TripNet: A Heuristic Algorithm for Constructing Rooted Phylogenetic Networks from Triplets

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Abstract

The problem of constructing an optimal rooted phylogenetic network from a set of rooted triplets is an NP-hard problem. In this paper, we present a heuristic algorithm called TripNet which tries to construct an optimal rooted phylogenetic network from an arbitrary set of triplets. We prove some theorems to justify the performance of the algorithm.

Index Terms

Rooted phylogenetic network, Rooted triplet, Quartet, Directed acyclic graph, Height function.

I. INTRODUCTION

Phylogenetic networks are a generalization of phylogenetic trees that permit the representation of non-tree-like underlying histories. A rooted phylogenetic network is a rooted directed acyclic graph in which no nodes has indegree greater than 2 and the outdegree of each node with indegree 2 is 1. Such nodes are called reticulation nodes. Mathematicians are interested in developing methods that infer a phylogenetic tree or network from basic building blocks. In the computation
of a rooted tree or network, one group of the basic building blocks are triplets, the rooted binary
trees on three taxa (1). In 1981, Aho et al., studied the problem of constructing a tree from a
set of triplets (2). They proposed an algorithm called the BUILD algorithm which shows that,
given a set of triplets, it is possible to construct in polynomial time a rooted tree that all the
input triplets are contained in it or decide that no such tree exists. When there is no tree for a
given set of triplets one may try to produce an optimal phylogenetic network. In this context, the
goal is to compute an optimal rooted phylogenetic network that contains all the rooted triplets.
One possible optimality criterion is to minimize the level of the network, which is defined as the
maximum number of reticulation nodes contained in any biconnected component of the network.
The other optimality criterion is to minimize the number of reticulation nodes (1). In (3) and
(4) the authors considered the problem of deciding whether, given a set of triplets as input, is
it possible to construct a level-1 phylogenetic network that contains all the input triplets? They
showed that, in general, this problem is NP-hard. However, in (4) the authors showed that when
the set of triplets is dense, which means that for each set of three taxa there is at least one triplet
in the input set, the problem can be solved in polynomial time. After their results, all research in
this new area has up to this point focused on constructing networks from dense triplet sets. The
algorithm by (5) can be used to find a level-1 or a level-2 phylogenetic network which minimizes
the number of reticulation nodes if such a network exists. In (6) the authors showed that given
a dense set of triplets \( \tau \) and a fixed number \( k \), it is possible to construct in time \( O(|\tau|^{k+1}) \) a
level-\( k \) phylogenetic network consistent with \( \tau \) or decides that no such network exists.

In this paper we present a heuristic algorithm called TripNet for constructing phylogenetic
networks from an arbitrary set of triplets. Despite of current methods that work for dense set of
triplets, a key innovation is the applicability of TripNet to non-dense set of triplets. The results of
the TripNet algorithm on biological sequences is presented in (7). Here we prove some theorems
to justify the performance of the algorithm. This paper is organized as follows. In section II we
present some definitions and notation. In section III we discuss triplet construction methods. In
section IV the directed graph \( G_\tau \) related to a set of triplets \( \tau \) is introduced. In section V the
concept of the height function of a tree is introduced, and we propose an algorithm to construct
a tree from its height function. Then we generalize the concept of the height function to the
networks. Finally, in section VI we present the TripNet algorithm.
II. Definitions and Notation

Let $X$ be a set of taxa. A rooted phylogenetic tree (tree for short) on $X$ is a rooted unordered leaf labeled tree whose leaves are distinctly labeled by $X$ and every node which is not a leaf has at least outdegree two. A directed acyclic graph (DAG) is a directed graph that is free of directed cycles. A directed acyclic graph $G$ is connected if there is an undirected path between any two nodes of $G$. It is biconnected if it contains no node whose removal disconnects $G$. A biconnected component of a graph $G$ is a maximal biconnected subgraph of $G$. A rooted phylogenetic network (network for short) on $X$ is a rooted directed acyclic graph in which root has indegree 0 and outdegree 2 and every node except the root satisfies one of the following conditions:

a) It has indegree 2 and outdegree 1. These nodes are called reticulation nodes.
b) It has indegree 1 and outdegree 2.
c) It has indegree 1 and outdegree 0. These nodes are called leaves and are distinctly labeled by $X$.

A reticulation leaf is a leaf whose parent is a reticulation node. A network is said to be a level-$k$ network if each of its biconnected component contains at most $k$ reticulation nodes. A tree can be considered as a level-0 network.

A rooted triplet (triplet for short) is a binary rooted unordered tree with three leaves. We use $ij|k$ to denote the triplet with taxa $i$ and $j$ on one side and $k$ on the other side of the root (Fig. 1(a)). A set of triplets $\tau$ is called dense if for each subset of three taxa, there is at least one triplet in $\tau$. A triplet $ij|k$ is consistent with a network $N$ or equivalently $N$ is consistent with $ij|k$ if $N$ contains a subdivision of $ij|k$, i.e. if $N$ contains distinct nodes $u$ and $v$ and pairwise internally node-disjoint paths $u \rightarrow i$, $u \rightarrow j$, $v \rightarrow u$ and $v \rightarrow k$. Fig. 1(b) shows an example of a network which is consistent with $ij|k$. A set $\tau$ of triplets is consistent with a network $N$ if all the triplets in $\tau$ are consistent with $N$. We use the symbols $\tau(N)$ and $L_N$ to represent the set of all triplets that are consistent with $N$ and the set of labels of its leaves respectively. For any set $\tau$ of triplets define $L(\tau) = \bigcup_{t \in \tau} L_t$. The set $\tau$ is called a set of triplets on $X$ if $L(\tau) = X$.

