'Lassoing' a phylogenetic tree I: basic properties, shellings, and covers

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Abstract A classical result, fundamental to evolutionary biology, states that an edge-weighted tree T with leaf set X, positive edge weights, and no vertices of degree 2 can be uniquely reconstructed from the leaf-to-leaf distances between any two elements of X. In biology, X corresponds to a set of taxa (e.g. extant species), the tree T describes their phylogenetic relationships, the edges correspond to earlier species evolving for a time until splitting in two or more species by some speciation/ bifurcation event, and their length corresponds to the genetic change accumulating over

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that time in such a species. In this paper, we investigate which subsets of $\binom{X}{2}$ suffice to determine ('lasso') the tree T from the leaf-to-leaf distances induced by that tree. The question is particularly topical since reliable estimates of genetic distance—even (if not in particular) by modern mass-sequencing methods—are, in general, available only for certain combinations of taxa.

1 Introduction

A metric D on a finite set X is said to be a 'tree metric' if there is a finite tree with leaf set X and non-negative edge weights so that, for all $x, y \in X$, $D(x, y)$ is the path distance in the tree between x and y. It is well known that not every metric is a tree metric. However, when a metric D is a tree metric, the tree (together with its edge weights) that provides a representation of D is—up to canonical isomorphism— unique if we also insist that the tree is an 'edge-weighted X-tree', i.e., that it has no vertices of degree 2 and that all of its interior edges have strictly positive edge weights. However, not all of the $\binom{|X|}{2}$ pairs of distances are required in order to reconstruct the underlying tree. Thus, it seems of some interest to investigate which subsets of $\binom{X}{2}$ suffice to determine ('lasso') the tree. In this first of a series of papers, we expound various aspects of this problem, present some relevant definitions, and collect some basic facts.

Our work is partly motivated by the widespread use of distance-based methods for reconstructing phylogenetic trees in evolutionary biology (Felsenstein 2004). A further reason is that asking similar questions for induced subtrees rather than for 'sparse' sets of distances gave rise to a rather appealing theory dealing with 'sparse' collections of induced subtrees that suffice to 'define' an X-tree (see e.g. Böcker et al. 1999; Dress et al. 2011b).

Provided one has access to all distances, and these are known to be sufficiently close to the distances induced by some (as yet unknown) tree, then that tree, together with its edge weighting, can be computed—with some degree of confidence—from those distances in polynomial time (for example, by using Neighbor-Joining, Atteson 1999). However, much of the data being generated—even by modern genomic methods— have patchy taxon coverage (Philippe et al. 2004) whereby only certain pairs of taxa have a known (or, at least, sufficiently reliable) distance. This raises interesting mathematical questions (besides the obvious statistical and algorithmic ones) concerning tree reconstruction from such incomplete data some of which we will address here.

More specifically, in this first of a series of papers, we want to explore the basic properties of 'edge-weight', 'topological', and 'strong lassos'—being primarily interested in the uniqueness question: Given the restriction of a tree metric D to some subset $\mathcal{L}$ of $\binom{X}{2}$, how much can we learn about the tree representing D from that restriction? In particular, we ask which subsets $\mathcal{L}$ of $\binom{X}{2}$ provide enough 'coverage'

Fig. 1 The set $\mathcal{L}_4 = \{\{a, b\}, \{c, d\}, \{a, c\}, \{b, d\}\}$ lassos the shape of the X_4-tree T_4 while $\mathcal{L}_4 \cup \{\{a, d\}\}$ and $\mathcal{L}_4 \cup \{\{b, c\}\}$ are strong lassos for T_4 (see *text* for details)
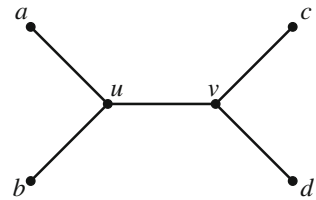
in order to fully determine an edge-weighted X-tree or, at least, its shape, or—given its shape—its edge lengths in terms of just the distances it induces between the pairs of taxa collected in $\mathcal{L}$. Or, put differently, how much 'missing data' (pairs of taxa x, y for which $D(x, y)$ is not known) can we allow and still be guaranteed to recover them from those distances that we can observe.

