearly, $C_0$ is the join of $A$ and $B$ in $P(C)$, and hence also their join in $P^0(C)$. Hence $P^0(C)$ is a lattice.

\[ \square \]

2.2 Planar Graphs

We shall assume that all sets and graphs are finite, and that all graphs are simple, that is, they contain neither loops nor parallel edges. For integers $m, n \geq 1$, let $K_{m,n}$ be the complete graph with $m$ vertices, and $K_{n,m}$ be the complete bipartite graph with $m$ vertices in one set and $n$ vertices in the other set.

We now recall some standard definitions for planar graphs and graph drawing, largely following [20] and [21]. A drawing $\Gamma = \Gamma(G)$ of a graph $G$ maps each vertex $v$ to a distinct point $\Gamma(v)$ of the euclidean plane (endowed with the $x$ and $y$ coordinates) and each edge $(u, v)$ to an arc $\Gamma(u,v)$, that is, a simple open Jordan curve with endpoints $\Gamma(u)$ and $\Gamma(v)$. For clarity, the points $\Gamma(v)$ corresponding to a vertex $v$ in $G$ will be referred to as a node in the drawing, to differentiate them from the points inside of the arcs. Such a drawing is called a straight-line drawing if each arc in the drawing is a straight line segment between its endpoints. A drawing is planar if there are no two distinct arcs intersect except, possibly, at common endpoints. A graph is planar if it admits a planar drawing. Note that such a drawing partitions the plane into connected regions called faces. There is precisely one unbounded face of $\Gamma$, referred to as the outer-face of $\Gamma$. If a planar graph has a drawing in which every vertex is contained in the outer-face, then the graph is called outer planar.

Given two graphs $G$ and $G'$, we say $G'$ is a minor of $G$ if $G'$ can be obtained from $G$ by repeated deletion (of vertices and edges) and contractions. Furthermore, we say $H$ is a subdivision of $G$ if $H$ is obtained from $G$ by replacing the (directed) edge of $G$ with (directed) paths between their ends (so that none of these paths has an inner vertex on another path or in $G$). The well-known Kuratowski theorem states that a graph $G$ is planar if and only if none of the subgraphs of $G$ is a subdivision of either $K_5$ or $K_{3,3}$, equivalently, the Wagner theorem states that $G$ is planar if and only if $G$ contains neither $K_5$ nor $K_{3,3}$ as a minor (see, e.g., [20, Theorem 4.4.6] for a proof of both theorems). Moreover, $G$ is outer planar if and only if no subgraph of $G$ is a subdivision of either $K_4$ or $K_{2,3}$, see, e.g., [22, p.117].

Note that if $G$ is a digraph, then each edge $(u, v)$ will be mapped to a directed arc from $\Gamma(u)$ to $\Gamma(v)$. Clearly, a digraph $G$ is planar if and only if its underlying graph $U(G)$ (e.g., the one obtained from $G$ by forgetting the directions of edges) is planar. Furthermore, a planar drawing of a digraph is called upward if each arc is a curve of monotonically nondecreasing in the $y$-coordinate. As noted in [23], a digraph $G$ is upward planar if it admits a straight-line upward planar drawing. Another useful result concerning upward-planar graphs is as follows. An st-digraph is an acyclic digraph with a single source, denoted by $s$, and a single sink, denoted by $t$, and the arc $(s,t)$. Then $G$ is upward-planar if and only if it is a spanning subgraph of a planar st-digraph, that is, directed edges can be added to $G$ such that the resulting digraph is a planar st-digraph [23, Theorem 1].

3 Planar Phylogenetic Networks

In the following we shall mainly use the definitions for phylogenetic networks presented in [11, Section 10]. A phylogenetic network on $X$, or simply a phylogenetic network when the underlying set $X$ is clear from the context, is an acyclic directed graph $N = (V, A)$ with $X \subseteq V$, a single source $\rho_N$ (the root), $X$ the set of sinks in $N$, and no vertices with indegree 1 and outdegree 1. In particular, each edge is directed away from the root of $N$. Two phylogenetic networks $N = (V, A)$ and $N' = (V', A')$ on $X$ are isomorphic if there exists a bijective map $f : V \rightarrow V'$ such that $(u, v) \in A$ if and only if $(f(u), f(v)) \in A'$, and for all $x \in X$, $f(x) = x$.