III. Triplets construction method

There are two main tree construction methods, character-based methods and distance-based methods. In character-based methods, the information of a set $X$ of biological sequences is
directly used for producing final tree. In distance-based methods first a distance matrix $D$ is computed from $X$ and then a rooted (or unrooted) tree $T$ is constructed from $D$ (1).

A weighted tree $(T, w)$ is a rooted (or unrooted) tree $T$ together with a function $w : E(T) \to \mathbb{R}$. We call $w(e)$ the weight of the edge $e$. For any two nodes $i$ and $j$ of $T$, let $l_{ij}$ denotes the unique path in $T$ from $i$ to $j$. Define

$$d_T(i, j) = \sum_{e \in l_{ij}} w(e).$$

If $T$ is an unweighted tree then we suppose that for each edge $e$ in $T$, $w(e) = 1$. Given a set of taxa $X$, let $(T, w)$ be a weighted tree on $X$ and $D_T$ be a matrix in which the entry of row $i$ and column $j$ is $d_T(i, j)$. We call $D_T$ the distance matrix related to $(T, w)$.

A quartet is a binary unrooted tree with four leaves. We use the symbol $ij|kl$ for a quartet on the set of taxa $\{i, j, k, l\}$ which have neighbor pairs $i, j$ and $k, l$. In a quartet $Q$ there is a unique edge such that its two end points are not leaves. We call this edge the *inner edge* of $Q$ (Fig. 1(c)). A weighted quartet is called *informative*, if the weight of its inner edge is positive. The following proposition holds for informative quartets.

**Proposition 1.** Given a set of four taxa $X = \{i, j, k, l\}$ and a distance matrix $D$ on $X$. For an informative quartet $ij|kl$, the equation $d(i, j) + d(k, l) < d(i, k) + d(j, l) = d(j, k) + d(i, l)$ holds.
The following proposition also holds (9).

**Proposition 2.** Given a set of four taxa $X$ and a distance matrix $D$ on $X$. There is a unique quartet $Q$ on $X$ for which $D_Q = D$.

Suppose that $X$ is a set of taxa in which each taxon is a biological sequence. Let $o_X$ be an outgroup for $X$ and $D$ be a distance matrix on $X \cup \{o_X\}$. In this paper to obtain a set of triplets, we use the method introduced in (5). For each set of four taxa that contains $o_X$, we construct the unique quartet which satisfies Proposition 2. Then, by removing $o_X$ from informative quartets we obtain the set of triplets. In the rest of paper we refer to this method by QOT.

**IV. The directed graph related to a set of triplets**

Let $\tau$ be a set of triplets. Define $G_\tau$, the directed graph related to $\tau$, by $V(G_\tau) = \{\{i, j\} : i, j \in L(\tau), i \neq j\}$ (we denote $\{i, j\}$ by $ij$ for short) and $E(G_\tau) = \{(ij, ik) : i|j|k \in \tau\} \cup \{(ij, jk) : i|j|k \in \tau\}$. The graph $G_\tau$ has an important role in the remaining of the paper and in this section we prove some basic properties of $G_\tau$.

Let $X$ be a set of sequences, $D = [d(i, j)]$ be a distance matrix on $X$ where for any pair $i, j \in X$, $d(i, j)$ denotes the distance between them, and $\tau$ be the set of triplets that is produced by QOT method. Here we define the concept of the closure of $\tau$. If $ij|k$ and $js|i$ are in $\tau$, then we have the quartets $ij|ko_X$ and $js|io_X$. According to the Proposition 1, $d(i, j) + d(k, o_X) < d(j, k) + d(i, o_X)$, $d(j, s) + d(i, o_X) < d(i, j) + d(s, o_X)$, and therefore $d(j, s) + d(k, o_X) < d(j, k) + d(s, o_X)$. It means that we should have the quartet $js|ko_X$. The equivalent triplet for this informative quartet is $js|k$. If this triplet is not in $\tau$ add it to $\tau$ and continue this procedure until one cannot add more triplets. We use the symbol $\overline{\tau}$ to show this new set of triplets and call it the closure of $\tau$.

The following lemma is an immediate consequence of the definition of $\overline{\tau}$.

**Lemma 1.** Let $X$ be a set of sequences and $\tau$ be the set of triplets which is produced by the QOT method. Then $\overline{\tau}$ contains at most one triplet for each $\{i, j, k\} \subseteq X$. 
Now we state the main results of this section.

**Theorem 1.** Let $X$ be a set of sequences and $\tau$ be the set of triplets which is produced by the QOT method. Then $G_\tau$ is a DAG.

**Proof:** We prove a stronger result and show that $G_\tau$ is a DAG. The proof proceeds by induction on the length of the shortest cycle in $G_\tau$. First we prove that $G_\tau$ dose not contain any cycle of length 3. Assume that $C$ is a cycle of length 3 in $G_\tau$. Let $(ij, ik)$ be an edge of $C$. The triplet which corresponds to this edge is $ij|k$. Suppose that the third node of the cycle is $st$. Thus the other edges of the cycle are $(st, ij)$ and $(ik, st)$. So $\{|i, j\} \cap \{s, t\} = \{|i, k\} \cap \{s, t\} = 1$.