2 Some basic definitions and facts

2.1 Trees and tree metrics

Consider any finite tree $T = (V, E)$ with vertex set V, leaf set $X \subseteq V$, and edge set $E \subseteq \binom{V}{2}$ together with an *edge weighting*—i.e., a map ω in the set $\Omega = \Omega_T := \mathbb{R}_{\geq 0}^E$ that assigns a non-negative length $\omega(e)$ to every edge $e \in E$. Any such pair (T, ω) induces a distance function:

$$D_\omega = D_{(T,\omega)} : \binom{X}{2} \to \mathbb{R}_{\geq 0} : \{x, y\} \mapsto D_\omega(x, y) := \omega_+ \left(E_T(x|y) \right) \qquad (1)$$

where $E_T(u|v)$ denotes, for any two vertices $u, v \in V$, the set of edges in E that 'separate' u and v in T (and, thus, together make up the path from u to v in T) and $\omega_+(F)$ denotes, for any non-empty subset F of E, the sum $\sum_{e \in F} \omega(e)$.

For example, in Fig. 1, we have $E_T(a|c) = \{\{a, u\}, \{u, v\}, \{v, c\}\}$ and, thus, $D_\omega(a, c) = 3$ for the binary tree $T := T_4$ with leaf set $X_4 := \{a, b, c, d\}$ and an interior edge that separates the leaves a, b from the leaves c, d provided unit edge length has been assigned to all edges of that tree.

While D_ω is clearly a (pseudo-)metric on X (and a proper metric if—but not necessarily only if—ω is strictly positive), not every metric on X can be represented in this way: The condition for an arbitrary metric D on X to have a *phylogenetic representation*, that is, to be representable in the form $D = D_\omega$ for some finite edge-weighted tree (T, ω) with leaf set X, is that D satisfies the well-known *four-point condition* which states that, for all $a, b, c, d \in X$, the larger two of the three distance sums $D(a, b) + D(c, d)$, $D(a, c) + D(b, d)$, $D(a, d) + D(b, c)$ coincide or, equivalently, if

$$D(ab|cd) := \max \{D(a, c) + D(b, d), \ D(a, d) + D(b, c)\} - D(a, b) - D(c, d)$$

$$(2)$$

is non-negative for all $a, b, c, d \in X$.

Such a metric D is said to be a *tree metric*, and any finite tree $T = (V, E)$ as above for which some $\omega \in \Omega_T$ with $D = D_\omega$ exists will be dubbed a *D-tree*. Furthermore, such a tree T will be said to be a *proper D-tree* if T has no vertices of degree 2 and it has a *proper* edge weighting ω with $D = D_\omega$, i.e., a map $\omega \in \Omega_T$ that is strictly positive on all interior edges of T.

Clearly, given any tree metric D, many non-equivalent D-trees T with edge weightings ω can exist such that $D = D_\omega$ holds, since adding zero-length edges and/or subdividing any edge of a D-tree by degree 2 vertices yields further D-trees. However, it has been well known since the 1960s (see, for instance, Barthélemy and Guéoche 1991; Semple and Steel 2003 and the references therein) that there is 'essentially' only one proper D-tree T for any tree metric D and, given T, only one edge weighting $\omega \in \Omega_T$ for which $D = D_\omega$ holds. This was actually one of the starting points of what currently is called *phylogenetic combinatorics*.

More specifically, recall that, given a finite set X of cardinality at least 3 (the set X typically represents the collection of 'taxa' under consideration—e.g. some extant species), a finite tree $T = (V, E)$ with vertex set V, leaf set $X \subseteq V$, and edge set $E \subseteq \binom{V}{2}$ having no vertices of degree 2 is said to be a *phylogenetic X-tree* or (in the context of this paper) more briefly an *X-tree* and that an X-tree for which every interior vertex has degree 3 is said to be a *binary X-tree*. With these definitions in hand, the following relationships are well-known and easily established.