A phylogenetic network on $X$ is called planar, outer planar or upward planar if as a digraph it satisfies each of these properties. Furthermore, we defined such a network to be terminal planar if it admits a planar drawing in which the set $\{\rho_N\} \cup X$ is contained in the outer-face (note that this is analogous to outer-labelled split networks [7], where the elements in $X$ must all lie in the outer face of the network). Clearly, if a phylogenetic network is outer planar, then it is terminal planar. Also, note that a phylogenetic network $N$ is outer planar (respectively terminal planar or planar) if and only if its underlying graph $U(N)$ is outer planar (respectively terminal planar or planar). In Fig. 2 we present some examples of these concepts; we shall prove that the networks in this figure have the stated properties in Theorems 3.2 and 4.1 below.

We now present a result relating terminal planar and upward planar phylogenetic networks on $X$. Given a phylogenetic network $N = (V,E)$ on $X$, we let $N'$ be the digraph with vertex set $V \cup \{t\}$ for some $t \notin V$ which will be referred to
to as the sink vertex, and directed edge set \( A \cup \{(x, t) : x \in X\} \). We call \( N^* \) the completion of \( N \).

**Theorem 3.1.** Suppose that \( N \) is a phylogenetic network on \( X \). Then \( N \) is terminal planar if and only if the completion \( N^* \) of \( N \) is upward planar.

**Proof.** Suppose first that \( N^* \) is upward planar. Fix an upward drawing \( \Gamma^* \) of \( N^* \). Consider the drawing \( \Gamma \) of \( N \) obtained from \( \Gamma(N^*) \) by removing the sink \( \Gamma^*(t) \) and the arcs incident with it. Then \( \Gamma \) is a planar drawing of \( N \) such that the set \( \{\rho_N\} \cup X \) is contained in the outer-face of \( \Gamma \). So \( N \) is terminal planar.

Conversely, suppose that \( N \) is terminal planar. Fix a planar drawing \( \Gamma \) of \( N \) in the plane such that the set \( \{\rho_N\} \cup X \) is contained in the outer-face. Without loss of generality, we may assume that the \( y \)-coordinate of each point in the drawing \( \Gamma \) is strictly positive. Take a point \( w \) in the interior of the outer-face in the plane whose \( y \)-coordinate is negative. Join this point to each element \( x \) of \( N \) with a curve \( \gamma_{w,x} \) contained in the outer-face such that \( \gamma_{w,x} \cap \gamma_{w,x'} = \{w\} \) for all \( x, x' \in X \). Then add in an arc between the \( \rho_N \) and \( w \) which does not intersect any existing arcs, except possibly in \( w \) or \( \rho_N \). This gives a planar drawing \( \Gamma' \) of the digraph

\[
N' = (V \cup \{t\}, A \cup \{(x, t) : x \in X\} \cup \{(\rho_N, t)\}),
\]

in which \( t \) is mapped to \( w \) under \( \Gamma' \). So \( N' \) is a planar st-digraph (with source \( s = \rho_N \) and sink \( t \)). It follows that \( N^* \) is upward planar by [23, Theorem 1] that we stated above. Finally, as \( N \) is a subgraph of \( N^* \), it follows that \( N \) is also upward planar. \( \square \)

Let \( \mathcal{P}_0(X), \mathcal{P}_1(X), \mathcal{P}_2(X), \mathcal{P}_n(X) \) denote the classes of planar, upward planar, terminal planar, and outer planar phylogenetic networks on \( X \), respectively. We now show how these classes are related to one another.

**Theorem 3.2.** For any \( X \), \( |X| \geq 2 \), we have

\[
\mathcal{P}_0(X) \subseteq \mathcal{P}_1(X) \subseteq \mathcal{P}_n(X) \subseteq \mathcal{P}_p(X).
\]

**Proof.** By definition we have \( \mathcal{P}_0(X) \subseteq \mathcal{P}_1(X) \) and \( \mathcal{P}_n(X) \subseteq \mathcal{P}_p(X) \). Furthermore, \( \mathcal{P}_1(X) \subseteq \mathcal{P}_n(X) \) follows from Theorem 3.1.

We now show that all of the set inclusions in the statement of the theorem are strict, for the cases \( \mathcal{P}_0 \subseteq \mathcal{P}_1 \) and \( \mathcal{P}_n \subseteq \mathcal{P}_p \), \( n \geq 3 \), which will complete the proof of the theorem.