There are two cases. Case 1: $s = i$ and $t \neq j, k$ (or $t = i$ and $s \neq j, k$). Case 2: $s = j$ and $t = k$ (or $s = k$ and $t = j$). For the first case, the edges of $C$ are $(ij, ik)$, $(ik, it)$ and $(it, ij)$. The three quartets which are corresponds to the triplets of these three edges are $(ij|ko_X, ik|to_X)$ and $(it|jo_X)$. According to Proposition 1, we have three inequalities $d(i, j) + d(k, o_X) < d(i, k) + d(j, o_X)$, $d(i, k) + d(t, o_X) < d(i, t) + d(k, o_X)$ and $d(i, t) + d(j, o_X) < d(i, j) + d(t, o_X)$. By summing up these inequalities, we obtain a contradiction. For the second case the edges of $C$ are $(ij, ik)$, $(ik, jk)$ and $(jk, ij)$. The three triplets corresponds to these three edges are $ij|k, ik|j$ and $jk|i$ which contradicts Lemma 1. So there is no cycle of length 3 in $G_\tau$. Now assume that there is no cycle of length $k \geq 3$ in $G_\tau$ and $C$ be a cycle of length $k + 1$ in it. First we claim that there is no path $s_1s_2 \rightarrow s_3s_4 \rightarrow s_5s_6$ in $C$ such that $\{|s_1, s_2\} \cap \{s_3, s_4\} \cap \{s_5, s_6\} = 1$. Suppose that there exists such a path. So this path is of the form $js \rightarrow ji \rightarrow jk$ and triplets $js|i$ and $ij|k$ are in $\tau$. The method of constructing $\tau$ implies that $js|k$ is in $\tau$ and the edge $js \rightarrow jk$ is in $G_\tau$. So we obtain a cycle of length $k$ in $G_\tau$, a contradiction.

Let $s_1s_2$ be a node of $C$. There exists a node $s_3$ such that the edge $s_1s_2 \rightarrow s_1s_3$ is in $C$ and $s_1s_3$ is connected to a node $s_1s_4$ or $s_3s_4$. If $s_1s_4 \in V(C)$ then $s_1s_2 \rightarrow s_1s_3 \rightarrow s_1s_4$ will be in $C$ which contradicts the above claim. So the cycle $C$ is of the form $s_1s_2 \rightarrow s_1s_3 \rightarrow s_3s_4 \rightarrow \ldots \rightarrow s_ks_k+1 \rightarrow s_{k+1}s_{k+2} \rightarrow s_1s_2$. For the edges $s_{k+1}s_{k+2} \rightarrow s_1s_2$ we obtain $|\{s_1, s_2\} \cap \{s_{k+1}, s_{k+2}\}| = 1$. For the cases $s_{k+1} = s_l, l \in \{1, 2\}$ or $s_{k+2} = s_1$ we have a cycle of length $k$ in $G_\tau$. So $s_{k+2} = s_2$ and triplets $s_1s_2|s_3, s_1s_3|s_4, s_3s_4|s_5, \ldots, s_{k-1}s_k|s_{k+1}, s_ks_{k+1}|s_2$ and $s_{k+1}s_2|s_1$ are in $\tau$. Equivalently, we have the following inequalities:

$$d(s_1, s_2) + d(s_3, o) < d(s_1, s_3) + d(s_2, o),$$
\[d(s_1, s_3) + d(s_4, o) < d(s_3, s_4) + d(s_1, o),\]
\[\vdots\]
\[d(s_k, s_{k+1}) + d(s_1, o) < d(s_{k+1}, s_1) + d(s_k, o),\]
\[d(s_{k+1}, s_1) + d(s_2, o) < d(s_1, s_2) + d(s_{k+1}, o).\]

Summing these inequalities, we obtain a contradiction. So there is no cycle of length \(k + 1\) in \(G_\tau\).

Let \(\tau\) be a set of triplets that is consistent with a tree. Let \(T_\tau\) denote the unique tree that is produced by the BUILD algorithm.

**Theorem 2.** Let \(\tau\) be a set of triplets that is consistent with a tree. Then \(G_\tau\) is a DAG.

**Proof:** The proof proceeds by induction on \(|L(\tau)|\). It is trivial when \(|L(\tau)| = 3\). Assume that theorem holds when \(|L(\tau)| \leq k\). Let \(|L(\tau)| = k + 1\) and \(T_1, T_2, \ldots, T_m\) be \(m\) subtrees that are obtained from \(T_\tau\) by removing its root. For each \(i, 1 \leq i \leq m\), let \(\tau_i = \tau|_{L_{T_i}}\) denotes the set of all triplets in \(\tau\) whose leaves are in \(L_{T_i}\). By the induction assumption for each \(i, 1 \leq i \leq m\), \(G_{\tau_i}\) is a DAG. Let \(\tau' = \bigcup_{1 \leq i \leq m} \tau_i\) and \(G' = \bigcup_{1 \leq i \leq m} G_{\tau_i}\). Apparently, \(G'\) is a DAG and \(G_{\tau'} = G'\).

The graph \(G_\tau\) can be obtained from \(G'\) by adding the nodes which belong to \(V(G_\tau) \setminus V(G')\) and the edges corresponds to the triplets in \(\tau \setminus \tau'\). If a triplet \(t = ab|c \in \tau \setminus \tau'\) then there is \(1 \leq i < j \leq m\) such that \(a, b \in L(\tau_i)\) and \(c \in L(\tau_j)\). It means that the edges corresponds to the triplets in \(\tau \setminus \tau'\) are of the form \((ab, ac)\) such that \(ac \in V(G_\tau) \setminus V(G')\). So all nodes in \(V(G_\tau) \setminus V(G')\) has outdegree zero and the edges in \(G_\tau \setminus G'\) are from \(V(G')\) to \(V(G_\tau) \setminus V(G')\). Now if there exists a cycle in \(G_\tau\) it should contain a node in \(V(G_\tau) \setminus V(G')\) which contradicts that these nodes have outdegree zero and the proof is complete.

**V. Height Function**

In this section first the concept of the height function of a tree and a DAG is introduced and then the BUILD algorithm is restated based on this concept.

Let \(\binom{X}{2}\) denotes the set of all subsets of \(X\) of size 2.