(i) $|E| \leq 2|X| - 3$ holds for every X-tree $T = (V, E)$; and
(ii) $|E| = 2|X| - 3$ holds if and only if T is a binary X-tree

Recall also that two X-trees $T = (V, E)$ and $T' = (V', E')$ are said to be (*topologically*) *equivalent* (written $T \simeq T'$) if there exists a (necessarily unique) graph isomorphism $\varphi : T \xrightarrow{\sim} T'$ that respects X, i.e., a bijection $\varphi : V \xrightarrow{\sim} V'$ with $E' = \{\{\varphi(u), \varphi(v)\} : \{u, v\} \in E\}$ and $\varphi(x) = x$ for all $x \in X$, and that T' is defined to be a *refinement* of T (written $T \leq T'$) if—up to equivalence—T can be obtained from T' by collapsing edges in T' (see Semple and Steel 2003). Furthermore, two edge-weighted X-trees $(T, \omega), (T', \omega')$ are said to be *isometric* $\big($written $(T, \omega) \equiv (T', \omega')\big)$ if there exists a graph isomorphism $\varphi : T \xrightarrow{\sim} T'$ as above that respects not only X, but also the edge lengths, i.e., also $\omega(\{u, v)\}) = \omega'(\{\varphi(u), \varphi(v)\})$ holds for all edges $\{u, v\} \in E$ of T. For example, denoting the 'all-one map' on a set A by $\mathbf{1}^A$, two X-trees $T = (V, E)$ and $T' = (V'E')$ are equivalent if and only if the corresponding edge-weighted X-trees $(T, \mathbf{1}^E)$ and $(T', \mathbf{1}^{E'})$ are isometric.

The basic result referred to above then states that, given any two X-trees T, T' with proper edge weightings $\omega \in \Omega_T$ and $\omega' \in \Omega_{T'}$, one has

$$D_\omega = D_{\omega'} \iff (T, \omega) \equiv (T', \omega') \tag{3}$$

and, therefore, also

$$D_\omega = D_{\omega'} \iff \omega = \omega' \tag{4}$$

for any fixed X-tree $T = (V, E)$ and all $\omega, \omega' \in \Omega_T$.

What we will be concerned with here is that, given (T, ω) and (T', ω') as above, we do not even always need the associated metrics D_ω and $D_{\omega'}$ to coincide on *all* pairs $\{x, y\} \in \binom{X}{2}$ to conclude

- that T' must be equivalent to (or at least a refinement of) T,
- that (T, ω) and (T', ω') must be isometric, or
- that $\omega = \omega'$ must hold in case $T = T'$.

Indeed, if T and T' are two X_4-trees, and ω and ω' are proper edge weightings of T and T', respectively, then

(i) T and T' must be equivalent whenever the two metrics $D := D_\omega$ and $D' := D_{\omega'}$ coincide on the four pairs $\{a, b\}, \{c, d\}, \{a, c\}$, and $\{b, d\}$, and $D(a, b) + D(c, d) < D(a, c) + D(b, d)$ holds (in which case, both must be equivalent to the tree depicted in Fig. 1);

(ii) (T, ω) and (T', ω') must be isometric or, equivalently, D and D' must coincide if these two maps coincide, in addition, on just one of the remaining two pairs $\{a, d\}$ or $\{b, c\}$.

2.2 Lassos

To deal with such matters, we define, given a subset $\mathcal{L}$ of $\binom{X}{2}$, two edge weighted X-trees (T, ω) and (T', ω') to be $\mathcal{L}$-*isometric* (written $(T, \omega) \overset{\mathcal{L}}{\equiv} (T', \omega')$) if $D|_\mathcal{L} = D'|_\mathcal{L}$ holds for $D := D_\omega$ and $D' := D_{\omega'}$. Then, given an X-tree T, it seems of some interest to study those subsets $\mathcal{L}$ of $\binom{X}{2}$ that have one of the following properties:

(L-i) $\omega = \omega'$ holds for all proper edge weightings ω, ω' of T with $(T, \omega) \overset{\mathcal{L}}{\equiv} (T, \omega')$;

(L-ii) $T \simeq T'$ holds for any X-tree T' for which there exist proper edge weightings ω of T and ω' of T' with $(T, \omega) \overset{\mathcal{L}}{\equiv} (T', \omega')$;

(L-ii′) $T \leq T'$ holds for any X-tree T' for which there exist proper edge weightings ω of T and ω' of T' with $(T, \omega) \overset{\mathcal{L}}{\equiv} (T', \omega')$;

(L-iii) $(T, \omega) \equiv (T', \omega')$ holds, for every given proper edge weighting ω of T, for any X-tree T' and any proper edge weighting ω' of T' with $(T, \omega) \overset{\mathcal{L}}{\equiv} (T', \omega')$.