First, consider the network \( N_2 \) on \( Y \) in Fig. 2 which is clearly contained in \( \mathcal{P}_n(Y) \). We claim that \( N_2 \not\in \mathcal{P}_1(Y) \). Indeed, if this were not the case, then \( N_2 \) is terminal planar, and hence its completion \( N_2^* \) is upward planar in view of Theorem 3.1. Therefore, \( N_2^* \) is a spanning subgraph of an st-digraph denoted by \( N_2 \). This implies that \( N_2 \) is a minor of \( U(N_2^*) \). However, \( G_2 \) contains \( K_{3,3} \) as one of its minors, and hence is not planar, a contradiction. Now, let \( T_0 = T(x_2, \ldots, x_n) \) be the binary tree on \( \{x_2, \ldots, x_n\} \) given by taking the Hasse diagram of the cluster system that contains all clusters of the form \( \{x_2, \ldots, x_k\} \), \( 3 \leq k \leq n \), and construct the phylogenetic network \( N_3^* \) on \( X \) by replacing \( x_2 \) with the tree \( T(x_2, \ldots, x_n) \) (see Fig. 3) for an example with \( n = 4 \). Since both \( N_2 \) and \( T(x_2, \ldots, x_n) \) are upward planar, it is straightforward to construct an upward planar drawing for \( N_3^* \). A similar to the proof that \( N_2 \) is not terminal planar then implies that \( N_3^* \not\in \mathcal{P}_n \). \( \square \)

Next, consider the network \( N_1 \) on \( Y \) in Fig. 2 which is clearly contained in \( \mathcal{P}_1(Y) \). Furthermore, \( N_1 \) is not outer planar because \( U(N_1) \) contains a subdivision of \( K_{2,3} \). Now we construct the phylogenetic network \( N_1^* \) on \( X \) by replacing \( x_2 \) with the tree \( T_0 \) as in the last paragraph. Since \( T_0 \) is outer planar and \( N_1 \) is terminal planar, we start with a planar drawing of \( N_1 \) whose outer-face contains the root and leaves of \( N_1 \) and then naturally extend it to a planar drawing of \( N_1^* \) whose outer-face contains the root and leaves of \( N_1^* \). It follows that \( N_1^* \) is terminal planar. Furthermore, \( N_1^* \) is not outer planar because \( U(N_1^*) \) again contains a subdivision of \( K_{2,3} \). Hence \( N_1^* \not\in \mathcal{P}_n \). \( \square \)

Finally, we claim that \( N_3 \) in Fig. 2, which is easily seen to be planar, is not in \( \mathcal{P}_0(Y) \). If not, then the directed graph \( G_2 \) (see Fig. 4) obtained from \( N_3 \) by removing the sinks \( x_1, x_2 \) and the directed edges incident with them is also upward planar. That is, \( G_3 \) is a spanning subgraph of an st-digraph \( G_3 \) and hence \( G_3 \) is a minor of \( U(G_3) \). However, \( G_3 \) contains \( K_{3,3} \) as its minor, a contradiction. We now construct a phylogenetic network \( N_3^* \) on \( X \) by replacing \( x_2 \) with the tree \( T_0 \) as above. Since \( T_0 \) is planar and it can be drawn in an arbitrary small neighborhood of \( x_2 \), it follows that \( N_3^* \) is also planar. An argument similar to the proof of that \( N_3 \) is not upward planar now implies \( N_3^* \not\in \mathcal{P}_p \). \( \square \)

We now consider some algorithmic aspects of planar phylogenetic networks. Our main result will follow more-or-less directly from some results in the literature concerning planar digraphs which we now briefly review. Suppose that \( G \) is a digraph with \( m \) vertices. Then it can be checked...
in $O(m)$ time if $G$ is planar/outer planar, and a straight-line-planar/outer-planar drawing for $G$ can be produced in $O(m)$ time in case it is (see [24]/[25],[26]). Similarly, there are also $O(m)$ algorithms for checking upward planarity and producing an upward planar drawing for $G$ in case $G$ has a single source (see [27], and also [23, Theorem 15]), although the decision problem for deciding whether or not a digraph is upward planar is NP-complete in general [28].

**Theorem 3.3.** Suppose $N$ is a phylogenetic network on $X$ with $m$ vertices. Then it can be checked in $O(m)$ time whether or not $N$ is planar/upward planar/outer planar/terminal planar, and a planar drawing with the corresponding property can be produced in $O(m)$ time if $N$ satisfies any of these properties. In particular, if the number of vertices in $N$ is bounded by some polynomial $p$ in $|X|$, then we can check if $N$ satisfies any of these planarity properties and if so produce a corresponding planar drawing in $O(p(|X|))$-time.

