Path lengths in tree-child time consistent hybridization networks

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Abstract. Hybridization networks are representations of evolutionary histories that allow for the inclusion of reticulate events like recombinations, hybridizations, or lateral gene transfers. The recent growth in the number of hybridization network reconstruction algorithms has led to an increasing interest in the definition of metrics for their comparison that can be used to assess the accuracy or robustness of these methods. In this paper we establish some basic results that make it possible the generalization to tree-child time consistent (TCTC) hybridization networks of some of the oldest known metrics for phylogenetic trees: those based on the comparison of the vectors of path lengths between leaves. More specifically, we associate to each hybridization network a suitably defined vector of 'splitted' path lengths between its leaves, and we prove that if two TCTC hybridization networks have the same such vectors, then they must be isomorphic. Thus, comparing these vectors by means of a metric for real-valued vectors defines a metric for TCTC hybridization networks. We also consider the case of fully resolved hybridization networks, where we prove that simpler, 'non-splitted' vectors can be used.

1 Introduction

An evolutionary history is usually modelled by means of a rooted phylogenetic tree, whose root represents a common ancestor of all species under study (or whatever other taxonomic units are considered: genes, proteins,...), the leaves, the extant species, and the internal nodes, the ancestral species. But phylogenetic trees can only cope with speciation events due to mutations, where each species other than the universal common ancestor has only one parent in the evolutionary history (its parent in the tree). It is clearly understood now that other speciation events, which cannot be properly represented by means of single arcs in a tree, play an important role in evolution [10]. These are reticulation events like genetic recombinations, hybridizations, or lateral gene transfers, where a species is the result of the interaction between two parent species. This has lead to the introduction of networks as models of phylogenetic histories that capture these reticulation events side by side with the classical mutations.

Contrary to what happens in the phylogenetic trees literature, where the basic concepts are well established, there is still some lack of consensus about terminology in the field of 'phylogenetic networks' [16]. Following [23], in this paper we use the term hybridization network to denote the most general model of reticulated evolutionary history:

a directed acyclic graph with only one root, which represents the last universal common ancestor and which we assume, thus, of out-degree greater than 1. In such a graph, nodes represent species (or any other taxonomy unit) and arcs represent direct descendance. A node with only one parent (a tree node) represents a species derived from its parent species through mutation, and a node with more than one parent (a hybrid node) represents a species derived from its parent species through some reticulation event.

The interest in representing phylogenetic histories by means of networks has lead to many hybridization network reconstruction methods [13, 14, 17–19, 21, 25, 28]. These reconstruction methods often search for hybridization networks satisfying some restriction, like for instance to have as few hybrid nodes as possible (in *perfect phylogenies*), or to have their reticulation cycles satisfying some structural restrictions (in galled trees and networks). Two popular and biologically meaningful such restrictions are the time consistency [1, 18], the possibility of assigning times to the nodes in such a way that tree children exist later than their parents and hybrid children coexist with their parents (and in particular, the parents of a hybrid species coexist in time), and the tree child condition [8,31], that imposes that every non-extant species has some descendant through mutation alone. The tree-child time consistent (TCTC) hybridization networks have been recently proposed as the class where meaningful phylogenetic networks should be searched [30]. Recent simulations (reported in [27]) have shown that over 64% of 4132 hybridization networks obtained using the coalescent model [15] under various population and sample sizes, sequence lengths, and recombination rates, were TCTC: the percentage of TCTC networks among the time consistent networks obtained in these simulations increases to 92.8%.

The increase in the number of available hybridization networks reconstruction algorithms has made it necessary the introduction of methods for the comparison of hybridization networks to be used in their assessment, for instance by comparing inferred networks with either simulated or true phylogenetic histories, and by evaluating the robustness of reconstruction algorithms when adding new species [18, 32]. This has lead recently to the definition of several metrics defined on different classes of hybridization networks [4–6,8,9,18,20]. All these metrics generalize in one way or another well-known metrics for phylogenetic trees.

Some of the most popular metrics for phylogenetic trees are based on the comparison of the vectors of path lengths between leaves [3,11,12,22,26,29]. Introduced in the early seventies, with different names depending on the author and the way these vectors are compared, they are globally known as nodal distances. Actually, these vectors of paths lengths only separate (in the sense that equal vectors means isomorphic trees), on the one hand, unrooted phylogenetic trees, and, on the other hand, fully resolved rooted phylogenetic trees, and therefore, as far as rooted phylogenetic trees goes, the distances defined through these vectors are only true metrics for fully resolved trees. These metrics were recently generalized to arbitrary rooted phylogenetic trees [7]. In this generalization, each path length between two leaves was replaced by the pair of distances from the leaves to their least common ancestor, and the vector of paths lengths between leaves was replaced by the splitted path lengths matrix obtained in this way. These matrices

separate arbitrary rooted phylogenetic trees, and therefore the *splitted nodal distances* defined through them are indeed metrics on the space of rooted phylogenetic trees.

In a recent paper [6] we have generalized these splitted nodal distances to TCTC hybridization networks with all their hybrid nodes of out-degree 1. The goal of this paper is to go one step beyond in two directions: to generalize to the TCTC hybridization networks setting both the classical nodal distances for fully resolved rooted phylogenetic trees and the new splitted nodal distances for rooted phylogenetic trees. Thus, on the one hand, we introduce a suitable generalization of the vectors of path lengths between leaves that separate fully resolved (where every non extant species has exactly two children, and every reticulation event involves exactly two parent species) TCTC hybridization networks. On the other hand, we show that if we split these new path lengths in a suitable way and we add a bit of extra information, the resulting vectors separate arbitrary TCTC hybridization networks. Then, the vectors obtained in both cases can be used to define metrics that generalize, respectively, the nodal distances for fully resolved rooted phylogenetic trees and the splitted nodal distances for rooted phylogenetic trees.

The key ingredient in the proofs of our main results is the use of sets of suitable reductions that applied to TCTC hybridization networks with n leaves and m internal nodes produce TCTC hybridization networks with either n-1 leaves or with n leaves and m-1 internal nodes (in the fully resolved case, the reductions we use are specifically tailored to make them remove always one leaf). Similar sets of reductions have already been introduced for TCTC hybridization networks with all their hybrid nodes of out-degree 1 [6] and for tree sibling (where every hybrid node has a tree sibling) time consistent hybridization networks with all their hybrid nodes of in-degree 2 and out-degree 1 [4], and they have been proved useful in those contexts not only to establish properties of the corresponding networks by algebraic induction, but also to generate in a recursive way all networks of the type under consideration. We hope that the reductions introduced in this paper will find similar applications elsewhere.

2 Preliminaries

2.1 Notations on DAGs

Let N = (V, E) denote in this subsection a directed acyclic (non-empty, finite) graph; a DAG, for short. A node $v \in V$ is a *child* of $u \in V$ if $(u, v) \in E$; we also say in this case that u is a *parent* of v. All children of the same parent are said to be *sibling* of each other.

Given a node $v \in V$, its in-degree $\deg_{in}(v)$ and its out-degree $\deg_{out}(v)$ are, respectively, the number of its parents and the number of its children. The type of v is the ordered pair $(\deg_{in}(v), \deg_{out}(v))$. A node v is a root when $\deg_{in}(v) = 0$, a tree node when $\deg_{in}(v) \leq 1$, a hybrid node when $\deg_{in}(v) \geq 2$, a leaf when $\deg_{out}(v) = 0$, internal when $\deg_{out}(v) \geq 1$, and elementary when $\deg_{in}(v) \leq 1$ and $\deg_{out}(v) = 1$. A tree arc (respectively, a hybridization arc) is an arc with head a tree node (respectively, a hybrid node). A DAG N is rooted when it has only one root.

A path on N is a sequence of nodes (v_0, v_1, \ldots, v_k) such that $(v_{i-1}, v_i) \in E$ for all $i = 1, \ldots, k$. We call v_0 the origin of the path, v_1, \ldots, v_{k-1} its intermediate nodes, and v_k its end. The length of the path (v_0, v_1, \ldots, v_k) is k, and it is non-trivial if $k \ge 1$. The acyclicity of N means that it does not contain cycles: non-trivial paths from a node to itself.

We denote by $u \leadsto v$ any path with origin u and end v. Whenever there exists a path $u \leadsto v$, we shall say that v is a descendant of u and also that u is an ancestor of v. When the path $u \leadsto v$ is non-trivial, we say that v is a proper descendant of u and that u is an proper ancestor of v. The distance from a node u to a descendant v is the length of a shortest path from u to v.

The height h(v) of a node v in a DAG N is the largest length of a path from v to a leaf. The absence of cycles implies that the nodes of a DAG can be stratified by means of their heights: the nodes of height 0 are the leaves, the nodes of height 1 are those nodes all whose children are leaves, the nodes of height 2 are those nodes all whose children are leaves and nodes of height 1, and so on. If a node has height m > 0, then all its children have height smaller than m, and at least one of them has height exactly m - 1.

A node v of N is a *strict descendant* of a node u if it is a descendant of it, and every path from a root of N to v contains the node u: in particular, we understand every node as a strict descendant of itself. When v is a strict descendant of u, we also say that u is a *strict ancestor* of v.

The following lemma will be used several times in this paper.

Lemma 1. Let u be a proper strict ancestor of a node v in a DAG N, and let w be an intermediate node in a path $u \rightsquigarrow v$. Then, u is also a strict ancestor of w.

Proof. Let $r \leadsto w$ be a path from a root of N to w, and concatenate to it the piece $w \leadsto v$ of the path $u \leadsto v$ under consideration. This yields a path $r \leadsto v$ that must contain u. Since u does not appear in the piece $w \leadsto v$, we conclude that it is contained in the path $r \leadsto w$. This proves that every path from a root of N to w contains the node w.

For every pair of nodes u, v of N:

- -CSA(u,v) is the set of all common ancestors of u and v that are strict ancestors of at least one of them;
- the least common semi-strict ancestor (LCSA) of u and v, in symbols [u, v], is the node in CSA(u, v) of minimum height.

The LCSA of two nodes u, v in a phylogenetic network is well defined and it is unique: it is actually the unique element of CSA(u, v) that is a descendant of all elements of this set [5]. The following result on LCSAs will be used often. It is the generalization to DAGs of Lemma 6 in [6], and we include its easy proof for the sake of completeness.

Lemma 2. Let N be a DAG and let u, v be a pair of nodes of N such that v is not a descendant of u. If u is a tree node with parent u', then [u, v] = [u', v].

Proof. We shall prove that CSA(u, v) = CSA(u', v).