To this end, given an X-tree T, we define a subset $\mathcal{L}$ of $\binom{X}{2}$ to be:

(i) an *edge-weight lasso for T* (or *to lasso the edge weights of T*) if (L-i) holds;
(ii) a *topological lasso for T* (or *to lasso the shape of T*) if (L-ii) holds;
(ii′) a *weak lasso for T* (or *to corall T*) if (L-ii′) holds; and
(iii) a *strong lasso for T* (or just *to lasso T*) whenever (L-iii) holds.

As we deal here with 'lassos', any 2-subset $\mathfrak{c} = \{x, y\} \in \binom{X}{2}$ of X will also be called a *cord*, often written more briefly as $\mathfrak{c} = xy$; also, we refer to the cords in a lasso $\mathcal{L}$ as the cords 'in' $\mathcal{L}$.

Using this terminology, we can rephrase the example discussed at the end of Sect. 2.1 as follows: The four cords ab, cd, ac and bd form a topological lasso $\mathcal{L}_4$ for the tree

T_4 depicted in Fig. 1, and adding either the cord ad or bc yields a strong lasso for that tree.

Clearly, a subset $\mathcal{L}$ is an edge-weight lasso for an X-tree $T = (V, E)$ if and only if $D = D'$ holds for any two tree metrics D, D' defined on X with $D|_{\mathcal{L}} = D'|_{\mathcal{L}}$ for which T is simultaneously a proper D- and a proper D'-tree: Indeed, if ω and ω' are proper edge weightings of T with $D = D_{\omega}$ and $D' = D_{\omega'}$, we have "$D|_{\mathcal{L}} = D'|_{\mathcal{L}} \iff (T, \omega) \overset{\mathcal{L}}{\equiv} (T, \omega')$" and "$D = D' \iff \omega = \omega'$" and, therefore, "$D|_{\mathcal{L}} = D'|_{\mathcal{L}} \Rightarrow D = D'$" if and only if "$(T, \omega) \overset{\mathcal{L}}{\equiv} (T, \omega') \Rightarrow \omega = \omega'$".

Similarly, $\mathcal{L}$ is a topological (or a weak) lasso for T if and only if every X-tree T' for which there exist tree metrics D and D' with $D|_{\mathcal{L}} = D'|_{\mathcal{L}}$ such that T is a proper D-tree and T' is a proper D'-tree is equivalent to (or a refinement of) T. And $\mathcal{L}$ is a strong lasso for T if and only if $D = D'$ holds for any two tree metrics D, D' defined on X with $D|_{\mathcal{L}} = D'|_{\mathcal{L}}$ for which T is a proper D-tree and, hence, if and only if it is both, an edge-weight lasso and a topological lasso for T.

In particular, if there exists a pair ω, ω' of edge weightings of T with $D_{\omega}|_{\mathcal{L}} = D_{\omega'}|_{\mathcal{L}}$ such that ω is a proper and ω' is not a proper edge weighting of T, then $\mathcal{L}$ is neither a topological lasso for T nor for the X-tree that results by 'collapsing' any of the interior edges e of T with $\omega'(e) = 0$.

2.3 Some further conventions, definitions, notations, and well-known facts

We end this section by listing some simple conventions, definitions, and well-known facts (see, e.g., Semple and Steel 2003) that will be used throughout.

2.3.1 Firstly, we will assume throughout that X is a finite set of cardinality $n \geq 3$ and we put $\bigcup \mathcal{L} := \bigcup_{\mathfrak{c} \in \mathcal{L}} \mathfrak{c}$ for any non-empty subset $\mathcal{L} \subseteq \binom{X}{2}$. We will refer to a subset $\mathcal{L}$ of $\binom{X}{2}$ as being 'connected', 'disconnected' or 'bipartite' etc. whenever the graph $\Gamma(\mathcal{L}) := (X, \mathcal{L})$ is connected, disconnected, or bipartite and so on, and a connected component of $\Gamma(\mathcal{L})$ will also be called a connected component of $\mathcal{L}$.

2.3.2 For every edge f of a tree $T = (V, E)$, we denote by $\delta_f \in \Omega_T$ the map defined by

$$\delta_f : E \to \mathbb{R} : e \mapsto \delta_{e,f} := \begin{cases} 1, & \text{if } e = f; \\ 0, & \text{otherwise.} \end{cases} \tag{5}$$

And for every leaf a of a tree T with at least 2 vertices, we denote by $e_a = e_a^T$ the unique edge of T containing a and by v_a the other (in case $|V| \geq 3$ necessarily interior) vertex of T contained in e_a.