**Definition 1.** Let \(X\) be an arbitrary finite set. A function \(h : \binom{X}{2} \to \mathbb{N}\) is called a height function on \(X\).
Let $T$ be a rooted tree with the root $r$, $c_{ij}$ be the lowest common ancestor of the leaves $i$ and $j$, and $l_T$ denotes the length of the longest path started from $r$.

**Definition 2.** The height function of $T$, $h_T$, is defined as $h_T(i, j) = l_T - d_T(c_{ij}, r)$ where $i$ and $j$ are two distinct leaves of $T$.

The following theorem represents the relation between the height function of a tree and a triplet consistent with it.

**Theorem 3.** Let $T$ be a tree. A triplet $ij|k$ is consistent with $T$ if and only if $h_T(i, j) < h_T(i, k)$ or $h_T(i, j) < h_T(j, k)$.

**Proof:** Let $ij|k$ be consistent with $T$. By definition $h_T(i, j) < h_T(i, k)$ and $h_T(i, j) < h_T(j, k)$. Now suppose that for the three arbitrary leaves $i, j$ and $k$, we have $h_T(i, j) < h_T(i, k)$ or $h_T(i, j) < h_T(j, k)$. Without loss of generality suppose that $h_T(i, j) < h_T(i, k)$. Since $c_{ij}$ and $c_{ik}$ are on a unique path from the root $r$ to $i$ and $d_T(c_{ij}, r) > d_T(c_{ik}, r)$, thus there is a path from the lowest common ancestor of $i, k$ to the lowest common ancestor of $i, j$ which follows that $ij|k$ is consistent with $T$.

Let $\tau$ be a set of triplets, $G_\tau$ be a DAG and $l_{G_\tau}$ denotes the length of the longest path in $G_\tau$. Since $G_\tau$ is a DAG, the set of nodes with outdegree zero is nonempty. Assign $l_{G_\tau} + 1$ to the nodes with outdegree zero and remove them from $G_\tau$. Assign $l_{G_\tau}$ to the nodes with outdegree zero in the resulting graph and continue this procedure until all nodes are removed.

**Definition 3.** For any two distinct $i, j \in L(\tau)$, define $h_{G_\tau}(i, j)$ as the value that is assigned by the above procedure to the node $ij$ and call it the height function related to $G_\tau$.

Let $\tau$ be a set of triplets that is consistent with a tree. By Theorem 2, $G_\tau$ is a DAG and $h_{G_\tau}$ is well-defined. The following theorem represents a method to obtain $h_{T_\tau}$ from $\tau$ using $h_{G_\tau}$.

**Theorem 4.** Let $\tau$ be a set of triplets which is consistent with a tree. Then $h_{G_\tau} = h_{T_\tau}$.

**Proof:** The proof proceeds by induction on $|L_{T_\tau}|$. It is trivial when $|L_{T_\tau}| = 3$. Assume that theorem holds when $|L_{T_\tau}| \leq k$. Let $|L_{T_\tau}| = k + 1$ and $T_1, T_2, \ldots, T_m$ be $m$ subtrees which are
obtained from $T_i$ by removing its root. For each $i, 1 \leq i \leq m$ let $\tau_i = \tau|_{T_{\tau_i}}$, and $r_i$ be the root of $T_i$. By the induction assumption for each $i, 1 \leq i \leq m$, $h_{G_{\tau_i}} = h_{T_{\tau_i}}$. Moreover we conclude from the BUILD algorithm that $T_i = T_{\tau_i}$, for $1 \leq i \leq m$. Thus $h_{G_{\tau_i}} = h_{T_{\tau_i}}$, for $1 \leq i \leq m$. So for $i, 1 \leq i \leq m$, the maximum length of the longest path in $T_i$ is $l_{T_{\tau_i}} - 1$. It means that for $i, 1 \leq i \leq m$, the maximum length of the longest path in $G_{\tau_i}$ is $l_{T_{\tau_i}} - 2$. Therefore by the proof of Theorem 2 the length of the longest path in $G_\tau$ is $l_{T_{\tau_i}} - 1$. Let $a, b \in L_{T_{\tau_i}}$. We have two cases.

**Case 1:** For some $i$ and $j$, $1 \leq i < j \leq m$, $a \in L_{T_i}$ and $b \in L_{T_j}$. Since the outdegree of $ab$ in $G_\tau$ is zero and $c_{ab} = r$, then $h_{T_{\tau_i}}(a, b) = l_{T_{\tau_i}} = h_{G_{\tau_i}}(a, b)$.

**Case 2:** For some $i$, $1 \leq i \leq m$, $a, b \in L_{T_i}$. By the induction assumption $h_{G_{\tau_i}}(a, b) = h_{T_{\tau_i}}(a, b)$. Therefore $h_{T_{\tau_i}}(a, b) = l_{T_{\tau_i}} - d_{T_{\tau_i}}(c_{ab}, r_i) = l_{T_{\tau_i}} - (d_{T_{\tau_i}}(c_{ab}, r_i) + 1) = (l_{T_{\tau_i}} - 1) + (l_{T_{\tau_i}} - d_{T_{\tau_i}}(c_{ab}, r_i) - 1) = (l_{T_{\tau_i}} - 1) + h_{T_{\tau_i}}(a, b) = (l_{T_{\tau_i}} - 1) + h_{G_{\tau_i}}(a, b) = h_{G_{\tau_i}}(a, b)$. The last equality is obtained by construction of $G_\tau$ from $G_{\tau_i}$ which is stated in the proof of Theorem 2. So for each $a, b \in L_{T_{\tau_i}}$, $h_{T_{\tau_i}}(a, b) = h_{G_{\tau_i}}(a, b)$ and the proof is complete.