Let $x \in CSA(u, v)$. Since u is not an ancestor of v, $x \neq u$ and hence any path $x \rightsquigarrow u$ is non-trivial. Then, since u' is the only parent of u, it appears in this path, and therefore x is also an ancestor of u'. This shows that x is a common ancestor of u' and v. Now, if x is a strict ancestor of v, we already conclude that $x \in CSA(u', v)$, while if x is a strict ancestor of u, it will be also a strict ancestor of u' by Lemma 1, and hence $x \in CSA(u', v)$, too. This proves that $CSA(u, v) \subseteq CSA(u', v)$

Conversely, let $x \in CSA(u',v)$. Since u' is the parent of u, it is clear that x is a common ancestor of u and v, too. If x is a strict ancestor of v, this implies that $x \in CSA(u,v)$. If x is a strict ancestor of u', then it is also a strict ancestor of u (every path $r \leadsto u$ must contain the only parent u' of u, and then x will belong to the piece $r \leadsto u'$ of the path $r \leadsto u$), and therefore $x \in CSA(u,v)$, too. This finishes the proof of the equality.

Let S be any non-empty finite set of *labels*. We say that the DAG N is *labeled in* S, or that it is an S-DAG, for short, when its leaves are bijectively labeled by elements of S. Although in real applications the set S would correspond to a given set of extant taxa, for the sake of simplicity we shall assume henceforth that $S = \{1, \ldots, n\}$, with n = |S|. We shall always identify, usually without any further notice, each leaf of an S-DAG with its label in S.

Two S-DAGs N, N' are *isomorphic*, in symbols $N \cong N'$, when they are isomorphic as directed graphs and the isomorphism maps each leaf in N to the leaf with the same label in N'.

2.2 Path lengths in phylogenetic trees

A phylogenetic tree on a set S of taxa is a rooted S-DAG without hybrid nodes and such that its root is non-elementary. A phylogenetic tree is fully resolved, or binary, when every internal node has out-degree 2. Since all ancestors of a node in a phylogenetic tree are strict, the LCSA [u, v] of two nodes u, v in a phylogenetic tree is simply their least common ancestor: the unique common ancestor of them that is a descendant of every other common ancestor of them.

Let T be a phylogenetic tree on the set $S = \{1, \ldots, n\}$. For every $i, j \in S$, we shall denote by $\ell_T(i, j)$ and $\ell_T(j, i)$ the lengths of the paths $[i, j] \leadsto i$ and $[i, j] \leadsto j$, respectively. In particular, $\ell_T(i, i) = 0$ for every $i = 1, \ldots, n$.

Definition 1. Let T be a phylogenetic tree on the set $S = \{1, ..., n\}$. The path length between two leaves i and j is

$$L_T(i,j) = \ell_T(i,j) + \ell_T(j,i).$$

The path lengths vector of T is the vector

$$L(T) = (L_T(i,j))_{1 \le i < j \le n} \in \mathbb{N}^{n(n-1)/2}$$

with its entries ordered lexicographically in (i, j).

The following result is a special case of Prop. 2 in [7].

Proposition 1. Two fully resolved phylogenetic trees on the same set S of taxa are isomorphic if, and only if, they have the same path lengths vectors.

The thesis in the last result is false for arbitrary phylogenetic trees. Consider for instance the phylogenetic trees with Newick strings (1,2,(3,4)); and ((1,2),3,4); depicted¹ in Fig. 1. It is straightforward to check that they have the same path lengths vectors, but they are not isomorphic.

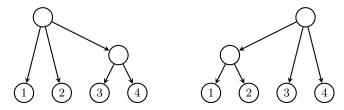


Fig. 1. Two non-isomorphic phylogenetic trees with the same path lengths vectors.

This problem was overcome in [7] by replacing the path lengths vectors by the following matrices of distances.

Definition 2. The splitted path lengths matrix of T is the $n \times n$ square matrix

$$\ell(T) = \left(\ell_T(i,j)\right)_{\substack{i=1,\dots,n\\j=1,\dots,n}} \in \mathcal{M}_n(\mathbb{N}).$$

Now, the following result is (again, a special case of) Theorem 11 in [7].

Proposition 2. Two phylogenetic trees on the same set S of taxa are isomorphic if, and only if, they have the same splitted path lengths matrices.

3 TCTC networks

While the basic notion of phylogenetic tree is well established, the notion of phylogenetic network is much less well defined [16]. The networks we consider in this paper are the (almost) most general possible ones: rooted S-DAGs with non-elementary root. Following [23], we shall call them *hybridization networks*. In these hybridization networks, every node represents a different species, and the arcs represent direct descendance, be it through mutation (tree arcs) or through some reticulation event (hybridization arcs).

It is usual to forbid elementary nodes in hybridization networks [23], mainly because they cannot be reconstructed. We allow them here for two reasons. On the one hand,

¹ Henceforth, in graphical representations of DAGs, hybrid nodes are represented by squares, tree nodes by circles, and indeterminate nodes, that is, nodes that can be of tree or hybrid type, by squares with rounded corners.

because allowing them simplifies considerably some proofs, as it will be hopefully clear in Section 5. On the other hand, because, as Moret et~al point out [18, §4.3], they can be useful both from the biological point of view, to include auto-polyploidy in the model, as well as from the formal point of view, to make a phylogeny satisfy other constraints, like for instance time consistency (see below) or the impossibility of successive hybridizations. Of course, our main results apply without any modification to hybridization networks without elementary nodes as well.

Following [5], by a *phylogenetic network* on a set S of taxa we understand a rooted S-DAG N with non-elementary root where every hybrid node has exactly one child, and it is a tree node. Although, from the mathematical point of view, phylogenetic networks are a special case of hybridization networks, from the point of view of modelling they represent in a different way evolutive histories with reticulation events: in a phylogenetic network, every tree node represents a different species and every hybrid node, a reticulation event that gives rise to the species represented by its only child.

A hybridization network N = (V, E) is time consistent when it allows a temporal representation [1]: a mapping

$$\tau: V \to \mathbb{N}$$

such that $\tau(u) < \tau(v)$ for every tree arc (u, v) and $\tau(u) = \tau(v)$ for every hybridization arc (u, v). Such a temporal representation can be understood as an assignment of times to nodes that strictly increases from parents to tree children and so that the parents of each hybrid node coexist in time.

Remark 1. Let N=(V,E) be a time consistent hybridization network, and let $N_1=(V_1,E_1)$ be a hybridization network obtained by removing from N some nodes and all their descendants (as well as all arcs pointing to any removed node). Then N_1 is still time consistent, because the restriction of any temporal representation $\tau:V\to\mathbb{N}$ of N to V_1 yields a temporal representation of N_1 .

A hybridization network satisfies the *tree-child condition*, or it is *tree-child*, when every internal node has at least one child that is a tree node (a *tree child*). So, tree-child hybridization networks can be understood as general models of reticulate evolution where every species other that the extant ones, represented by the leaves, has some descendant through mutation. Tree-child hybridization networks include galled trees [13, 14] as a particular case [8].

A tree path in a tree-child hybridization network is a non-trivial path such that its end and all its intermediate nodes are tree nodes. A node v is a tree descendant of a node u when there exists a tree path from u to v. By [9, Lem. 2], every internal node u of a tree-child hybridization network has some tree descendant leaf, and by [9, Cor. 4] every tree descendant v of u is a strict descendant of u and the path $u \leadsto v$ is unique.

To simplify the notations, we shall call TCTC-networks the tree-child time consistent hybridization networks: these include the tree-child time consistent phylogenetic networks, which were the objects dubbed TCTC-networks in [5,6]. Every phylogenetic tree is also a TCTC-network. Let $TCTC_n$ denote the class of all TCTC-networks on $S = \{1, \ldots, n\}$.

We prove now some basic properties of TCTC-networks that will be used later.

Lemma 3. Let u be a node of a TCTC-network N, and let v be a child of u. The node v is a tree node if, and only if, it is a strict descendant of u.

Proof. Assume first that v is a tree child of u. Since u is the only parent of v, every non-trivial path ending in v must contain u. This shows that u is a strict ancestor of v.

Assume now that v is a hybrid child of u that is also a strict descendant of it, and let us see that this leads to a contradiction. Indeed, in this case the set H(u) of hybrid children of u that are strict descendants of it is non-empty, and we can choose a node v_0 in it of largest height. Let v_1 be any parent of v_0 other than u. Since u is a strict ancestor of v_0 , it must be an ancestor of v_1 , and since u and v_1 have the hybrid child v_0 is common, they must have the same temporal representation, and therefore v_1 as well as all intermediate nodes in any path $u \leadsto v_1$ must be hybrid. Moreover, since u is a strict ancestor of v_0 , it is also a strict ancestor of v_1 as well as of any intermediate node in any path $u \leadsto v_1$ (by Lemma 1). In particular, the child of u in a path $u \leadsto v_1$ will belong to H(u) and its height will be larger than the height of v_0 , which is impossible.

Corollary 1. All children of the root of a TCTC-network are tree nodes.

Proof. Every node in a hybridization network is a strict descendant of the root. Then, Lemma 3 applies.

The following result is the key ingredient in the proofs of our main results; it generalizes to hybridization networks Lemma 3 in [6], which referred to phylogenetic networks. A similar result was proved in [4] for *tree-sibling* (that is, where every hybrid node has a sibling that is a tree node) time consistent phylogenetic networks with all its hybrid nodes of in-degree 2.

Lemma 4. Every TCTC-network with more than one leaf contains at least one node v satisfying one of the following properties:

- (a) v is an internal tree node and all its children are tree leaves.
- (b) v is a hybrid internal node, all its children are tree leaves, and all its siblings are leaves or hybrid nodes.
- (c) v is a hybrid leaf, and all its siblings are leaves or hybrid nodes.

Proof. Let N be a TCTC-network and τ a temporal representation of it. Let v_0 be an internal node of highest τ -value and, among such nodes, of smallest height. The tree children of v_0 have strictly higher τ -value than v, and therefore they are leaves. And the hybrid children of v_0 have the same τ -value than v_0 but smaller height, and therefore they are also leaves.

Now:

- If v_0 is a tree node all whose children are tree nodes, taking $v = v_0$ we are in case (a).

- If v_0 is a hybrid node all whose children are tree nodes, then its parents have its same τ -value, which, we recall, is the highest one. This implies that their children (v_0 's siblings) cannot be internal tree nodes, and hence they are leaves or hybrid nodes. So, taking $v = v_0$, we are in case (b).
- If v_0 has some hybrid child, take as the node v in the statement this hybrid child: it is a leaf, and all its parents have the same τ -value as v_0 , which implies, arguing as in the previous case, that all siblings of v are leaves or hybrid nodes. Thus, v satisfies (c).

We introduce now some reductions for TCTC-networks. Each of these reductions applied to a TCTC-network with n leaves and m internal nodes produces a TCTC-network with either n-1 leaves and m internal nodes or with n leaves and m-1 internal nodes, and given any TCTC-network with more than two leaves, it will always be possible to apply to it some of these reductions. This lies at the basis of the proofs by algebraic induction of the main results in this paper.

Let N be a TCTC-network with $n \ge 3$ leaves.

(U) Let i be one tree leaf of N and assume that its parent has only this child. The U(i) reduction of N is the network $N_{U(i)}$ obtained by removing the leaf i, together with its incoming arc, and labeling with i its former parent; cf. Fig. 2. This reduction removes the only child of a node, and thus it is clear that $N_{U(i)}$ is still a TCTC-network, with the same number of leaves but one internal node less than N.