**Proof.** The results concerning planar, upper planar, or outer planar follow from the results mentioned before the statement of the theorem.

To check whether $N$ is terminal planar, we can construct its completion $N^*$ which contains $m + 1$ vertices in $O(m)$ time. Since it can be checked in $O(m)$ time whether or not $N^*$ is upper planar, by Theorem 3.1 we can check whether $N$ is terminal planar in $O(m)$ time. Furthermore, when $N$ is terminal planar, a terminal planar drawing of $N$ can be obtained from an upper planar drawing of $N^*$ in $O(m)$ time using the procedure in the proof of Theorem 3.1.

Using Theorem 3.3, we can now say something more about checking planarity for some well-known classes of phylogenetic networks. We begin by recalling some definitions (see e.g., [11, Chapter 10]). A vertex in a phylogenetic network is either a tree vertex (i.e., a vertex of indegree 1 or the root vertex) or a reticulation vertex (i.e., a vertex of indegree 2 or more). Furthermore, a phylogenetic network is called binary if the root has outdegree 2, the leaves have indegree 1, and all of the all other vertices have indegree 1 and outdegree 2 or indegree 2 and outdegree 1.

Now, a tree-child network is a phylogenetic network for which every non-leaf vertex has a child that is a tree vertex (note a vertex $v$ in a phylogenetic network $N$ is a child of a vertex $u$ in $N$ if $(u, v)$ is an arc in $N$). A vertex $v$ is said to be visible if there is a leaf $x_v \in X$ so that every directed path from the root to $x_v$ passes through $v$. A reticulation-visible network is a phylogenetic network for which each reticulation vertex is visible. Since a phylogenetic network is tree-child if and only if each vertex is visible, it follows that a tree-child network is necessarily reticulation-visible. In particular, the corollary below concerning reticulation-visible networks also holds for tree-child networks. Finally, a phylogenetic network is normal if it is tree-child and has it does not contain any arc $(u, v)$ such that there is another directed path from $u$ to $v$ (these are know as redundant arcs).

It is known that a binary reticulate-visible network on $X$ has $O(|X|)$ vertices (see e.g., [11, Theorem 10.10]), and that a normal network on $X$ has $O(|X|^2)$ vertices (see [11, Proposition 10.11], and the discussion directly after). Hence by Theorem 3.3 we immediately see that the following holds:

**Corollary 3.4.** Suppose that $N$ is a phylogenetic network on $X$. If $N$ is binary and reticulate-visible, or normal (not necessarily binary), then it can be checked in $O(|X|)$ or $O(|X|^2)$ time, respectively, whether $N$ is planar, upper planar, outer planar or terminal planar and in case $N$ satisfies any of these properties, a planar drawing can be produced with the corresponding property in the same asymptotic time.

**Remark.** There are non-binary, terminal planar, tree-child networks on a set $X$ that do not have a polynomial number of vertices in $|X|$ (see e.g., [11, Fig. 10.5 (ii)]).

### 4 Level-k Networks

In this section, we shall consider planarity of level-$k$ networks [16], which are defined as follows. A biconnected component in a graph is a maximal subgraph that does not contain any cut vertex (i.e., a vertex whose removal disconnects the graph). A phylogenetic network is level-$k$, $k \geq 0$, if it is binary and it can be converted into a tree by deleting at most $k$ directed edges from each biconnected component [11, p.247]. Clearly, a level-0 phylogenetic network is necessarily a tree, and a binary phylogenetic network $N$ is level-$k$ if and only if $U(N)$ can be converted into a tree by deleting at most $k$ edges from each biconnected component of $U(N)$.

We let $L_i(X)$ denote the set of level-$k$ phylogenetic networks on $X$ for $k \geq 0$, so that $L_i(X) \subseteq L_k(X)$ clearly holds for all $0 \leq i \leq k$.

To prove the first main result of this section we will use the following observation [29]: A connected single-source digraph is upward planar if and only if all of its biconnected components are upward planar (see also [23, Lemma 4]). Since each phylogenetic network on $X$ is a connected and single-source, it follows that $N$ is upward planar if and only if all the biconnected components of $N$ are upward planar.