Now we describe an algorithm similar to BUILD algorithm, using height function. We refer to this algorithm by $HBUILD$. Let $h$ be a height function on $X$. Define a weighted complete graph $(G, h)$ where $V(G) = X$ and edge $\{i, j\}$ has weight $h(i, j)$. Remove the edges with maximum weight from $G$. If removing these edges results a connected graph the algorithm stops. Otherwise, the process of removing the edges with maximum weight is continued in each connected component until each connected component contains only one node. At the end of this procedure one can reconstruct the tree by reversing the steps of the algorithm similar to BUILD algorithm (see Fig. 2). The algorithm above decides in polynomial time whether a tree with height function $h$ exists.

Now if $\tau$ is a set of triplets which is consistent with a tree, by Theorems 2 and 4, $G_\tau$ is a DAG and $h_{G_\tau} = h_{T_\tau} = h$ and HBUILD algorithm constructs $T_\tau$.

Now we generalize the concept of height function from trees to networks. This generalization is not straightforward because the concept of (lowest) common ancestor of two leaves of a network is not well-defined. Let $N$ be a network with the root $r$ and $l_N$ be the length of the longest directed path from $r$ to the leaves. For each node $u$ consider $d(u, r)$ as the length of the longest directed path from $r$ to $u$. For any two nodes $u$ and $v$, we call $u$ an ancestor of $v$, if there exists a directed path from $u$ to $v$. If $u$ is an ancestor of $v$ then we say that $v$ is lower
Fig. 2. The steps of constructing $T_\tau$ from the given set $\tau = \{kl|j, kl|i, jk|i, jl|i\}$. (a) The graph $G_\tau$. (b) The graph $(G, h)$. (c) Removing maximum weights from the graph $(G, h)$. (d) Constructing $T_\tau$ using step c.

than $u$. Lowest common ancestor of two leaves in a network is not necessarily unique. For any two leaves $i$ and $j$, let $C_{ij}$ be the set of all lowest common ancestors of $i$ and $j$.

**Definition 4.** For each pair of leaves $i$ and $j$, define $h_N(i, j) = \min\{l_N - d(c, r) : c \in C_{ij}\}$ and call it the height function of $N$.

Obviously, every network $N$ indicates a unique height function $h_N$. But two different networks may have the same height function (see Fig. 3(a)) .

Fig. 3. (a) Two different networks with the same height function. $h_N = h_T = h$. $h(j, k) = 1, h(i, j) = h(i, k) = 2$ and $h(i, l) = h(j, l) = h(k, l) = 3$. (b) $T_2$ is a binarization of $T_1$.

In the following proposition we prove that for a given height function $h$ there is a network $N$ such that $h_N = h$.

**Proposition 3.** Let $X$ be an arbitrary finite set and $h$ be a height function on $X$. Then there
exists a network \( N \) not necessarily binary, such that \( h_N = h \).

**Proof:** Let \( h_{\text{max}} = \max\{h(x,y) : x, y \in X\} \). Let \( r \) be the root of \( N \). For each pair of nodes \( x \) and \( y \) with \( h(x,y) = h_{\text{max}} \), we connect \( x \) and \( y \) to \( r \). For each pair of nodes \( x \) and \( y \) with \( h(x,y) < h_{\text{max}} \), we consider a new node and connect this node to \( r \) by \( h_{\text{max}} - h(x,y) \) edges. By deleting multiple edges we obtain a network \( N \) with \( h_N = h \). \( \blacksquare \)

The following theorem shows the relation between height function of a network and the triplet consistency with it.

**Theorem 5.** Let \( N \) be a network, \( i, j, \) and \( k \) be its three distinct leaves. If \( h_N(i,j) < h_N(i,k) \) or \( h_N(i,j) < h_N(j,k) \) then \( i|j|k \) is consistent with \( N \).

**Proof:** Suppose that \( h_N(i,j) < h_N(i,k) \). Let \( v_{ij} \) and \( v_{ik} \) be common ancestors of \( i, j \) and \( i, k \) respectively, such that \( h_N(i,j) = l_N - d(v_{ij}, r) \) and \( h_N(i,k) = l_N - d(v_{ik}, r) \). Let \( l_i \) and \( l_j \) be two distinct paths from \( v_{ij} \) to \( i \) and \( j \), respectively. Let \( l_k \) be an arbitrary path from \( v_{ik} \) to \( k \). If \( l_i \cap l_k \neq \emptyset \) then it follows that \( h_N(i,j) \geq h_N(i,k) \) which is a contradiction. So \( i|j|k \) is consistent with \( N \). \( \blacksquare \)

The reverse of the above theorem is not necessarily true. For example, consider the network of Fig. 1(e). The triplet \( i|j|k \) is consistent with it, but \( h(i,j) = h(i,k) = 3 \) and \( h(j,k) = 2 \).

The basic idea of the TripNet algorithm is to find a height function as an intermediate computational step that yields the minimum amount of information required to construct the network from a set of triplets. So it is important to find a way for computing \( h_N \) from a set of triplets. In the rest of this section we introduce a computational method for computing \( h_N \) using Integer Programming. Let \( \tau \) be a set of triplets with \( |L(\tau)| = n \). Inspiring from Theorems 3 and 5, for each triplet \( i|j|k \in \tau \), define two inequalities \( h(i,k) - h(i,j) \geq 1 \) and \( h(j,k) - h(i,j) \geq 1 \). Since the number of variables in such inequalities are at most \( c(n,2) \), we obtain the following
system of inequalities from $\tau$.

$$
\begin{align*}
  h(i, k) - h(i, j) &\geq 1 \quad ij|k \in \tau, \\
  h(j, k) - h(i, j) &\geq 1 \quad ij|k \in \tau, \\
  0 < h(i, j) &\leq c(n, 2) \quad 1 \leq i, j \leq n.
\end{align*}
$$

Let $s$ be an integer. Define the following Integer Programming and call it IP($\tau, s$).