Fig. 2. The U(i)-reduction.

- (T) Let i, j be two sibling tree leaves of N (that may, or may not, have other siblings). The T(i;j) reduction of N is the network $N_{T(i;j)}$ obtained by removing the leaf i, together with its incoming arc; cf. Fig. 3. This reduction procedure removes one tree leaf, but its parent u keeps at least another tree child, and if u was the root of N then it would not become elementary after the reduction, because $n \ge 3$ and therefore, since j is a leaf, u should have at least another child. Therefore, $N_{T(i;j)}$ is a TCTC-network with the same number of internal nodes as N and n-1 leaves.
- (H) Let i be a hybrid leaf of N, let v_1, \ldots, v_k , with $k \geq 2$, be its parents, and assume that each one of these parents has (at least) one tree leaf child: for every $l = 1, \ldots, k$, let j_l be a tree leaf child of v_l . The $H(i; j_1, \ldots, j_k)$ reduction of N is the network $N_{H(i;j_1,\ldots,j_k)}$ obtained by removing the hybrid leaf i and its incoming arcs; cf. Fig. 4. This reduction procedure preserves the time consistency and the tree-child condition (it removes a hybrid leaf), and the root does not become elementary: indeed, the



Fig. 3. The T(i; j)-reduction.

only possibility for the root to become elementary is to be one of the parents of i, which is impossible by Corollary 1. Therefore, $N_{H(i;j_1,...,j_k)}$ is a TCTC-network with the same number of internal nodes as N and n-1 leaves.



Fig. 4. The $H(i; j_1, \ldots, j_k)$ -reduction.

We shall call the inverses of the U, T, and H reduction procedures, respectively, the U⁻¹, T⁻¹, and H⁻¹ expansions, and we shall denote them by $U^{-1}(i)$, $R^{-1}(i;j)$, and $H^{-1}(i;j_1,\ldots,j_k)$. More specifically, for every TCTC-network N:

- If N has some leaf labeled i, the expansion $U^{-1}(i)$ can be applied to N and the resulting network $N_{U^{-1}(i)}$ is obtained by unlabeling the leaf i and adding to it a tree leaf child labeled with i. $N_{U^{-1}(i)}$ is always a TCTC-network.
- If N has no leaf labeled with i and some tree leaf labeled with j, the expansion $T^{-1}(i;j)$ can be applied to N, and the resulting network $N_{T^{-1}(i;j)}$ is obtained by adding to the parent of the leaf j an new tree leaf child labeled with i. $N_{T^{-1}(i;j)}$ is always a TCTC-network.
- If N has no leaf labeled with i and some tree leaves labeled with $j_1, \ldots, j_k, k \geq 2$, that are not sibling of each other, the expansion $H^{-1}(i; j_1, \ldots, j_k)$ can be applied to N and the resulting network $N_{H^{-1}(i;j_1,\ldots,j_k)}$ is obtained by adding a new hybrid node labeled with i and arcs from the parents of j_1,\ldots,j_k to i. $N_{H^{-1}(i;j_1,\ldots,j_k)}$ is always a tree child hybridization network, but it need not be time consistent, as the parents of j_1,\ldots,j_k may have different temporal representations in N (for instance, one of them could be a tree descendant of another one).

The following result is easily deduced from the explicit descriptions of the reduction and expansion procedures, and the fact that isomorphisms preserve labels and parents.

Lemma 5. Let N and N' be two TCTC-networks. If $N \cong N'$, then the result of applying to both N and N' the same U reduction (respectively, T reduction, H reduction, U^{-1}

expansion, T^{-1} expansion, or H^{-1} expansion) are again two isomorphic hybridization networks.

Moreover, if we apply an U reduction (respectively, T reduction, or H reduction) to a TCTC-network N, and then we apply to the resulting TCTC-network the inverse U^{-1} expansion (respectively, T^{-1} expansion, or H^{-1} expansion), we obtain a TCTC-network isomorphic to N.

As we said above, every TCTC-network with at least 3 leaves allows the application of some reduction.

Proposition 3. Let N be a TCTC-network with more than two leaves. Then, at least one U, R, or H reduction can be applied to N.

Proof. By Lemma 4, N contains either an internal (tree or hybrid) node v all whose children are tree leaves, or a hybrid leaf i all whose siblings are leaves or hybrid nodes. In the first case, we can apply to N either the reduction U(i) (if v has only one child, and it is the tree leaf i) or T(i;j) (if v has at least two tree leaf children, i and j). In the second case, let v_1, \ldots, v_k , with $k \ge 2$, be the parents of i. By the tree child condition, each v_l , with $l = 1, \ldots, k$, has some tree child, and by the assumption on i, it will be a leaf, say j_l . Then, we can apply to N the reduction $H(i; j_1, \ldots, j_k)$.

Therefore, every TCTC-network with $n \ge 3$ leaves and m internal nodes is obtained by the application of an U^{-1} , T^{-1} , or H^{-1} expansion to a TCTC-network with either n-1 leaves or n leaves and m-1 internal nodes. This allows the recursive construction of all TCTC-networks from TCTC-networks (actually, phylogenetic trees) with 2 leaves and 1 internal node.

Example 1. Fig. 5 shows how a sequence of reductions transforms a certain TCTC-network N with 4 leaves into a phylogenetic tree with 2 leaves. The sequence of inverse expansions would then generate N from this phylogenetic tree. This sequence of expansions generating N is, of course, not unique.

4 Path lengths vectors for fully resolved networks

Let N be a hybridization network on $S = \{1, ..., n\}$. For every pair of leaves i, j of N, let $\ell_N(i, j)$ and $\ell_N(j, i)$ be the distance from [i, j] to i and to j, respectively.

Definition 3. The LCSA-path length between two leaves i and j in N is

$$L_N(i, j) = \ell_N(i, j) + \ell_N(j, i).$$

The LCSA-path lengths vector of N is

$$L(N) = (L_N(i,j))_{1 \le i < j \le n} \in \mathbb{N}^{n(n-1)/2},$$

with its entries ordered lexicographically in (i, j).

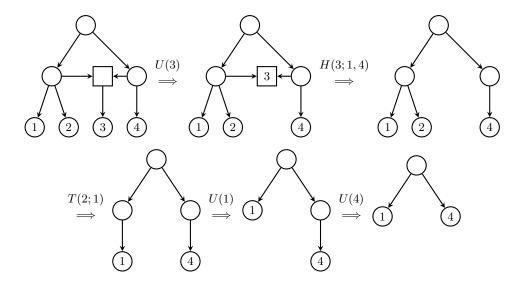


Fig. 5. A sequence of reductions.

Notice that $L_N(i,j) = L_N(j,i)$, for every pair of leaves $i, j \in S$.

If N is a phylogenetic tree, the LCSA-path length between two leaves is the path length between them as defined in $\S 2.2$, and therefore the vectors L(N) defined therein and here are the same. But, contrary to what happens in phylogenetic trees, the LCSA-path length between two leaves i and j in a hybridization network need not be the smallest sum of the distances from a common ancestor of i and j to these leaves (that is, the distance between these leaves in the undirected graph associated to the network).

Example 2. Consider the TCTC-network N depicted in Fig. 6. Table 4 gives, in its upper triangle, the LCSA of every pair of different leaves, and in its lower triangle, the LCSA-path length between every pair of different leaves.

Notice that, in this network, [3,5] = r, because the root is the only common ancestor of 3 and 5 that is strict ancestor of some of them, and hence $L_N(3,5) = 8$, but e is a common ancestor of both leaves and the length of both paths $e \rightsquigarrow 3$ and $e \rightsquigarrow 5$ is 3. Similarly, f is also a common ancestor of both leaves and the length of both paths $f \rightsquigarrow 3$ and $f \rightsquigarrow 5$ is 3. This is an example of LCSA-path length between two leaves that is largest than the smallest sum of the distances from a common ancestor of these leaves to each one of them.

In a fully resolved phylogeny with reticulation events, every non extant species should have two direct descendants, and every reticulation event should involve two parent species, as such an event corresponds always to the exchange of genetic information between two parents: as Semple points out [23], hybrid nodes with in-degree greater than 2 actually represent "an uncertainty of the exact order of 'hybridization'." Depending on whether we use hybridization or phylogenetic networks to model phylogenies, we distinguish between:

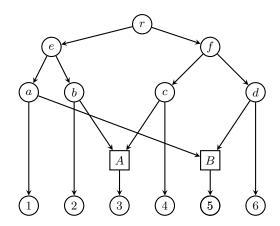


Fig. 6. The network N in Example 2.

Table 1. For every $1 \le i < j \le 6$, the entry (i, j) of this table is [i, j], and the entry (j, i) is $L_N(i, j)$, with N the network in Fig. 6.

	1	2	3	4	5	6
1		e	e	r	a	r
2	4		b	r	e	r
3	5	3		c	r	f
4	6	6	3		f	f
5	3	5	8	5		d
6	6	6	5	4	3	

- Fully resolved hybridization networks: hybridization networks with all their nodes of types (0,2), (1,0), (1,2), (2,0), or (2,2).
- Fully resolved phylogenetic networks: phylogenetic networks with all their nodes of types (0,2), (1,0), (1,2), or (2,1).

To simplify the language, we shall say that a hybridization network is *quasi-binary* when all its nodes are of types (0,2), (1,0), (1,2), (2,0), (2,1), or (2,2). These quasi-binary networks include as special cases the fully resolved hybridization and phylogenetic networks.

Our main result in this section establishes that the LCSA-path lengths vectors separate fully resolved (hybridization or phylogenetic) TCTC-networks, thus generalizing Proposition 1 from trees to networks. To prove this result, we shall use the same strategy as the one developed in [4] or [6] to prove that the metrics introduced therein were indeed metrics: algebraic induction based on reductions. Now, we cannot use the reductions defined in the last section as they stand, because they may generate elementary nodes that are forbidden in fully resolved networks. Instead, we shall use certain suitable combinations of them that always reduce in one the number of leaves.

So, consider the following reduction procedures for quasi-binary TCTC networks N with n leaves:

(R) Let i, j be two sibling tree leaves of N. The R(i; j) reduction of N is the quasi-binary TCTC-network $N_{R(i;j)}$ obtained by applying first the T(i; j) reduction to N and then the U(j) reduction to the resulting network. The final result is that the leaves i and j are removed, together with their incoming arcs, and then their former common parent, which now has become a leaf, is labeled with j; cf. Fig. 7.

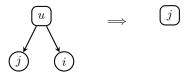


Fig. 7. The R(i; j)-reduction.