**Theorem 4.1.** The following statements hold:

i) All level-1 networks are outer-planar, that is, $L_1(X) \subseteq P_p(X)$.

ii) All level-2 networks are upward planar, but some level-2 networks are not terminal planar, that is, $L_2(X) \subseteq P_u(X)$ and $L_2(X) \setminus P_p(X) \neq \emptyset$.

iii) All level-3 networks are planar, but some level-3 networks are not upward planar, that is $L_3(X) \subseteq P_p(X)$ and $L_3(X) \setminus P_p(X) \neq \emptyset$.

iv) Some level-4 networks are non-planar, that is, $L_4(X) \setminus P_p(X) \neq \emptyset$.

**Proof.** (i) Assume that $N$ is a level-1 network on $X$ and consider its underlying undirected graph $U(N)$. Since each non-trivial biconnected component of $U(N)$ is a cycle, it follows that none of the subgraphs of $U(N)$ is a subdivision of either $K_1$ or $K_{2,5}$, and hence $U(N)$ is outer planar. Thus $N$ is also outer planar.

(ii) Assume that $N$ is a level-2 network on $X$. To show that $N$ is upward planar, it is sufficient to establish the claim that each biconnected component of $N$ is upward planar. To this end, consider an arbitrary biconnected component $H$ of $N$. Without loss of generality we may further assume that $H$ contains more than one cycle as otherwise the claim clearly holds. Using the results in [30, Section 4] concerning the generators of level-2...
networks, it follows that $H$ is a subdivision of one of the four digraphs in Fig. 5. Since each of these four digraphs in Fig. 5 is upward planar, it follows that $H$ is also upward planar, as required.

Finally, note that the network $N_0'$ constructed in the proof of Theorem 3.2 is clearly contained in $L_3(X) \setminus P_1(X)$.

(iii) First, we shall show that $L_3(X) \subseteq P_1(X)$. If not, consider a level-3 phylogenetic network $N$ on $X$ such that $N$ is not planar. Then $U(N)$ contains either $K_{3,3}$ or $K_5$ as its minor. We shall only consider the case where $U(N)$ contains $K_{3,3}$ as a minor; the proof for $K_5$ a minor is similar. In this case, there exists a biconnected component $B$ of $U(N)$ such that $B$ contains $K_{3,3}$ as a minor. This implies that we need to delete at least 4 edges from $B$ to convert it into a tree, in contradiction to the assumption that $N$ is level-3.

Finally note that for the network $N_0'$ constructed in the proof of Theorem 3.2 we clearly have $N_0' \in L_3(X) \setminus P_1(X)$.

(iv) This follows since the network $N_1$ on the set $\{x_1, x_2\}$ in Fig. 2 is level-4 but not planar as $K_{3,3}$ is a minor of $U(N_1)$.

Now construct a phylogenetic network $N_1'$ on $X$ by replacing $x_1$ with any binary rooted phylogenetic tree on $\{x_1, x_3, ..., x_7\}$. Then it is straightforward to see that $N_1' \in L_3(X) \setminus P_1(X)$. □

In the last theorem we showed that all level-1 networks are outer planar. In the second main result of this section, we show that for a level-2 network outer planarity of the network is equivalent to it being terminal planar, and characterize those level-2 networks that have this property.

**Theorem 4.2.** Suppose that $N$ is a level-2 phylogenetic network on $X$. Then the following statements are equivalent:

i) $N$ is terminal planar.

ii) $N$ is outer planar.

iii) $N$ does not contain any subdivision of any of the four digraphs of Theorem 6.

iv) $U(N)$ does not contain a subdivision of $K_{2,3}$.

**Proof.** Since (ii) ⇒ (i) clearly holds, it suffices to show that (i) ⇒ (iii) ⇒ (iv) ⇒ (ii).

(i) ⇒ (iii): First assume that $N$ contains a subdivision of $H_i'$ in Fig. 6. Since $N$ is a binary network, it follows that there exists two elements $x_1$ and $x_2$ in $X$ such that for $i = 1, 2$, there exists a directed path from $v_i$ to $x_i$ which does not contain any directed edge in $H_i'$. Now an argument similar to the proof of Theorem 4.1(ii) (see also Fig. 3) shows that $N$ is not terminal planar, a contradiction. The other three cases can be established in a similar manner.

(iii) ⇒ (iv): Assume that $U(N)$ contains a subdivision of $K_{2,3}$. We need to show that $N$ contains a subdivision of one of the four digraphs in Fig. 6. Let $H$ be a biconnected component in $N$ such that $U(H)$ contains a subdivision of $K_{2,3}$, which must clearly exist. Then $H$ contains a subdivision of one of the four digraphs $H_i$ in Fig. 5. We assume that $H$ contains a subdivision of $H_2$; the other cases can be established in a similar manner.