Maximize $\sum_{1 \leq i, j \leq n} h(i, j)$,

Subject to:

$$
\begin{align*}
  h(i, k) - h(i, j) &\geq 1 \quad ij|k \in \tau, \\
  h(j, k) - h(i, j) &\geq 1 \quad ij|k \in \tau, \\
  0 < h(i, j) &\leq s \quad 1 \leq i, j \leq n.
\end{align*}
$$

Intuitively if IP($\tau, s$) has a feasible solution, we expect that the optimal solution to this integer programming is an approximation of the height function of an optimal network $N$ consistent with $\tau$. The following theorems support this intuition.

**Theorem 6.** Let $\tau$ be a set of triplets. Then $G_\tau$ is a DAG if and only if for some integer $s$, the IP($\tau, s$) has a feasible solution. In this case the minimum number $s$, for which IP($\tau, s$) has a feasible solution, is $l_{G_\tau} + 1$.

**Proof:** Let $G_\tau$ be a DAG. Without loss of generality assume that $G_\tau$ is connected. The proof proceeds by induction on $l_{G_\tau}$. If $l_{G_\tau} = 1$ then obviously for $s = 1$, IP($\tau, s$) has no feasible solution and for each $s \geq 2$, IP($\tau, s$) has a feasible solution. Assume that the theorem holds for $l_{G_\tau} \leq k$. Suppose that $\tau$ is a set of triplets with $l_{G_\tau} = k + 1$. Let $A$ be the set of the terminal nodes of all longest paths in $G_\tau$. For each $ij \in A$ there is some $x \in L(\tau)$ such that $ix|j \in \tau$. Let $B$ be the set of all such triplets and $\tau' = \tau \setminus B$. Apparently, $B \neq \emptyset$ and the length of the longest path in $G_{\tau'}$ is $k$. By the induction assumption the minimum number $s$ for which IP($\tau', s$) has a feasible solution, is $l_{G_{\tau'}} + 1 = l_{G_\tau}$. Consider IP($\tau, l_{G_\tau} + 1$). Define $h(i, j) = l_{G_\tau} + 1$, for each $ij \in A$ and $h(t, l) = h'(t, l)$, for each $tl \notin A$. $h$ is a feasible solution to IP($\tau, l_{G_\tau} + 1$). Now if $s$ be a solution for IP($\tau, s$) then $s - 1$ is a solution for IP($\tau', s - 1$). So $l_{G_\tau} + 1$ is minimum solution for IP($\tau, s$). Now suppose that $\tau$ is a set of triplets and for some integer $s$, IP($\tau, s$) has
a feasible solution $h$. Assume that $G_{\tau}$ has a cycle $C = i_1j_1 \rightarrow i_2j_2 \rightarrow \ldots \rightarrow i_mj_m \rightarrow i_1j_1$. Corresponds to $C$ we have inequalities $h(i_1, j_1) < h(i_2, j_2) < \ldots < h(i_m, j_m) < h(i_1, j_1)$ which is a contradiction and the proof is complete.

Let $\tau$ be a set of triplets consistent with a tree. By Theorems 2, 3, and 6, $h_{T_{\tau}}$ is a feasible solution to IP($\tau$, $l_{G_{\tau}} + 1$). In the following theorem we prove the uniqueness of this solution.

**Theorem 7.** Let $\tau$ be a set of triplets consistent with a tree. Then $h_{T_{\tau}}$ is the unique optimal solution to IP($\tau$, $l_{G_{\tau}} + 1$).

**Proof:** By Theorem 2, $G_{\tau}$ is a DAG. So $l_{G_{\tau}}$ is well defined. The proof proceeds by induction on $l_{G_{\tau}}$. Without loss of generality assume that $G_{\tau}$ is connected. The theorem is trivial when $l_{G_{\tau}} = 1$. Let for each set of triplets consistent with a tree, $h_{T_{\tau}}$ be the unique optimal solution to IP($\tau$, $l_{G_{\tau}} + 1$) where $l_{G_{\tau}} = k \geq 1$. Suppose that $\tau$ is a set of triplets consistent with a tree and $l_{G_{\tau}} = k + 1$. Let $\tau'$ be the set of triplets which is introduced in the proof of Theorem 6. By the induction assumption $h_{T_{\tau'}}$ is the unique optimal solution to IP($\tau'$, $l_{G_{\tau'}} + 1$). By Theorem 6 the minimum $s$ for which IP($\tau$, $s$) has a feasible solution is $l_{G_{\tau}} + 1$. Also $l_{G_{\tau'}} + 1 = l_{G_{\tau}}$. It follows that $h_{T_{\tau}}$ is the unique optimal solution to the IP($\tau$, $l_{G_{\tau}} + 1$) and the proof is complete.

The BUILD tree is not necessarily a binary tree. To obtain a binary tree consistent with a set of triplets we do the following procedure.

Let $T$ be a tree and $x$ be a node of $T$ with $x_1, x_2, \ldots, x_k$, $k \geq 3$ as its childs. Consider a new node $y$. Construct $T'$ by removing the edges $(x, x_1), (x, x_2), \ldots, (x, x_{k-1})$ from $T$ and adding the edges $(x, y), (y, x_1), (y, x_2), \ldots, (y, x_{k-1})$ to $T$. Continuing the same method for each node with outdegree more than 2 we obtain a binary tree which we call it a binarization of $T$ (see Fig. 3(b)). Obviously, we can obtain different binarization of $T$. The proof of the following theorem is easy and we omit it.