2.3.3 Two distinct leaves, a and b, in a tree T with $v_a = v_b$ will be said to form a *T-cherry*, and they will be said to form a *T-proper cherry* if, in addition, $v_a(= v_b)$ has degree 3; for example, the two pairs a, b and c, d form proper cherries in the tree T_4
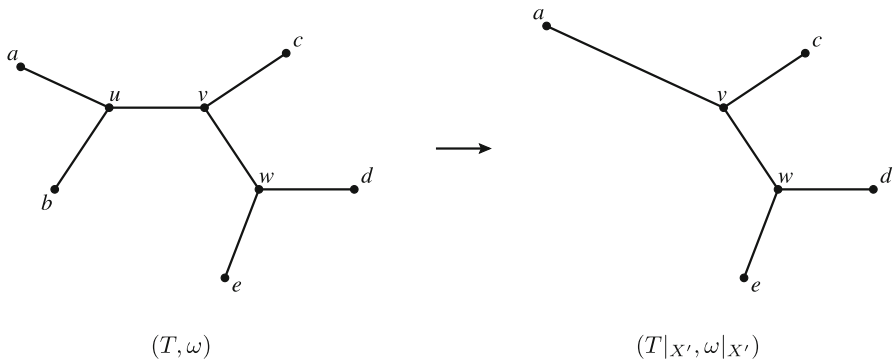
Fig. 2 For $X' := \{a, c, d, e\} \subset X_5 = \{a, b, c, d, e\}$, the X'-tree on the right is obtained from the X_5-tree T_5 on the left by restricting its leaf set to X'. The associated induced edge weighting $\omega_{|X'}$ is also indicated

depicted in Fig. 1. A *caterpillar tree* is a binary X-tree that has exactly two proper cherries (see, for example the tree T_6 in Fig. 4, or the tree in Fig. 7).

2.3.4 The *median* of three vertices u, v, and w of a tree $T = (V, E)$ is the unique vertex in V that is simultaneously contained in the three paths connecting any two of u, v, and w in T, and will be denoted by $\mathrm{med}_T(u, v, w)$. For example, the vertex u in Fig. 1 is the median of the three leaves a, b, c.

Given an X-tree $T = (V, E)$ and any subset X' of X, the *restriction* of T to X' (i.e., the tree with vertex set $\mathrm{med}_T(X') := \{\mathrm{med}_T(x, y, z) : x, y, z \in X'\}$ and edge set the set of all pairs $\{u, v\} \in \binom{\mathrm{med}_T(X')}{2}$ for which $\mathrm{med}_T(u, v, x) \in \{u, v\}$ holds for all $x \in X'$) will be denoted by $T|_{X'}$, and its vertex and edge sets by $V|_{X'}$ and $E|_{X'}$, respectively. And, given any edge weighting ω of T, the *induced* edge weighting of T', i.e., the edge weighting that maps any edge $\{u, v\} \in E|_{X'}$ onto the sum $\omega_+ (E_T(u|v))$, will also be denoted by $\omega_{|X'}$. These concepts are illustrated in Fig. 2 for the caterpillar tree T_5 with leaf set $X_5 := \{a, b, c, d, e\}$ and the two cherries a, b and d, e depicted in Fig. 2 on the left.

It is well known and easily seen that $T|_{X'}$ is a (binary) X'-tree for every (binary) X-tree T and every subset X' of X of cardinality at least 3.

2.3.5 An *X-split* is a 'split' or 'bipartition' of X into two disjoint non-empty subsets. A *quartet* is a bipartition of a 4-set into two disjoint subsets of cardinality 2. In case a, a', b, b' are any 4 distinct elements, the quartet $\{\{a, a'\}, \{b, b'\}\}$ is also denoted, for short, by $aa'\|bb'$ while $a|a'|b|b'$ stands for the partition of $\{a, a', b, b'\}$ into the four one-element sets $\{a\}, \{a'\}, \{b\}, \{b'\}$.