We shall show that $H$ contains a subdivision of $H_2'$. To this end, label the vertices and edges in $H_2$ as in Fig. 7 A. Since $U(H)$ contains a subdivision of $K_{2,3}$, there exists two vertices $u, v$ in $U(H)$ such that there are three internally disjoint paths between them and each of these three paths contains at least two edges. Noting that $H_2'$ is obtained from $H_2$ by subdividing the edge $e_2 = \{u_1, u_2\}$ with the path $u_1, v_1, u_2$, it is now sufficient to establish the following claim:

**Claim.** Under the above assumptions, $\{u, v\} = \{u_1, u_2\}$.

To establish the claim we consider the following subcases based on the size of intersection $\{u, v\} \cap V(H_2)$.

Case (a): Neither $u$ nor $v$ is contained in $V(H_2)$. Then both $u$ and $v$ are contained in edges of $H_2$ and are added in the subdivision step when obtaining $H$ from $H_2$. We have two subcases to consider. The first one assumes that both $u$ and $v$ are contained in the same edge. We assume that both of them are contained in $e_1$; the other cases are similar (see Fig. 7 B for an illustration). Then at most one path between $u$ and $v$ in $U(H)$ does not contain the vertex $u_2$, and hence $U(H)$ does not contain a subdivision of $K_{2,3}$, a contradiction. The second subcase assumes that $u$ and $v$ are contained in two different edges. We assume $v$ is contained in $e_1$ and $u$ is contained in $e_2$; the other cases are similar (see Fig. 7 C for an illustration). Then each path between $u$ and $v$ in $U(H)$ contains either $u_1$ or $u_2$, and hence $U(H)$ does not contain a subdivision of $K_{2,3}$, a contradiction.

Case (b): Precisely one of the vertices between $u$ and $v$ is contained in $V(H_2)$. Without loss of generality, we assume $u \in V(H_2)$ and $v \notin V(H_2)$. Then there are 30 combinations to consider: five choices for $u$, and six choices for $v$. Here we consider the combination $u = u_1$ and $v$ is contained in $e_1$ (see Fig. 7 D for an illustration); the other combinations can be proved similarly. For this combination, each path between $u$ and $v$ in $U(H)$ contains either $u_1$ or $u_2$, and hence $U(H)$ does not contain a subdivision of $K_{2,3}$, a contradiction.

Case (c): Both vertices are contained in $V(H_2)$, that is, $\{u, v\} \subseteq V(H_2)$. Since $\{u, v\} \neq \{u_1, u_2\}$, then an argument similar to the proof of Case (a) shows that $U(H)$ does not contain a subdivision of $K_{2,3}$, a contradiction. This completes the proof of the claim, and hence also the implication (iii) ⇒ (iv).
(iv) ⇒ (ii): Since $N$ is outer planar if and only if $U(N)$ does not contain a subdivision of $K_{2,3}$ or $K_4$, it remains to show that $N$ does not contain a subdivision of $K_4$. If this were not the case, then there must exist a biconnected component $B$ of $U(N)$ such that $B$ contains a subdivision of $K_4$. This implies that we need to delete at least 3 edges from $B$ to convert it into a tree, in contradiction to the assumption that $N$ is level-2.

Remark. Note that the condition that $N$ is level-2 is optimal in Theorem 4.2 in the following sense: The network $N_1$ in Fig. 2 is level-3 and terminal planar, but not outer planar.

5 Regular Networks

In this section, we shall consider planarity of regular phylogenetic networks [17] that are defined as follows. First, note that given any cluster system $C$ on $X$, we can regard the Hasse diagram $H(C)$ as a phylogenetic network on $X$, where the root is the vertex corresponding to the cluster $X$, and each element $x \in X$ corresponds to the singleton set $\{x\}$. Conversely, given a phylogenetic network $N = (V, A)$ on $X$, consider the partial ordering $\leq_N$ on $V$ (or $\leq$ for short) given by taking $u \leq_N v$ for $u, v \in V$ if there exists a directed path from $u$ to $v$ (which includes the special case that $u = v$). The cluster induced by a vertex $v$ in $N$, denoted by $C(v)$, is the set of elements $x \in X$ such that $v \leq x$ (so $u \leq_N v, u, v \in V$ if and only if $C(v) \subseteq C(u)$), and the cluster system $C(N)$ induced by $N$ consists of all clusters induced by the vertices in $N$. A phylogenetic network $N$ on $X$ is regular if $N$ is isomorphic to $H(C(N))$ [11, p.252].