(**H**₀) Let i be a hybrid leaf, let v_1 and v_2 be its parents and assume that the other children of these parents are tree leaves j_1 and j_2 , respectively. The $H_0(i;j_1,j_2)$ reduction of N is the quasi-binary TCTC-network $N_{H_0(i;j_1,j_2)}$ obtained by applying first the reduction $H(i;j_1,j_2)$ to N and then the reductions $U(j_1)$ and $U(j_2)$ to the resulting network. The overall effect is that the hybrid leaf i and the tree leaves j_1,j_2 are removed, together with their incoming arcs, and then the former parents v_1,v_2 of j_1 and j_2 are labeled with j_1 and j_2 , respectively; cf. Fig. 8.

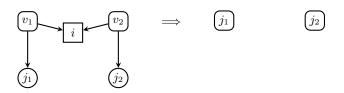


Fig. 8. The $H_0(i; j_1, j_2)$ -reduction.

(**H**₁) Let A be a hybrid node with only one child i, that is a tree node. Let v_1 and v_2 be the parents of A and assume that the other children of these parents are tree leaves j_1 and j_2 , respectively. The $H_1(i;j_1,j_2)$ reduction of N is the TCTC-network $N_{H_1(i;j_1,j_2)}$ obtained by applying first the reduction U(i) to N, followed by the reduction $H_0(i;j_1,j_2)$ to the resulting network. The overall effect is that the leaf i, its parent A and the leaves j_1,j_2 are removed, together with their incoming arcs, and then the former parents v_1,v_2 of j_1 and j_2 are labeled with j_1 and j_2 , respectively; cf. Fig. 9.

We use H₀ and H₁ instead of H and U because, for our purposes in this section, it has to be possible to decide whether or not we can apply a given reduction to a given fully

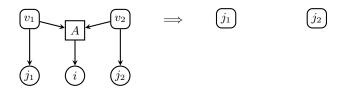


Fig. 9. The $H_1(i; j_1, j_2)$ -reduction.

resolved network N from the knowledge of L(N), and this cannot be done for the U reduction, while, as we shall see below, it is possible for H_0 and H_1 .

 H_0 reductions cannot be applied to fully resolved phylogenetic networks (they don't have hybrid leaves) and H_1 reductions cannot be applied to fully resolved hybridization networks (they don't have out-degree 1 hybrid nodes). The application of an R or an H_0 reduction to a fully resolved TCTC hybridization network is again a fully resolved TCTC hybridization network, and the application of an R or an H_1 reduction to a fully resolved TCTC phylogenetic network.

We shall call the inverses of the R, H_0 and H_1 reduction procedures, respectively, the R^{-1} , H_0^{-1} and H_1^{-1} expansions, and we shall denote them by $R^{-1}(i;j)$, $H_1^{-1}(i;j_1,j_2)$ and $H_0^{-1}(i;j_1,j_2)$. More specifically, for every quasi-binary TCTC-network N with no leaf labeled i:

- the expansion $R^{-1}(i;j)$ can be applied to N if it has a leaf labeled j, and the resulting network $N_{R^{-1}(i;j)}$ is obtained by unlabeling the leaf j and adding to it two leaf tree children labeled with i and j;
- the expansion $H_0^{-1}(i; j_1, j_2)$ can be applied to N if it has a pair of leaves labeled j_1, j_2 , and the resulting network $N_{H_0^{-1}(i; j_1, j_2)}$ is obtained by adding a new hybrid leaf labeled with i, and then, for each l = 1, 2, unlabeling the leaf j_l and adding to it a new tree leaf child labeled with j_l and an arc to i.
- the expansion $H_1^{-1}(i; j_1, j_2)$ can be applied to N if it has a pair of leaves labeled j_1, j_2 , and the resulting network $N_{H_1^{-1}(i; j_1, j_2)}$ is obtained by adding a new node A, a tree leaf child i to it, and then, for each l = 1, 2, unlabeling the leaf j_l and adding to it a new tree leaf child labeled with j_l and an arc to A.

A R⁻¹(i;j) expansion of a quasi-binary TCTC-network is always a quasi-binary TCTC-network, but an $H_0^{-1}(i;j_1,j_2)$ or an $H_1^{-1}(i;j_1,j_2)$ expansion of a quasi-binary TCTC-network, while still being always quasi-binary and tree child, needs not be time consistent: for instance, the leaves j_1 and j_2 could be a hybrid leaf and a tree sibling of it. Moreover, we have the following result, which is a direct consequence of Lemma 5 and we state it for further reference.

Lemma 6. Let N and N' be two quasi-binary TCTC-networks. If $N \cong N'$, then the result of applying to both N and N' the same R reduction (respectively, H_0 reduction, H_1 reduction, R^{-1} expansion, H_0^{-1} expansion, or H_1^{-1} expansion) is again two isomorphic networks.

Moreover, if we apply an R reduction (respectively, H_0 reduction or H_1 reduction) to a quasi-binary TCTC-network N, and then we apply to the resulting network the inverse R^{-1} expansion (respectively, H_0^{-1} expansion or H_1^{-1} expansion), we obtain a quasi-binary TCTC-network isomorphic to N.

We have moreover the following result.

Proposition 4. Let N be a quasi-binary TCTC-network with more than one leaf. Then, at least one R, H_0 , or H_1 reduction can be applied to N.

Proof. If N contains some internal node with two tree leaf children i and j, then the reduction R(i;j) can be applied. If N does not contain any node with two tree leaf children, then, by Lemma 4, it contains a hybrid node v that is either a leaf (say, labeled with i) or it has only one child, which is a tree leaf (say, labeled with i), and such that all siblings of v are leaves or hybrid nodes. Now, the quasi-binarity of N and the tree child condition entail that v has two parents, that each one of them has exactly one child other than v, and that this second child is a tree node. So, v has exactly two siblings, and they are tree leaves, say j_1 and j_2 . Then, the reduction $H_0(i; j_1, j_2)$ (if v is a leaf) or $H_1(i; j_1, j_2)$ (if v is not a leaf) can be applied.

Corollary 2. (a) If N is a fully resolved TCTC hybridization network with more than one leaf, then, at least one R or H_0 reduction can be applied to it.

(b) If N is a fully resolved TCTC phylogenetic network with more than one leaf, then, at least one R or H_1 reduction can be applied to it.

We shall prove now that the application conditions for the reductions introduced above can be read from the LCSA-path lengths vector of a fully resolved TCTC-network and that they modify in a specific way the LCSA-path lengths of the network which they are applied to. This will entail that if two fully resolved (hybridization or phylogenetic) TCTC-networks have the same LCSA-path lengths vectors, then the same reductions can be applied to both networks and the resulting fully resolved TCTC-networks still have the same LCSA-path lengths vectors. This will be the basis of the proof by induction on the number of leaves that two TCTC hybridization or phylogenetic networks with the same LCSA-path lengths vectors are always isomorphic.

Lemma 7. Let i, j be two leaves of a quasi-binary TCTC-network N. Then, i and j are siblings if, and only if, $L_N(i, j) = 2$.

Proof. If $L_N(i,j) = 2$, then the paths $[i,j] \rightsquigarrow i$ and $[i,j] \rightsquigarrow j$ have length 1, and therefore [i,j] is a parent of i and j. Conversely, if i and j are siblings and u is a parent in common of them, then, by the quasi-binarity of N, they are the only children of u, and by the tree-child condition, one of them, say i, is a tree node. But then, u is a strict ancestor of i, an ancestor of j, and no proper descendant of u is an ancestor of both i and j. This implies that u = [i, j] and hence that $L_N(i, j) = 2$.

Lemma 8. Let N be a quasi-binary TCTC-network on a set S of taxa.

- (1) The reduction R(i;j) can be applied to N if, and only if, $L_N(i,j) = 2$ and, for every $k \in S \setminus \{i,j\}$, $L_N(i,k) = L_N(j,k)$.
- (2) If the reduction R(i;j) can be applied to N, then

$$L_{N_{R(i;j)}}(j,k) = L_N(j,k) - 1 \quad \text{for every } k \in S \setminus \{i,j\}$$

$$L_{N_{R(i;j)}}(k,l) = L_N(k,l) \quad \text{for every } k,l \in S \setminus \{i,j\}$$

Proof. As far as (1) goes, R(i;j) can be applied to N if, and only if, the leaves i and j are siblings and of tree type. Now, if i and j are two tree sibling leaves and u is their parent, then on the one hand, $L_N(i,j) = 2$ by Lemma 7, and on the other hand, since, by Lemma 2, [i,k] = [u,k] = [j,k] for every leaf $k \neq i,j$, we have that

$$\ell_N(i,k) = \ell_N(j,k) = 1 + \text{distance from } [u,k] \text{ to } u$$

 $\ell_N(k,i) = \ell_N(k,j) = \text{distance from } [u,k] \text{ to } k$

and therefore $L_N(i,k) = L_N(j,k)$ for every $k \in S \setminus \{i,j\}$.

Conversely, assume that $L_N(i,j)=2$ and that $L_N(i,k)=L_N(j,k)$ for every $k \in S \setminus \{i,j\}$. The fact that $L_N(i,j)=2$ implies that i and j share a parent u. If one of these leaves, say i, is hybrid, then the tree child condition implies that the other, j, is of tree type. Let now v be the other parent of i and k a tree descendant leaf of v, and let k be the length of the unique path $v \leadsto k$. Then k is a strict ancestor of k and an ancestor of k, and no proper tree descendant of k can possibly be an ancestor of k: otherwise, there would exist a path from a proper tree descendant of k to k, and then the time consistency property would forbid k and k to have a hybrid child in common. Therefore k is an k-and k-and

As far as (2) goes, in $N_{R(i;j)}$ we remove the leaf i and we replace the leaf j by its parent. By Lemma 2, this does not modify the LCSA [j,k] of j and any other remaining leaf k, and since we have shortened in 1 any path ending in j, we deduce that $L_{N_{R(i;j)}}(j,k) = L_N(j,k) - 1$ for every $k \in S \setminus \{i,j\}$. On the other hand, for every $k,l \in S \setminus \{i,j\}$, the reduction R(i;j) has affected neither the LCSA [k,l] of k and l, nor the paths $[k,l] \leadsto k$ or $[k,l] \leadsto l$, which implies that $L_{N_{R(i;j)}}(k,l) = L_N(k,l)$

Lemma 9. Let N be a fully resolved TCTC hybridization network on a set S of taxa.