**Theorem 8.** Let $\tau$ be a set of triplets that is consistent with a tree $T_1$, and $T_2$ be a binarization of $T_1$. Then $\tau$ is consistent with $T_2$. 
VI. **TripNet Algorithm**

Now we describe the TripNet algorithm in nine steps. In this algorithm the input is a set of triplets $\tau$ and the output is a network consistent with $\tau$. Also if $\tau$ is consistent with a tree the algorithm constructs a binarization of $T_\tau$.

**Step 1:** In this step we find a height function $h$ on $L(\tau)$. If $G_\tau$ is a DAG we set $G'_\tau = G_\tau$. If $G_\tau$ is not a DAG we remove some edges from $G_\tau$ in such a way that the resulting graph $G'_\tau$ is a DAG. Set $h = h_{G'_\tau}$.

If $\tau$ is obtained from biological sequences using the QOT method, then Theorems 2 shows that $G_\tau$ is a DAG. Removing minimum number of edges from a directed graph to make it a DAG is known as the *minimum Feedback Arc Set* problem which is NP-hard (10). Thus, using a greedy algorithm, we try to remove as minimum number of edges as possible from $G_\tau$ in order to lose minimum information. However, any such missing information will be recaptured in Step 9.

**Step 2:** In this step TripNet first apply HBUILD on $h$. If the result is a tree, TripNet constructs a binarization of this tree. Otherwise TripNet goes to Step 3.

Note that if $\tau$ is consistent with a tree, by Theorem 4, $h_{G_\tau} = h_{T_\tau}$ and TripNet constructs a binarization of $T_\tau$.

**Step 3:** Remove all the maximum-weight edges from $G$. The process of removing all the maximum-weight edges from the graph continues until the resulting graph is disconnected.

In (3) and (4) the authors introduced the concept of $SN$-sets for a set of triplets $\tau$. A subset $S$ of $L(\tau)$ is an *$SN$-set* if there is no triplet $ij|k \in \tau$ such that $i \notin S$ and $j, k \in S$. In (4) it is shown that if $\tau$ is dense then the maximal $SN$-sets partition $L(\tau)$ and can be found in polynomial time. By contracting each of the $SN$-set to a single node and assuming a common ancestor for all of these leaves, the size of the problem is reduced. In these papers, for finding the maximal $SN$-sets in polynomial time, the authors use the high density of the input triplet sets. TripNet
algorithm uses the concept of height function as an auxiliary tool to obtain $SN$-sets instead of the high density assumption.

**Step 4:** For each connected component obtaining in Step 3, which is not an $SN$-set we apply Step 3. This process continues until all of the resulting components are $SN$-sets. Let \( \{S_1, S_2, \ldots, S_k\} \) be the set of resulting $SN$-sets. If each $SN$-set contains only one node, HBUILD is applied and if the result is a tree TripNet constructs a binary tree and goes to Step 6. Otherwise TripNet goes to Step 5. If for some \( i \), \( |S_i| > 1 \), contract each \( S_i \) to a single node \( s_i \) and set \( S = \{s_1, s_2, \ldots, s_k\} \). Update the set of triplets by defining \( \tau_S = \{s_is_j|s_k : \exists \ xy \ y \in S_j \text{ and } \} \). Constructs a weighted complete graph \((G_S, w_S)\) with \( V(G_S) = S \) and \( w_S(s_i, s_j) = \min \{h(x, y) : x \in S_i \text{ and } y \in S_j\} \). Set \((G, w) = (G_S, w_S)\) and TripNet goes to Step 3.

The following theorem is consequence of definition $SN$-set for \((G_S, w_S)\).

**Theorem 9.** Applying Steps 3 and 4 on \((G_S, w_S)\) and \(\tau_S\), each resulting $SN$-set has one member.

*Proof:* Suppose that \( S = \{s_1, s_2, s_3, \ldots, s_r\} \) is an $SN$-set in \((G_S, w_S)\). Now assume that in the procedure of Step 3 by removing the edges with weight \( l \), \( S_1 \) separates from \( S_2 \). Thus there exists \( k > l \) such that by removing the edges with weight at least \( k \) in \((G_S, w_S)\), the connected component \( S \) separates from other components of \( G_S \). It means that by removing the edges with weight at least \( k \) in \( G \), we obtain the $SN$-set \( S_1 \cup \ldots \cup S_r \) in \( \tau \) which is a contradiction. $\blacksquare$

In the next step the reticulation leaves are recognized using the following three criteria:

**Criterion I:** Let \( m_i \) and \( M_i \) be the minimum and maximum weight of the edges in \((G, h)\) with exactly one end in \( S_i \). Choose the node with minimum \( m_i \) and if there is more than one node with minimum \( m_i \) then choose among them the nodes which has minimum \( M_i \). Let \( R_1 \) denotes the set of such nodes.

**Criterion II:** Let \( w_{\min} = \min \{w(s_i, s_j) : 1 \leq i, j \leq k\} \). In \( G_S \) consider the induced subgraph on the edges with the weight \( w_{\min} \). Choose the nodes of \( R_1 \) with the maximum degree in this induced subgraph. Let \( R_2 \) denotes the set of such nodes.

**Criterion III:** For each node \( s \in R_2 \), remove it from \( G_S \) and find $SN$-sets for this new graph
using Steps 3 and 4. Let \( n_s \) be the number of \( SN \)-sets of this new graph with cardinality greater than one. Choose the nodes in \( R_2 \) with maximum \( n_s \). Let \( R_3 \) denotes the set of such nodes.

We state an example to show the idea behind these three criteria.