Interestingly, there is a special type of planar, regular phylogenetic network on $X$ that first appeared sometime ago in the literature [18] (using different terminology). Following [31], a cluster system $C$ of $X$ is a prepyramid if it can be represented as a family of intervals, that is, there exists a bijective mapping $f$ from $X$ to $[n] := \{1, \ldots, n\}$ such that $f(A)$ is an interval of $\{1, \ldots, n\}$ for each cluster $A$ in $C$, and a pyramid if it is both pre-pyramid and closed under intersection [18]. Here we use the convention that singleton sets are also intervals. We define a (pre)pyramid network to be a phylogenetic network on $X$ of the form $H(C)$ for a (pre)pyramid on $X$. In [18] pyramid networks were implicitly defined and shown to be planar. An example of such a network also appeared recently in [32, Fig 2]. Note that pyramids are closely related to the so-called circular split systems (see e.g., [31]), the type of split systems that underpin the NeighborNet algorithm mentioned in the introduction.

In this section, we shall show that terminal planar regular networks and pyramidal networks are in fact one and the same thing. To prove this, we shall use the following three results rephrased in our terminology: (F1) the poset induced by a planar digraph with one source and one sink is a lattice [23, Theorem 5], (F2) a lattice is upward planar if and only if it has dimension at most 2 [33, Proposition 5.2], and (F3) if $C$ is a pyramidal on $X$, then the poset $(C, \subseteq)$ has dimension at most 2 [19, Theorem 3.6.1].

Theorem 5.1. Suppose that $N$ is regular phylogenetic network on $X$. Then $N$ is terminal planar if and only if $N$ is pyramidal.

Proof. Let $N$ be a regular network on $X$. Denote its cluster system by $C = C(N)$ so that, since $N$ is regular, $N \cong H(P(C))$. Clearly the isomorphism between $N$ and $H(P(C))$ can be extended to give a digraph isomorphism between the completion $N^*$ of $N$ and the Hasse diagram $H(P^*(C))$, by mapping the sink vertex $t$ in $N^*$ to the vertex in $H(P^*(C))$ associated with the bottom element.

For the ‘if’ direction, suppose that $N$ is pyramidal, so that $C$ is a pyramid. Then by Lemmas 2.1 and the fact (F3) above, $P^*(C)$ is a lattice with dimension at most 2. It follows that $H(P^*(C))$ is upward planar by the fact (F2) above. Hence, as $N^*$ is isomorphic to $H(P^*(C))$, it follows that $N^*$ is upward planar, and so $N$ is terminal planar by Theorem 3.1.

Now, for the ‘only if’ direction, suppose that $N$ is terminal planar. By Theorem 3.1 $N^*$ is upward planar. As $N^*$ is isomorphic to $H(P^*(C))$, by the fact (F1) above it follows that $P^*(C)$ is a lattice. Therefore, $C$ is closed under intersection, that is, for any two vertices $u$ and $v$ in $N$ with $C(u) \cap C(v) \neq \emptyset$, there exists a vertex $w$ in $N$ such that $C(u) \cap C(v) = C(w)$.

Fix an upward planar drawing $G^*$ of $N^*$, and let $\Gamma$ be the terminal planar drawing of $N$ induced by $\Gamma^*$, that is, $\Gamma$ is obtained from $\Gamma^*$ by removing the node corresponding to the sink vertex in $N^*$ and all arcs incident with it. Consider the ordering of the elements in $X$ obtained from the drawing $\Gamma$ of $N$ by following the outer-face of $\Gamma$ in a clockwise direction starting from the node associated with the root of $N$. This gives a bijective map $f$ from $X$ to $\{1, \ldots, n\}$, where $n = |X|$. For simplicity, we may further assume that the elements in $X$ are enumerated in a way such that $f(x_i) = i$ holds for all $1 \leq i \leq n$. We claim that for each cluster $A$ in $C$, $f(A)$ is an interval of $\{1, \ldots, n\}$ which, as $C$ is closed under intersection, will complete the proof of the theorem.

To establish the claim, consider an arbitrary vertex $v$ in $N$. Without loss of generality, we suppose that $a < b$ are two numbers in $\{1, \ldots, n\}$ with $a < b - 1$ and both $x_a \leq v$ and $x_b \leq v$ hold for $x_a := f^{-1}(a)$ and $x_b := f^{-1}(b)$, as otherwise the claim clearly holds. It suffices to show that for each $c$ with $a < c < b$ we have $x_c \leq v$ for the leaf $x_c := f^{-1}(c)$. This clearly holds if $v$ is the root of $N$, and
hence we may assume that \( v \) is not the root for the remainder of the proof of the claim.