- (1) The reduction $H_0(i; j_1, j_2)$ can be applied to N if, and only if, $L_N(i, j_1) = L_N(i, j_2) = 2$.
- (2) If the reduction $H_0(i; j_1, j_2)$ can be applied to N, then

$$\begin{split} &L_{N_{H_0(i;j_1,j_2)}}(j_1,j_2) = L_N(j_1,j_2) - 2 \\ &L_{N_{H_0(i;j_1,j_2)}}(j_1,k) = L_N(j_1,k) - 1 \quad \text{for every } k \in S \setminus \{i,j_1,j_2\} \\ &L_{N_{H_0(i;j_1,j_2)}}(j_2,k) = L_N(j_2,k) - 1 \quad \text{for every } k \in S \setminus \{i,j_1,j_2\} \\ &L_{N_{H_0(i;j_1,j_2)}}(k,l) = L_N(k,l) \quad \text{for every } k,l \in S \setminus \{i,j_1,j_2\} \end{split}$$

Proof. As far as (1) goes, the reduction $H_0(i; j_1, j_2)$ can be applied to N if, and only if, i is a hybrid sibling of the tree leaves j_1 and j_2 . If this last condition happens, then $L_N(i, j_1) = 2$ and $L_N(i, j_2) = 2$ by Lemma 7. Conversely, $L_N(i, j_1) = L_N(i, j_2) = 2$ implies that i, j_1 and i, j_2 are pairs of sibling leaves. Since no node of N can have more than 2 children, and at least one of its children must be of tree type, this implies that i is a hybrid node (with two different parents), and j_1 and j_2 are tree nodes.

As far as (2) goes, the tree leaves j_1 and j_2 are replaced by their parents. By Lemma 7, this does not affect any LCSA and it only shortens in 1 the paths ending in j_1 or j_2 . Thus, the $H_0(i; j_1, j_2)$ reduction does not affect the LCSA-path length between any pair of remaining leaves other than j_1 and j_2 , it shortens in 1 the LCSA-path length between j_1 or j_2 and any remaining leaf other than j_1 or j_2 , and it shortens in 2 the LCSA-path length between j_1 and j_2 .

Lemma 10. Let N be a fully resolved TCTC phylogenetic network on a set S of taxa.

```
(1) The reduction H<sub>1</sub>(i; j<sub>1</sub>, j<sub>2</sub>) can be applied to N if, and only if,

- L<sub>N</sub>(i, j<sub>1</sub>) = L<sub>N</sub>(i, j<sub>2</sub>) = 3,

- L<sub>N</sub>(j<sub>1</sub>, j<sub>2</sub>) ≥ 4,

- if L<sub>N</sub>(j<sub>1</sub>, j<sub>2</sub>) = 4, then L<sub>N</sub>(j<sub>1</sub>, k) = L<sub>N</sub>(j<sub>2</sub>, k) for every k ∈ S \ {j<sub>1</sub>, j<sub>2</sub>, i}.
(2) If the reduction H<sub>1</sub>(i; j<sub>1</sub>, j<sub>2</sub>) can be applied to N, then
L<sub>NH<sub>1</sub>(i;j<sub>1</sub>,j<sub>2</sub>)</sub>(j<sub>1</sub>, j<sub>2</sub>) = L<sub>N</sub>(j<sub>1</sub>, j<sub>2</sub>) - 2

L<sub>NH<sub>1</sub>(i;j<sub>1</sub>,j<sub>2</sub>)</sub>(j<sub>1</sub>, k) = L<sub>N</sub>(j<sub>1</sub>, k) - 1 for every k ∈ S \ {i, j<sub>1</sub>, j<sub>2</sub>}

L<sub>NH<sub>1</sub>(i;j<sub>1</sub>,j<sub>2</sub>)</sub>(j<sub>2</sub>, k) = L<sub>N</sub>(j<sub>2</sub>, k) - 1 for every k ∈ S \ {i, j<sub>1</sub>, j<sub>2</sub>}

L<sub>NH<sub>1</sub>(i;j<sub>1</sub>,j<sub>2</sub>)</sub>(k, l) = L<sub>N</sub>(k, l) for every k ∈ S \ {i, j<sub>1</sub>, j<sub>2</sub>}
```

Proof. As far as (1) goes, the reduction $H_1(i; j_1, j_2)$ can be applied to N if, and only if, j_1 and j_2 are tree leaves that are not siblings and they share a sibling hybrid node that has the tree leaf i as its only child. Now, if this application condition for $H_1(i; j_1, j_2)$ is satisfied, then $L_N(i, j_1) = 3$, because the parent of j_1 is an ancestor of i, a strict ancestor of j_1 , and clearly no proper descendant of it is an ancestor of i and j_1 ; by a similar reason, $L_N(i, j_2) = 3$. Moreover, since j_1 and j_2 are not sibling, $L_N(j_1, j_2) \ge 3$. But if $L_N(j_1, j_2) = 3$, then there would exist an arc from the parent of j_1 to the parent of j_2 , or vice versa, which would entail a node of out-degree 3 that cannot exist in the fully resolved network N. Therefore, $L_N(j_1, j_2) \ge 4$. Finally, if $L_N(j_1, j_2) = 4$, this means that the parents x and y of j_1 and j_2 (that are tree nodes, because they have out-degree 2 and N is a phylogenetic network) are sibling: let u be their parent in common. In this case, no leaf other than j_1, j_2, i is a descendant of u, and therefore, for every $k \in S \setminus \{j_1, j_2, i\}$,

$$[j_1, k] = [x, k] = [u, k] = [y, k] = [j_2, k]$$

by Lemma 4, and thus

$$\ell_N(j_1, k) = \ell_N(j_2, k) = 2 + \text{distance from } [u, k] \text{ to } u$$

 $\ell_N(k, j_1) = \ell_N(k, j_2) = \text{distance from } [u, k] \text{ to } k,$

which implies that $L_N(j_1, k) = L_N(j_2, k)$.

Conversely, assume that $L_N(i, j_1) = L_N(i, j_2) = 3$, that $L_N(j_1, j_2) \ge 4$, and that if $L_N(j_1, j_2) = 4$, then $L_N(j_1, k) = L_N(j_2, k)$ for every $k \in S \setminus \{j_1, j_2, i\}$. Let x, y and z be the parents of j_1 , j_2 and i, respectively. Notice that these parents are pairwise different (otherwise, the LCSA-path length between a pair among j_1, j_2, i would be 2). Moreover, since N is a phylogenetic network, j_1, j_2 and i are tree nodes. Then, $L_N(i, j_1) = L_N(i, j_2) = 3$ implies that there must exist an arc between the nodes x and z and an arc between the nodes y and z.

Now, if these arcs are (z, x) and (z, y), the node z would have out-degree 3, which is impossible. Assume now that (x, z) and (z, y) are arcs of N. In this case, both z and x have out-degree 2, which implies (recall that N is a phylogenetic network) that they are tree nodes. Then, $x = [j_1, j_2]$ (it is an ancestor of j_2 , a strict ancestor of j_1 , and no proper descendant of it is an ancestor of j_1 and j_2) and therefore $L_N(j_1, j_2) = 4$. In this case, we assume that $L_N(j_1, k) = L_N(j_2, k)$ for every $k \in S \setminus \{j_1, j_2, i\}$. Now we must distinguish two cases, depending on the type of node y:

- If y is a tree node, let p be its child other than j_2 , and let k be a tree descendant leaf of p. In this case, $[j_1, k] = x$ and $[j_2, k] = y$ (by the same reason why x is $[j_1, j_2]$), and hence $L_N(j_1, k) = L_N(j_2, k) + 2$, against the assumption $L_N(j_1, k) = L_N(j_2, k)$.
- If y is a hybrid node, let p be its parent other than z, and let k be a tree descendant leaf of p ($k \neq j_2$, because j_2 is not a tree descendant of p). In this case, $[j_2, k] = p$ (because p is an ancestor of j_2 and a strict ancestor of k, and the time consistency property implies that no intermediate node in the path $p \rightsquigarrow k$ can be an ancestor of y). Now, if the length of the (only) path $p \rightsquigarrow k$ is h, then $L_N(j_2, k) = h + 2$, and for the equality $L_N(j_1, k) = h + 2$ to hold, either the arc (x, p) belongs to N, which is impossible because x would have out-degree 3, or a node in the path $p \rightsquigarrow k$ is an ancestor of x, which is impossible because of the time consistency property.

In both cases we reach a contradiction that implies that the arcs (x, z), (z, y) do not exist in N. By symmetry, the arcs (y, z), (z, x) do not exist in N, either. Therefore, the only possibility is that N contains the arcs (x, z), (y, z), that is, that z is hybrid child of the nodes x and y. This finishes the proof of (1).

As far as (2) goes, it is proved as in Lemma 9.

Now we can prove the main results in this section.

Proposition 5. Let N and N' be two fully resolved TCTC hybridization networks on the same set S of taxa. Then, L(N) = L(N') if, and only if, $N \cong N'$.

Proof. The 'if' implication is obvious. We prove the 'only if' implication by induction on the number n of elements of S.

The cases n = 1 and n = 2 are straightforward, because there exist only one TCTC-network on $S = \{1\}$ and one TCTC-network on $S = \{1, 2\}$: the one-node graph and the phylogenetic tree with leaves 1,2, respectively.

Assume now that the thesis is true for fully resolved TCTC hybridization networks with n leaves, and let N and N' be two fully resolved TCTC hybridization networks on the same set S of n+1 labels such that L(N)=L(N'). By Corollary 2.(a), an R(i;j) or a $H_0(i;j_1,j_2)$ can be applied to N. Moreover, since the possibility of applying one such reduction depends on the LCSA-path lengths vector by Lemmas 8.(1) and 9.(1), and L(N)=L(N'), it will be possible to apply the same reduction to N'. So, let N_1 and N_1' be the fully resolved TCTC hybridization networks obtained by applying the same R or H_0 reduction to N and N'.

From Lemmas 8.(2) and 9.(2) we deduce that $L(N_1) = L(N'_1)$ and hence, by the induction hypothesis, $N_1 \cong N'_1$. Finally, if we apply to N_1 and N'_1 the R^{-1} or H_0^{-1} expansion that is inverse to the reduction applied to N and N', then, by Lemma 6, we obtain again N and N' and they are isomorphic.

A similar argument, using Lemmas 8 and 10, proves the following result.

Proposition 6. Let N and N' be two fully resolved TCTC phylogenetic networks on the same set S of taxa. Then, L(N) = L(N') if, and only if, $N \cong N'$.

Remark 2. The LCSA-path lengths vectors do not separate quasi-binary TCTC-networks. Indeed, consider the TCTC-networks N, N' depicted in Fig. 10. They are quasi-binary (but neither fully resolved phylogenetic networks nor fully resolved hybridization networks), and a simple computation shows that

$$L(N) = L(N') = (3, 6, 3, 3, 6, 3).$$

The network N in Fig. 10 also shows that Lemma 10.(1) is false for quasi-binary hybridization networks.

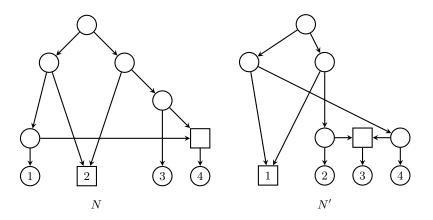


Fig. 10. These two quasi-binary TCTC-networks have the same LCSA-path length vectors.

Let FRH_n (respectively, FRP_n) denote the classes of fully resolved TCTC hybridization (respectively, phylogenetic) networks on $S = \{1, ..., n\}$. We have just proved that the mappings

$$L: FRH_n \to \mathbb{R}^{n(n-1)/2}, \quad L: FRP_n \to \mathbb{R}^{n(n-1)/2}$$

are injective, and therefore they can be used to induce metrics on FRH_n and FRP_n from metrics on $\mathbb{R}^{n(n-1)/2}$.