A *quartet tree* is a binary tree T with exactly four leaves—and, therefore, exactly two cherries. We will also say that such a tree T is a *quartet tree of type* $aa'\|bb'$ if its two cherries are formed by the leaves a, a' and b, b', i.e., $\{a, a', b, b'\}$ is the 4-set that forms the leaf set of T, and T has a (necessarily interior and necessarily unique) edge that separates a, a' from b, b' (so, as stated in Fig. 1, the tree T_4 depicted in that figure is a quartet tree of type $ab\|cd$). In addition, a tree T with exactly four leaves

a, a', b, b' will be said to be a tree of type $a|a'|b|b'$ if it is non-binary, so that any tree T with leaf set $\{a, a', b, b'\}$ is either a tree of type $a|a'|b|b'$ or a quartet tree of type $aa'\|bb'$, $ab\|a'b'$, or $ab'\|a'b$.

Further, an X-tree T is said to *display* a quartet $xx'\|yy'$ (or, respectively, the partition $x|x'|y|y'$) if $\{x, x', y, y'\}$ is a 4-subset of X and $T|_{\{x,x',y,y'\}}$ is a quartet tree of type $xx'\|yy'$ (or, respectively, a tree of type $x|x'|y|y'$). By abuse of notation, T will also be said to display $xx'|yy'$ if it either displays $xx'\|yy'$ or $x|x'|y|y'$ or, equivalently, neither $xy\|x'y'$ nor $xy'\|x'y$. The collection of all quartets displayed by T will be denoted by $\mathcal{Q}(T)$.

Recall also that, given any five distinct elements $x, x', y, y', y'' \in X$, T displays $xx'\|yy''$ (or $xx'|yy''$, respectively) if it displays $xx'\|yy'$ and $xx'\|y'y''$ (or $xx'|yy'$ and $xx'|y'y''$) (Colonius and Schulze 1981). In addition, given any proper edge weighting ω of T, T displays

- $xx'\|yy'$ if and only if $D_\omega(xx'|yy') > 0$ holds,[1]
- $x|x'|y|y'$ if and only if $D_\omega(x, y) + D_\omega(x', y') = D_\omega(x, y') + D_\omega(x', y) = D_\omega(x, x') + D_\omega(y, y')$ holds; and
- $xx'|yy'$ if and only if $D_\omega(x, y) + D_\omega(x', y') = D_\omega(x, y') + D_\omega(x', y)$ holds.

Furthermore (see for instance Chapter 7 in Dress et al. 2011b), one has

$$\min\left\{D_\omega(xx'|yy'), D_\omega(xx'|y'y'')\right\} \leq D_\omega(xx'|yy'') \tag{6}$$

for all x, x', y, y', y'' as above whenever T displays $xx'|yy'$ and $xx'|y'y''$.

In consequence,

$$D_\omega(xx'|yz) = D_\omega(xx'|y'z) \tag{7}$$

holds for all $x, x', y, y', z \in X$ with $D_\omega(xx'|yy') > D_\omega(xx'|yz)$ and, given any six elements $x, x', y, y',$ and z, z', one has

$$D_\omega(xx'|yz) = D_\omega(xx'|y'z) = D_\omega(xx'|yz') = D_\omega(xx'|y'z') \tag{8}$$

whenever $D_\omega(xx'|yy'), D_\omega(xx'|zz') > D_\omega(xx'|yz)$ holds.

2.3.6 Next, given any two non-empty subsets A and B of X, an X-tree T is said to *display* $A\|B$ (or $A|B$, respectively), if A and B are disjoint and T displays $aa'\|bb'$ (or $aa'|bb'$, respectively) for any two distinct elements $a, a' \in A$ and $b, b' \in B$ or, equivalently, if this holds for some fixed $a \in A$ and $b \in B$ and all $a' \in A - \{a\}$ and $b' \in B - \{b\}$.

If T displays $A\|B$ and $A \cup B = X$ holds, the pair A, B will also be called a *T-split*, and a *non-trivial T-split* if, in addition, $|A|, |B| \geq 2$ holds. Similarly, if T displays $A|B$ and $A \cup B = X$ holds, the pair A, B will also be referred to as a *virtual T-split*, and a *non-trivial* virtual T-split if, in addition, $|A|, |B| \geq 2$ holds.

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[1] Recall that $D_\omega(ab|cd) = \max\{D(a, c) + D(b, d),\ D(a, d) + D(b, c)\} - D(a, b) - D(c, d)$ for $D = D_\omega$.