Let \( \tau = \{ij|l, jk|i, kl|j, no|m, lo|k, jl|o, mn|l, mn|j, no|k, mo|i, jk|n, ij|o, ik|m, il|n\} \). \( \tau \) is not consistent with a tree but it is consistent with the network \( N \) shown in Fig. 4(a). Obviously, \( N \) is an optimal network consistent with \( \tau \). In order to find \( SN \)-sets we construct \( G'_\tau \) and \( (G, h) \), and find \( SN \)-sets from \( (G, h) \) using Steps 3 and 4 (Figs. 4(b) to 4(g)). It follows that \( S = \{\{i\}, \{j\}, \{k\}, \{l\}, \{m\}, \{n, o\}\} \). Now in \( G_S \) (Fig 4(h)). we expect that the reticulation is in \( R_1 \). In this example both \( k \) and \( l \) are in \( R_1 \). Also we expect that if there is a reticulation leaf, it belongs to \( R_2 \) which again both \( k \) and \( l \) are in \( R_2 \). Now just \( l \) belongs to \( R_3 \). Thus we consider \( l \) as the reticulation leaf (Figs 4(i) to 4(n)). Remove triplets from \( \tau_S \) which contain \( l \) and denote the new set of triplets by \( \tau'_S \). Obviously, \( \tau'_S \) is consistent with a tree. We add this reticulation leaf to a binarization of \( T_{\tau'_S} \) such that the resulting network is consistent with \( \tau_S \). Note that if we consider each node except than \( l \) as the reticulation leaf then final network consistent with \( \tau_S \) has at least two reticulation leaves.

**Step 5** : In this step the reticulation leaf is recognized using three criteria. Do the criterion

- **I.** If \( |R_1| = 1 \) then choose the node \( x \in R_1 \) as the reticulation node. Otherwise if \( |R_1| > 1 \) do the criterion II.
- **II.** If \( |R_2| = 1 \) then choose the node \( x \in R_2 \) as the reticulation node. Otherwise if \( |R_2| > 1 \) do the criterion III.
- **III.** If \( |R_3| = 1 \) then choose the node \( x \in R_3 \) as the reticulation node. Otherwise if \( |R_3| > 1 \) then by the speed options we choose the reticulation node as follows.

**Slow:** Each node in \( R_3 \) is examined as the reticulation leaf.

**Normal:** Two nodes in \( R_3 \) are selected randomly and each of these two nodes is examined as the reticulation leaf.

**Fast:** One node in \( R_3 \) selected randomly as the reticulation leaf.

Let \( x \) be a node which is considered as a reticulation leaf. Remove \( x \) from \( G_S \) and all of the triplets which contain \( x \) from \( \tau_S \). Define \( G = G \setminus \{x\} \) and go to Step 3.

Note that for the Fast option the running time of the algorithm is polynomial. For biological data almost always the criteria I and II find a unique reticulation leaf. So on real data the running time of TripNet is almost always polynomial.
Step 6: Let $x_1, x_2, \ldots, x_m$ be $m$ reticulation leaves which are obtained in Step 5 with this order and $T$ be the tree that is constructed in Step 4. Now add these $m$ nodes in the reverse order to $T$ as what follows. Let $e_1$ and $e_2$ be two edges of $T$. Consider two new nodes $y_1$ and $y_2$ in the middle of $e_1$ and $e_2$. Connect $y_1$ and $y_2$ to a new node $y_3$ and connect the reticulation leaf $x_m$ to $y_3$. Do this procedure for all pairs of edges and choose a pair such that the resulting network is consistent with maximum number of triplets in $\tau$. Triplet continue this procedure until all the reticulation nodes are added.
Step 7: For each $SN$-set, $S_i$, and the set $\tau_{S_i}$ of triplets we run the algorithm again.

Step 8: Replace each $SN$-set in the network of Step 6 with its related network constructed in Step 7 to obtain a network $N'$. Let $\tau' \in \tau$ be the set of the triplets which are not consistent with $N'$. For each pair of leaves $a$ and $b$ assume that $\tau'_{ab}$ is the set of triplets in $\tau'$ which are of the form $ab|c$. Consider the pair of leaves $i$ and $j$ such that $\tau'_{ij}$ has the maximum cardinality. Assume that $p_i$ and $p_j$ are the parents of $i$ and $j$, respectively.

Step 9: Create two new nodes in the middle of the edges $p_i i$ and $p_j j$ and connect them with a new edge. This new edge creates a reticulation node and all of the triplets in $\tau'_{ij}$ will be consistent with the new network. All consistent triplets with the new network are removed from $\tau'$ and this procedure will continue until $\tau'$ becomes empty.

Fig. 5 presents an example of the algorithm with all of its Steps.

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The (G, h) graph

Remove edges with weights 5 and 4. Continue the process on non SN-set {2, 3, 4, 5, 6}.

Updated graph on SN-sets. Updated triplets:

\{3, 4\} \{5, 6\}\{3, 4\}\{5, 6\}\{3, 4\}\{5, 6\}\{3, 4\}\{5, 6\}\{3, 4\}\{5, 6\}\{3, 4\}\{5, 6\}\{3, 4\}\{5, 6\}\{3, 4\}\{5, 6\}.

Remove first and second selected reticulations {5, 6} and {3, 4} to obtain a tree.

Add {5, 6} to the network.

Add {3, 4} to the network.

Replace SN-sets.

Fig. 5. Steps of our algorithm for input triplets: 2 3|1, 4 1|2, 5 2|1, 2 6|1, 3 4|1, 1 3|5, 1 3|6, 5 4|1, 4 6|1, 5 6|1, 3 4|2, 3 5|2, 2 6|3, 4 5|2, 2 4|6, 5 6|2, 3 4|5, 3 4|6, 5 6|3, 5 6|4.

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