Proposition 7. For every $n \ge 1$, let D be any metric on $\mathbb{R}^{n(n-1)/2}$. The mappings d: $\mathrm{FRH}_n \times \mathrm{FRH}_n \to \mathbb{R}$ and d: $\mathrm{FRP}_n \times \mathrm{FRP}_n \to \mathbb{R}$ defined by $d(N_1, N_2) = D(L(N_1), L(N_2))$ satisfy the axioms of metrics up to isomorphisms:

- (1) $d(N_1, N_2) \ge 0$,
- (2) $d(N_1, N_2) = 0$ if, and only if, $N_1 \cong N_2$,
- (3) $d(N_1, N_2) = d(N_2, N_1),$
- (4) $d(N_1, N_3) \leq d(N_1, N_2) + d(N_2, N_3)$.

Proof. Properties (1), (3) and (4) are direct consequences of the corresponding properties of D, while property (2) follows from the separation axiom for D (which says that $D(M_1, M_2) = 0$ if, and only if, $M_1 = M_2$) and Proposition 5 or 6, depending on the case.

For instance, using as D the Manhattan distance on $\mathbb{R}^{n(n-1)/2}$, we obtain the metric on FRH_n or FRP_n

$$d_1(N_1, N_2) = \sum_{1 \le i < j \le n} |L_{N_1}(i, j) - L_{N_2}(i, j)|,$$

and using as D the Euclidean distance we obtain the metric

$$d_2(N_1, N_2) = \sqrt{\sum_{1 \le i < j \le n} (L_{N_1}(i, j) - L_{N_2}(i, j))^2}.$$

These metrics generalize to fully resolved TCTC (hybridization or phylogenetic) networks the classical distances for fully resolved phylogenetic trees introduced by Farris [11] and Clifford [29] around 1970.

5 Splitted path lengths vectors for arbitrary networks

As we have seen in §2.2 and Remark 2, the path lengths vectors do not separate arbitrary TCTC-networks. Since to separate arbitrary phylogenetic trees we splitted the path lengths (Definition 2), we shall use the same strategy in the networks setting. In this connection, we already proved in [6] that the matrix

$$\ell(N) = \left(\ell_N(i,j)\right)_{\substack{i=1,\dots,n\\j=1,\dots,n}}$$

separates TCTC phylogenetic networks on $S = \{1, ..., n\}$ with tree nodes of arbitrary out-degree and hybrid nodes of arbitrary in-degree. But it is not true for TCTC hybridization networks, as the following example shows.

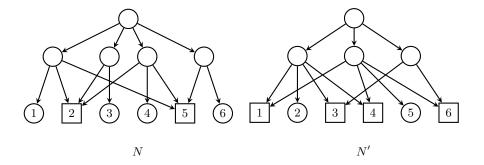


Fig. 11. These two hybridization TCTC-networks are such that $\ell_N(i,j) = \ell_{N'}(i,j)$, for every pair of leaves i,j.

Example 3. Consider the pair of non-isomorphic TCTC-networks N and N' depicted in Fig. 11. A simple computation shows that

$$\ell(N) = \ell(N') = \begin{pmatrix} 0 & 1 & 2 & 2 & 1 & 2 \\ 1 & 0 & 1 & 1 & 2 & 2 \\ 2 & 1 & 0 & 2 & 2 & 2 \\ 2 & 1 & 2 & 0 & 1 & 2 \\ 1 & 2 & 2 & 1 & 0 & 1 \\ 2 & 2 & 2 & 2 & 1 & 0 \end{pmatrix}$$

So, in order to separate arbitrary TCTC-networks we need to add some extra information to the distances $\ell_N(i,j)$ from LCSAs to leaves. The extra information we shall use is whether the LCSA of each pair of leaves is a strict ancestor of one leaf or the other (or both). So, for every pair of different leaves i,j of N, let $h_N(i,j)$ be -1 if [i,j] is a strict ancestor of i but not of i, 1 if [i,j] is a strict ancestor of j but not of i, and 0 if [i,j] is a strict ancestor of both i and j. Notice that $h_N(j,i) = -h_N(i,j)$.

Definition 4. Let N be a hybridization network on the set $S = \{1, ..., n\}$. For every $i, j \in S$, the splitted LCSA-path length from i to j is the ordered 3-tuple

$$L_N^s(i,j) = (\ell_N(i,j), \ell_N(j,i), h_N(i,j)).$$

The splitted LCSA-path lengths vector of N is

$$L^s(N) = \left(L_N^s(i,j)\right)_{1\leqslant i < j \leqslant n} \in (\mathbb{N} \times \mathbb{N} \times \{-1,0,1\})^{n(n-1)/2}$$

with its entries ordered lexicographically in (i, j).

Example 4. Consider the quasi-binary TCTC-networks N and N' depicted in Fig. 10. Then

$$L^s(N) = ((2,1,-1), (3,3,0), (1,2,-1), (1,2,1), (2,4,0), (1,2,-1))$$

 $L^s(N') = ((1,2,1), (2,4,0), (1,2,1), (1,2,-1), (3,3,0), (2,1,1))$

Example 5. Consider the TCTC-networks N and N' depicted in Fig. 11. Then

$$L^{s}(N) = ((1,1,-1),(2,2,0),(2,2,0),(1,1,-1),(2,2,0),(1,1,1),(1,1,1),(2,2,0),(2,2,0),(2,2,0),(2,2,0),(2,2,0),(1,1,-1),(2,2,0),(1,1,1))$$

$$L^{s}(N') = ((1,1,1),(2,2,0),(2,2,0),(1,1,1),(2,2,0),(1,1,-1),(1,1,-1),(2,2,0),(2,2,0),(2,2,0),(2,2,0),(2,2,0),(1,1,1),(2,2,0),(1,1,1),(2,2,0),(1,1,-1))$$

Remark 3. If N is a phylogenetic tree on S, then $h_N(i,j) = 0$ for every $i,j \in S$.

We shall prove now that these splitted LCSA-path lengths vectors separate arbitrary hybridization TCTC-networks. The master plan for proving it is similar to the one used in the proof of Proposition 5: induction based on the fact that the application conditions for the reductions introduced in Section 3 can be read in the splitted LCSA-path lengths vectors of TCTC-networks and that these reductions modify in a controlled way these vectors.

Lemma 11. Let N be a TCTC-network on a set S of taxa.

- (1) The reduction U(i) can be applied to N if, and only if, $\ell_N(i,j) \ge 2$ for every $j \in S \setminus \{i\}$.
- (2) If the reduction U(i) can be applied to N, then

$$L_{N_{U(i)}}(i,j) = L_N(i,j) - (1,0,0) \quad \text{for every } j \in S \setminus \{i\}$$

$$L_{N_{U(i)}}(j,k) = L_N(j,k) \quad \text{for every } j,k \in S \setminus \{i\}$$

Proof. As far as (1) goes, the reduction U(i) can be applied to N if, and only if, the leaf i is a tree node and the only child of its parent. Let us check now that this last condition is equivalent to $\ell_N(i,j) \ge 2$ for every $j \in S \setminus \{i\}$. To do this, we distinguish three cases:

- Assume that i is a tree node and the only child of its parent x. Then, for every $j \in S \setminus \{i\}$, the LCSA of i and j is a proper ancestor of x, and therefore $\ell_N(i,j) \ge 2$.
- Assume that i is a tree node and that it has a sibling y. Let x be the parent of i and y and let j be a tree descendant leaf of y. Then [i,j]=x, because x is a strict ancestor of i, an ancestor of j and clearly no descendant of x is an ancestor of both i and j. Therefore, in this case, $\ell_N(i,j)=1$ for this leaf j.
- Assume that i is a hybrid node. Let x be any parent of i and let j be a tree descendant of x. Then, [i,j]=x, because x is a strict ancestor of j, an ancestor of i, and no intermediate node in the unique path $x \rightsquigarrow j$ is an ancestor of i (it would violate the time consistency property). Therefore, in this case, $\ell_N(i,j)=1$ for this leaf j, too.

Since these three cases cover all possibilities, we conclude that i is a tree node without siblings if, and only if, $\ell_N(i,j) \ge 2$ for every $j \in S \setminus \{i\}$. This finishes the proof of (1).

As far as (2) goes, in $N_{U(i)}$ we replace the tree leaf *i* by its parent. By Lemma 2, this does not modify any LCSA, and it only shortens in 1 any path ending in *i*. Therefore

$$\ell_{N_{U(i)}}(i,j) = \ell_{N}(i,j) - 1, \ \ell_{N_{U(i)}}(j,i) = \ell_{N}(j,i) \text{ for every } j \in S \setminus \{i\}$$

$$\ell_{N_{U(i)}}(j,k) = \ell_{N}(j,k), \ \ell_{N_{U(i)}}(k,j) = \ell_{N}(k,j) \text{ for every } j,k \in S \setminus \{i\}$$

As far as the h component of the splitted LCSA-path lengths goes, notice that a node u is a strict ancestor of a tree leaf i if, and only if, it is a strict ancestor of its parent x (because every path ending in i contains x). Therefore, an internal node of $N_{U(i)}$ is a strict ancestor of the leaf i in $N_{U(i)}$ if, and only if, it is a strict ancestor of the leaf i in N. On the other hand, replacing a tree leaf without siblings by its only parent does not affect any path ending in another leaf, and therefore an internal node of $N_{U(i)}$ is a strict ancestor of a leaf $j \neq i$ in $N_{U(i)}$ if, and only if, it is a strict ancestor of the leaf j in N.

So, by Lemma 2, the LCSA of a pair of leaves in N and in $N_{U(i)}$ is the same, and we have just proved that this LCSA is a strict ancestor of exactly the same leaves in both networks: this implies that

$$h_{N_{U(i)}}(i,j) = h_N(i,j)$$
 for every $j \in S \setminus \{i\}$
 $h_{N_{U(i)}}(j,k) = h_N(j,k)$ for every $j,k \in S \setminus \{i\}$

Lemma 12. Let N be a TCTC-network on a set S of taxa.

- (1) The reduction T(i;j) can be applied to N if, and only if, $L_N^s(i,j) = (1,1,0)$.
- (2) If the reduction T(i;j) can be applied to N, then

$$L_{N_{T(i:j)}}^{s}(k,l) = L_{N}^{s}(k,l)$$
 for every $k,l \in S \setminus \{i\}$

Proof. As far as (1) goes, T(i;j) can be applied to N if, and only if, the leaves i and j are tree nodes and sibling. Let us prove that this last condition is equivalent to $\ell_N(i,j) = \ell_N(j,i) = 1$ and $h_N(i,j) = 0$. Indeed, if the leaves i and j are tree nodes and sibling, then their parent is their LCSA and moreover it is a strict ancestor of both of them, which implies that $\ell_N(i,j) = \ell_N(j,i) = 1$ and $h_N(i,j) = 0$. Conversely, assume that $\ell_N(i,j) = \ell_N(j,i) = 1$ and $h_N(i,j) = 0$. The equalities $\ell_N(i,j) = \ell_N(j,i) = 1$ imply that [i,j] is a parent of i and j, and $h_N(i,j) = 0$ implies that this parent of i and j is a strict ancestor of both of them, and therefore, by Lemma 3, that i and j are tree nodes. This finishes the proof of (1).