Fix two directed paths \( H_a \) and \( H_b \) in \( N^* \) between \( v \) and \( x_a \) and \( x_b \), respectively. Furthermore, let \( e_a = (x_a, t) \) and \( e_b = (x_b, t) \) denote the two directed edges connecting \( x_a \) and \( x_b \) to the sink element \( t \), respectively. Without loss of generality, we may further assume that \( v \) is the only common vertex contained in both \( H_a \) and \( H_b \), as otherwise we can replace \( v \) by the lowest vertex in \( H_a \) that is also contained in \( H_b \).

Let \( L_a = \Gamma^+(H_a) \) and \( L_b = \Gamma^+(H_b) \) be the curves in the drawing \( \Gamma^+ \) corresponding to \( H_a \) and \( H_b \), respectively. Then the curve \( L = L_a \cup L_b \cup \Gamma^+(e_a) \cup \Gamma^+(e_b) \) forms a closed Jordan curve in the plane. By the Jordan Curve Theorem (see e.g., [20, Theorem 4.1.1]), it follows that \( L \) partitions the plane into precisely two connected components, one containing the node corresponding to root \( \rho \), and the other containing the node corresponding to vertex \( x_e \).

Now, fix a path \( H_e \) in \( N^* \) from the root \( \rho \) to \( x_e \). Then, as \( L \) partitions the plane into precisely two connected components, \( \Gamma^+(H_e) \) must intersect at least one node in \( L \). That is, there exists a vertex \( u \) in \( N^* \) such that \( \Gamma^+(u) \in L \cap \Gamma^+(H_e) \). Since \( \Gamma^+ \) is an upward planar drawing of \( N^* \), we can further assume \( u \notin \{x_a, x_b, t\} \). Since \( v \preceq u \preceq x_e \), it follows that \( x_e \in \mathcal{C}(u) \), which completes the proof of the claim.

Note that there are regular networks on \( X \) have can have \( 2^{|X|} - 1 \) vertices (see, e.g., [11, Section 10.3.4]), but by Theorem 5.1, the number of vertices in any terminal planar regular network is less than or equal to \( |X|^2 \), the number of intervals of \( \{1, 2, \ldots, |X|\} \). Thus by Theorem 3.3 we have:

\section{Discussion}

In this paper, we have considered the concept of planar phylogenetic networks, and shown that the theory and algorithms coming from the area of planar digraphs can be very useful for handling and understanding these structures. There remain several open questions. For example:

- Further elucidate planarity for additional classes of rooted phylogenetic networks, such as galled and tree-based networks (see e.g., [34] for a recent review).
- Given a planar phylogenetic network on \( X \), let \( \bar{N} \) be the digraph obtained from \( N \) by adding an additional arc \((x, \rho)\) for each element \( x \) in \( X \) if \((\rho, x)\) is not already an arc in \( N \). If \( N \) is terminal planar, then it is straight-forward to see that \( N \) is planar, but does the converse hold?
- Given a normal network \( N \), we define \( \text{Comp}(N) \) to be the network which is obtained from \( N \) by collapsing any arc \((u, v)\) in \( N \), where \( u \) has indegree 1 and \( v \) has indegree 1. Note that that \( \text{Comp}(N) \) must be regular (see e.g., [11, p.253]). Is \( N \) is terminal planar if and only \( \text{Comp}(N) \) is terminal planar?
- Is there a prepyramid cluster system \( C \) such that \( H(C) \) is not upward planar?
- Although there are some general algorithms for drawing planar, upper planar, terminal planar and outer planar networks (Theorem 3.3), are there more specific algorithms for drawing special types of planar phylogenetic networks such as tree-child networks?

More generally, the phylogenetic networks that we have considered in this paper did not have arc weights. It would be interesting to understand how arc weights might affect our results, especially when we want to make a straight-line drawing where the length of an arc is proportional to its weights. A special case that could be considered first are temporal phylogenetic networks which incorporate a natural vertical time axis which provides timings for past evolutionary events (see e.g., [11, p. 250]). This concept appears to be related to upward planarity, and it would be interesting to further investigate this relationship. Moreover, in general as the theory of phylogenetic networks continues to grow it could be worthwhile to develop new algorithms to produce planar phylogenetic networks from biological data.

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