As far as (2) goes, in $N_{T(i;j)}$ we simply remove the leaf i without removing anything else. Therefore, no path ending in a remaining leaf is affected, and as a consequence no $L^s(k,l)$ with $k,l \neq i$, is modified.

Lemma 13. Let N be a TCTC-network on a set S of taxa.

- (1) The reduction $H(i; j_1, \ldots, j_k)$ can be applied to N if, and only if,
 - $-L_N^s(i,j_l)=(1,1,1), \text{ for every } l \in \{1,\ldots,k\}.$
 - $-\ell_N(j_a,j_b) \geqslant 2 \text{ or } \ell_N(j_b,j_a) \geqslant 2 \text{ for every } a,b \in \{1,\ldots,k\}.$
 - For every $s \notin \{j_1, \ldots, j_k\}$, if $\ell_N(i, s) = 1$ and $h_N(i, s) = 1$, then $\ell_N(j_l, s) = 1$ and $h_N(j_l, s) = 0$ for some $l \in \{1, \ldots, k\}$.
- (2) If the reduction $H(i; j_1, \ldots, j_k)$ can be applied to N, then

$$L_{N_{H(i;j_1,...,j_k)}}(s,t) = L_N(s,t)$$
 for every $s,t \in S \setminus \{i\}$

Proof. As far as (1) goes, $H(i; j_1, ..., j_k)$ can be applied to N if, and only if, $j_1, ..., j_k$ are tree leaves that are not sibling of each other, the leaf i is a hybrid sibling of $j_1, ..., j_k$, and the only parents of i are those of $j_1, ..., j_k$. Now:

- For each l = 1, ..., k, the condition $L_N^s(i, j_l) = (1, 1, 1)$ says that i and j_l are sibling, and that their parent in common is a strict ancestor of j_l but not of i. Using Lemma 3, we conclude that this condition is equivalent to the fact that i and j_l are sibling, j_l is a tree node, and i a hybrid node.
- Assume that j_1, \ldots, j_k are tree leaves, with parents v_1, \ldots, v_k , respectively. In this case, the condition $\ell_N(j_a, j_b) \geqslant 2$ or $\ell_N(j_b, j_a) \geqslant 2$ is equivalent to the fact that j_a, j_b are not sibling. Indeed, if j_a and j_b are sibling, then $\ell_N(j_a, j_b) = \ell_N(j_b, j_a) = 1$. Conversely, if j_a and j_b are not sibling, then there are two possibilities: either v_a is an ancestor of j_b , but not its parent, in which case $v_a = [j_a, j_b]$ and $\ell_N(j_b, j_a) \geqslant 2$, or v_a is not an ancestor of j_b , in which case $[j_a, j_b]$ is a proper ancestor of v_a and hence $\ell_N(j_a, j_b) \geqslant 2$.
- Assume that j_1, \ldots, j_k are tree leaves, with parents v_1, \ldots, v_k , respectively, and that i is a hybrid sibling of them. Let us see that the only parents of i are v_1, \ldots, v_k if, and only if, for every $s \notin \{j_1, \ldots, j_k\}$, $\ell_N(i, s) = 1$ and $h_N(i, s) = 1$ imply that $\ell_N(j_l, s) = 1$ and $h_N(j_l, s) = 0$ for some $l = 1, \ldots, k$.

 Indeed, assume that the only parents of i are v_1, \ldots, v_k , and let $s \notin \{j_1, \ldots, j_k\}$ be a leaf such that $\ell_N(i, s) = 1$ and $h_N(i, s) = 1$. Since $\ell_N(i, s) = 1$, some parent of i, say v_l , is the LCSA of i and s, and $h_N(i, s) = 1$ implies that v_l is a strict ancestor of s. But then v_l will be the LCSA of its tree leaf j_l and s and strict ancestor of both of them, and thus $\ell_N(j_l, s) = 1$ and $h_N(j_l, s) = 0$.

Conversely, assume that, for every $s \notin \{j_1, \ldots, j_k\}, \ \ell_N(i,s) = 1$ and $h_N(i,s) = 1$ imply that $\ell_N(j_l,s)=1$ and $h_N(j_l,s)=0$ for some $l=1,\ldots,k$. Let v be a parent of i, and let s be a tree descendant leaf of v. Then, v = [i, s] (v is a strict ancestor of s, an ancestor of i, and no intermediate node in the unique path $v \leadsto s$ is an ancestor of i, by the time consistency property) and thus $\ell_N(i,s)=1$; moreover, $h_N(i,s)=1$ by Lemma 3. Now, if $s = j_l$, for some $l = 1, \ldots, k$, then $v = v_l$. On the other hand, if $s \notin \{j_1, \ldots, j_k\}$, then by assumption, there will exist some j_l such that $\ell_N(j_l, s) = 1$ and $h_N(j_l,s)=0$, that is, such that v_l is a strict ancestor of s. This implies that $v=v_l$. Indeed, if $v\neq v_l$, then either v_l is an intermediate node in the path $v\leadsto s$, and in particular a tree descendant of v, which is forbidden by the time consistency because v and v_l have the hybrid child i in common, or v is a proper descendant of v_l through a path where v_l and all the intermediate nodes are hybrid (if some of these nodes were of tree type, the temporal representation of v would be greater than that of v_l , contradicting again the time consistency), in which case the child of v_l in this path would be a hybrid child of v_l that is a strict descendant of it (because it is intermediate in the path $v_l \rightsquigarrow v \rightsquigarrow s$ and s is a strict descendant of v_l), which is impossible by Lemma 3.

This finishes the proof of (1).

As far as (2) goes, in $N_{H(i;j_1,...,j_k)}$ we simply remove the hybrid leaf i without removing anything else, and therefore no splitted LCSA-path length of a pair of remaining leaves is affected.

Theorem 1. Let N and N' be two TCTC-networks on the same set S of taxa. Then, $L^s(N) = L^s(N')$ if, and only if, $N \cong N'$.

Proof. The 'if' implication is obvious. We prove the 'only if' implication by double induction on the number n of elements of S and the number m of internal nodes of N.

As in Proposition 5, the cases n = 1 and n = 2 are straightforward, because both $TCTC_1$ and $TCTC_2$ consist of a single network.

On the other hand, the case when m=1, for every n, is also straightforward: assuming $S=\{1,\ldots,n\}$, the network N is in this case the phylogenetic tree with Newick string $(1,2,\ldots,n)$;, consisting only of the root and the leaves, and in particular $L_N^s(i,j)=(1,1,0)$ for every $1\leqslant i< j\leqslant n$. If $L^s(N)=L^s(N')$, we have that $L_{N'}^s(i,j)=(1,1,0)$ for every $1\leqslant i< j\leqslant n$, and therefore all leaves in N' are tree nodes and sibling of each other by Lemma 3. Since the root of a hybridization network cannot be elementary, this says that N' is also a phylogenetic tree with Newick string $(1,2,\ldots,n)$; and hence it is isomorphic to N.

Let now N and N' two TCTC-networks with $n \ge 3$ leaves such that $L^s(N) = L^s(N')$ and N has $m \ge 2$ internal nodes. Assume as induction hypothesis that the thesis in the theorem is true for pairs of TCTC-networks N_1, N_1' with n-1 leaves or with n leaves and such that N_1 has m-1 internal nodes.

By Proposition 3, a reduction U(i), T(i;j) or $H(i;j_1,\ldots,j_k)$ can be applied to N. Since the application conditions for such a reduction depend only on the splitted LCSA-path lengths vectors by Lemmas 11.(1), 12.(1) and 13.(1), and $L^s(N) = L^s(N')$, we conclude that we can apply the same reduction to N'.

Now, we apply the same reduction to N and N' to obtain new TCTC-networks N_1 and N'_1 , respectively. If the reduction was of the form U(i), N_1 and N'_1 have n leaves and N_1 has m-1 internal nodes; if the reduction was of the forms T(i;j) or $H(i;j_1,\ldots,j_k)$, N_1 and N'_1 have n-1 leaves. In all cases, $L^s(N_1) = L^s(N'_1)$ by Lemmas 11.(2), 12.(2) and 13.(2), and therefore, by the induction hypothesis, $N_1 \cong N'_1$.

Finally, by Lemma 5, N and N' are obtained from N_1 and N'_1 by applying the same expansion U^{-1} , T^{-1} , or H^{-1} , and they are isomorphic.

The vectors of splitted LCSA-path lengths vectors do not separate hybridization networks much more general than the TCTC, as we following examples show.

Remark 4. The vectors of splitted distances do not separate arbitrary (that, is, possibly time inconsistent) tree-child phylogenetic networks. Indeed, the non-isomorphic tree-child binary phylogenetic networks N and N' depicted in Fig. 12 have the same L^s vectors:

$$L^{s}(N) = L^{s}(N') = ((2,1,1), (4,1,1), (3,1,1)).$$

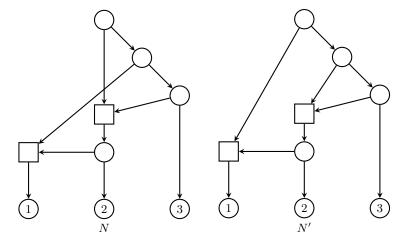


Fig. 12. These two tree-child binary phylogenetic networks have the same splitted LCSA-path lengths vectors.

Remark 5. The splitted LCSA-path lengths vectors do not separate tree-sibling time consistent phylogenetic networks, either. Consider for instance the tree-sibling time consistent fully resolved phylogenetic networks N and N' depicted in Figure 13. A simple computation shows that they have the same L^s vectors, but they are not isomorphic.

As in the fully resolved case, the injectivity of the mapping

$$L^s: \mathrm{TCTC}_n \to \mathbb{R}^{3n(n-1)/2}$$

makes it possible to induce metrics on $TCTC_n$ from metrics on $\mathbb{R}^{3n(n-1)/2}$. The proof of the following result is similar to that of Proposition 7.

Proposition 8. For every $n \ge 1$, let D be any metric on $\mathbb{R}^{3n(n-1)/2}$. The mapping $d^s : \mathrm{TCTC}_n \times \mathrm{TCTC}_n \to \mathbb{R}$ defined by $d(N_1, N_2) = D(L^s(N_1), L^s(N_2))$ satisfies the axioms of metrics up to isomorphisms.

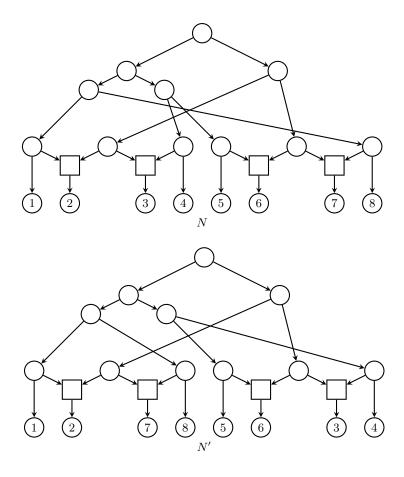


Fig. 13. These two tree-sibling time consistent binary phylogenetic networks have the same splitted LCSA-path lengths vectors.

For instance, using as D the Manhattan distance or the Euclidean distance, we obtain, respectively, the metrics on TCTC_n

$$\begin{split} d_1^s(N_1,N_2) &= \sum_{1 \leqslant i < j \leqslant n} \left(|\ell_{N_1}(i,j) - \ell_{N_2}(i,j)| + |\ell_{N_1}(j,i) - \ell_{N_2}(j,i)| \right. \\ &+ |h_{N_1}(i,j) - h_{N_2}(i,j)| \right) \\ &= \sum_{1 \leqslant i \neq j \leqslant n} \left(|\ell_{N_1}(i,j) - \ell_{N_2}(i,j)| + \frac{1}{2} |h_{N_1}(i,j) - h_{N_2}(i,j)| \right) \\ d_2^s(N_1,N_2) &= \left(\sum_{1 \leqslant i < j \leqslant n} \left((\ell_{N_1}(i,j) - \ell_{N_2}(i,j))^2 + (\ell_{N_1}(j,i) - \ell_{N_2}(j,i))^2 \right. \\ &+ \left. \left(h_{N_1}(i,j) - h_{N_2}(i,j) \right)^2 \right) \right]^{\frac{1}{2}} \\ &= \sqrt{\sum_{1 \leqslant i \neq j \leqslant n} \left((\ell_{N_1}(i,j) - \ell_{N_2}(i,j))^2 + \frac{1}{2} (h_{N_1}(i,j) - h_{N_2}(i,j))^2 \right)} \end{split}$$

These metrics generalize to TCTC-networks the splitted nodal metrics for arbitrary phylogenetic trees defined in [7]. and the nodal metric for TCTC *phylogenetic* networks defined in [6].

6 Conclusions

A classical result of Smolenskii [24] establishes that the vectors of distances between pairs of leaves separate unrooted phylogenetic trees on a given set of taxa. This result generalizes easily to fully resolved rooted phylogenetic trees [7], and it lies at the basis of the classical definitions of nodal distances for unrooted as well as for fully resolved rooted phylogenetic trees based on the comparison of these vectors [3,11,12,22,26,29]. But these vectors do not separate arbitrary rooted phylogenetic trees, and therefore they cannot be used to compare the latter in a sound way. This problem was overcome in [7] by introducing the splitted path lengths matrices and showing that they separate arbitrary rooted phylogenetic trees on a given set of taxa. It is possible then to define splitted nodal metrics for arbitrary rooted phylogenetic trees by comparing these matrices.

In this paper we have generalized these results to the class $TCTC_n$ of tree-child time consistent hybridization networks (TCTC-networks) with n leaves. For every pair i, j of leaves in a TCTC-network N, we have defined the LCSA-path length $L_N(i,j)$ and the splitted LCSA-path length $L_N^s(i,j)$ between i and j and we have proved that the vectors $L(N) = (L_N(i,j))_{1 \le i < j \le n}$ separate fully resolved networks in $TCTC_n$ and the vectors $L^s(N) = (L_N^s(i,j))_{1 \le i < j \le n}$ separate arbitrary TCTC-networks.

The vectors L(N) and $L^s(N)$ can be computed in low polynomial time by means of simple algorithms that do not require the use of sophisticated data structures. Indeed, let n be the number of leaves and m the number of internal nodes in N. As we explained in $[5, \S V.D]$, for each internal node v and for each leaf i, it can be decided whether v is a strict or a non-strict ancestor of i, or not an ancestor of it at all, by computing by breadth-first search the shortest paths from the root to each leaf before and after removing each of the m nodes in turn, because a non-strict descendant of a node will still be reachable from the root after removing that node, while a strict descendant will not. All this information can be computed in O(m(n+m)) time, and once it has been computed the least common semi-strict ancestor of two leaves can be computed in O(m) time by selecting the node of least height among those which are ancestors of the two leaves and strict ancestors of at least one of them. This allows the computation of L(N) and $L^s(N)$ in $O(m^2 + n^2m)$ time.

These vectors L(N) and $L^s(N)$ can be used then to define metrics for fully resolved and arbitrary TCTC-networks, respectively, from metrics for real-valued vectors. The metrics obtained in this way can be understood as generalizations to TCTC_n of the (non-splitted or splitted) nodal metrics for phylogenetic trees and they can be computed in low polynomial time if the metric used to compare the vectors can be done so: this is the case, for instance, when this metric is the Manhattan or the Euclidean metric (in the last case, computing the square root with $O(10^{m+n})$ significant digits [2], which should be more than enough).

It remains to study the main properties of the metrics defined in this way, like for instance their diameter or the distribution of their values. It is important to recall here that these are open problems even for the classical nodal distances for fully resolved rooted phylogenetic trees.

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References

- 1. M. Baroni, C. Semple, M. Steel, Hybrids in real time, Syst. Biol. 55 (2006) 46-56.
- P. Batra, Newton's method and the computational complexity of the fundamental theorem of algebra, Electron. Notes Theor. Comput. Sci. 202 (2008) 201–218.
- 3. J. Bluis, D.-G. Shin, Nodal distance algorithm: Calculating a phylogenetic tree comparison metric, in: Proc. 3rd IEEE Symp. BioInformatics and BioEngineering, 2003.
- G. Cardona, M. Llabrés, F. Rosselló, G. Valiente, A distance metric for a class of tree-sibling phylogenetic networks, Bioinformatics 24 (13) (2008) 1481–1488.
- 5. G. Cardona, M. Llabrés, F. Rosselló, G. Valiente, Metrics for phylogenetic networks I: Generalizations of the Robinson-Foulds metric, submitted (2008).
- 6. G. Cardona, M. Llabrés, F. Rosselló, G. Valiente, Metrics for phylogenetic networks II: Nodal and triplets metrics, submitted (2008).
- G. Cardona, M. Llabrés, F. Rosselló, G. Valiente, Nodal metrics for rooted phylogenetic trees, submitted, available at arxiv.org/abs/0806.2035 (2008).
- 8. G. Cardona, F. Rosselló, G. Valiente, Comparison of tree-child phylogenetic networks, IEEE T. Comput. Biol. preprint, 30 June 2008, doi:10.1109/TCBB.2007.70270.
- G. Cardona, F. Rosselló, G. Valiente, Tripartitions do not always discriminate phylogenetic networks, Math. Biosci. 211 (2) (2008) 356–370.
- W. F. Doolittle, Phylogenetic classification and the universal tree, Science 284 (5423) (1999) 2124– 2128.
- J. S. Farris, A successive approximations approach to character weighting, Syst. Zool. 18 (1969) 374–385.
- 12. J. S. Farris, On comparing the shapes of taxonomic trees, Syst. Zool. 22 (1973) 50-54.
- D. Gusfield, S. Eddhu, C. Langley, The fine structure of galls in phylogenetic networks, INFORMS J. Comput. 16 (4) (2004) 459–469.
- 14. D. Gusfield, S. Eddhu, C. Langley, Optimal, efficient reconstruction of phylogenetic networks with constrained recombination, J. Bioinformatics Comput. Biol. 2 (1) (2004) 173–213.
- J. Hein, M. H. Schierup, C. Wiuf, Gene Genealogies, Variation and Evolution: A Primer in Coalescent Theory, Oxford University Press, 2005.
- D. H. Huson, D. Bryant, Application of Phylogenetic Networks in Evolutionary Studies, Mol. Biol. Evol. 23 (2) (2006) 254–267.
- D. H. Huson, T. H. Klöpper, Beyond galled trees decomposition and computation of galled networks, in: Proceedings RECOMB 2007, vol. 4453 of Lecture Notes in Computer Science, Springer-Verlag, 2007.
- 18. B. M. E. Moret, L. Nakhleh, T. Warnow, C. R. Linder, A. Tholse, A. Padolina, J. Sun, R. Timme, Phylogenetic networks: Modeling, reconstructibility, and accuracy, IEEE T. Comput. Biol. 1 (1) (2004) 13–23.
- L. Nakhleh, J. Sun, T. Warnow, C. R. Linder, B. M. E. Moret, A. Tholse, Towards the development of computational tools for evaluating phylogenetic network reconstruction methods, in: Proc. 8th Pacific Symp. Biocomputing, 2003.

- L. Nakhleh, J. Sun, T. Warnow, C. R. Linder, B. M. E. Moret, A. Tholse, Towards the development of computational tools for evaluating phylogenetic network reconstruction methods, in: Proc. 8th Pacific Symp. Biocomputing, 2003.
- L. Nakhleh, T. Warnow, C. R. Linder, K. S. John, Reconstructing reticulate evolution in species: Theory and practice, J. Comput. Biol. 12 (6) (2005) 796–811.
- 22. J. B. Phipps, Dendrogram topology, Syst. Zool. 20 (1971) 306-308.
- 23. C. Semple, Hybridization networks, in: O. Gascuel, M. Steel (eds.), Reconstructing evolution: New mathematical and computational advances, Oxford University Press, 2008, pp. 277–314.
- Y. A. Smolenskii, A method for the linear recording of graphs, USSR Computational Mathematics and Mathematical Physics 2 (1963) 396–397.
- Y. S. Song, J. Hein, Constructing minimal ancestral recombination graphs, J. Comput. Biol. 12 (2) (2005) 147–169.
- M. A. Steel, D. Penny, Distributions of tree comparison metrics—some new results, Syst. Biol. 42 (2) (1993) 126–141.
- 27. G. Valiente, Phylogenetic networks, course at the Int. Summer School on Bioinformatics and Computational Biology Lipari (June 14–21, 2008).
- L. Wang, K. Zhang, L. Zhang, Perfect phylogenetic networks with recombination, J. Comput. Biol. 8 (1) (2001) 69–78.
- 29. W. T. Williams, H. T. Clifford, On the comparison of two classifications of the same set of elements, Taxon 20 (4) (1971) 519–522.
- 30. S. J. Willson, Restrictions on meaningful phylogenetic networks, contributed talk at the EMBO Workshop on Current Challenges and Problems in Phylogenetics (Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, 3–7 September 2007).
- 31. S. J. Willson, Reconstruction of certain phylogenetic networks from the genomes at their leaves, J. Theor. Biol. 252 (2008) 338–349.
- 32. S. M. Woolley, D. Posada, K. A. Crandall, A comparison of phylogenetic network methods using computer simulation, Plos ONE 3 (4) (2008) e1913.