Notice that if T displays both $A\|B$ and $A'\|B'$ (or $A\|B$ and $A'|B'$ or $A|B$ and $A'\|B'$) then one of the four intersections $A \cap A'$, $A \cap B'$, $B \cap A'$, and $B \cap B'$ is empty. Any two X-splits that satisfy this last property are said to be *compatible*, otherwise they are *incompatible*.

Further, given—in addition—any edge weighting ω of T, we put

$$D_\omega(A|B) := \min \left\{ D_\omega(aa'|bb') : a, a' \in A, b, b' \in B \right\}$$

so that T displays $A\|B$ if and only if $D_\omega(A|B) > 0$ holds for one or, equivalently, for every proper edge weighting ω of T—note that this notation is consistent with our previous notation as, in view of the triangle inequality, we have $D_\omega(aa'|bb') = D_\omega(\{a, a'\}|\{b, b'\})$ for all a, a', b, b' in X.

Clearly, two leaves $a, a' \in X$ form a proper T-cherry if and only if the pair $\{a, a'\}$, $X - \{a, a'\}$ forms a T-split or, equivalently, if and only if T displays $\{a, a'\}\|X - \{a, a'\}$; and they form just a T-cherry if and only if the pair $\{a, a'\}$, $X - \{a, a'\}$ forms a virtual T-split or, equivalently, if and only if T displays $\{a, a'\}|X - \{a, a'\}$. So, both trees depicted in Fig. 2 display the quartet $ac\|de$; and the pair $\{a, b, c\}$, $\{d, e\}$ forms a T_5-split.

2.3.7 It is also well known that an X-tree T displays $A\|B$ for two disjoint non-empty subsets A and B of X if and only if there exists some edge $e \in E$ with $e \in E_T(a|b)$ for all $a \in A$ and $b \in B$ and, hence, if and only if there exists a T-split A^*, B^* of X with $A \subseteq A^*$ and $B \subseteq B^*$. Furthermore, if A, B is a T-split, there is exactly one edge $e = e_{A\|B} \in E$ with $e \in E_T(a|b)$ for all $a \in A$ and $b \in B$. And associating, to each T-split A, B, the edge $e_{A\|B}$ defines a canonical one-to-one correspondence between the collection $\mathcal{S}(T)$ of all T-splits and the edge set E of T as well as between the collection $\mathcal{S}_{nt}(T)$ of all non-trivial T-splits and the set of all interior edges of T.

Furthermore, given any bipartition S' of X into two disjoint and non-empty subsets A', B' of X and any X-tree T, the following assertions are equivalent:

– the pair A', B' forms a virtual T-split;
– $S' = \{A', B'\}$ is compatible with every T-split $S \in \mathcal{S}(T)$;
– there exists an X-tree T' with $\mathcal{S}(T') = \mathcal{S}(T) \cup \{S'\}$ such that collapsing the edge $e_{A'\|B'}$ in T' yields—up to canonical isomorphism—the tree T.

And putting $A(a|bx) := \{a' \in X : a' = a$ or $aa'\|bx \in \mathcal{Q}(T)\}$ for any three distinct elements $a, b, x \in X$, the pair $A(a|bx)$, $X - A(a|bx)$ always forms a T-split and the pair $A(a|bx) \cup A(b|ax)$, $X - (A(a|bx) \cup A(b|ax))$ forms a virtual T-split. Furthermore, there exist, for every T-split $S = A|B$ with $|B| > 1$, two distinct elements $b, x \in B$ such that S coincides with the pair $A(a|bx)$, $X - A(a|bx)$ for one or, equivalently, for every $a \in A$. Also, given any element $x' \in X - \{a, b, x\}$ with $ab\|xx' \in \mathcal{Q}(T)$, one has $a' \in A(a|bx)$ for some $a' \in X - \{a, b, x\}$ if and only if one has $D_\omega(aa'|xx') > D_\omega(ab|xx')$ for some or, equivalently, for every proper edge weighting ω of T. In particular, given any bipartition S of X into two disjoint and non-empty subsets A, B of X, some $a \in A$ and two distinct elements $x, x' \in B$, the pair A, B forms a T-split if and only if one has $D_\omega(aa'|xx') > D_\omega(ab|xx')$ for all $a' \in A$ and $b \in B$ (see Fig. 3).
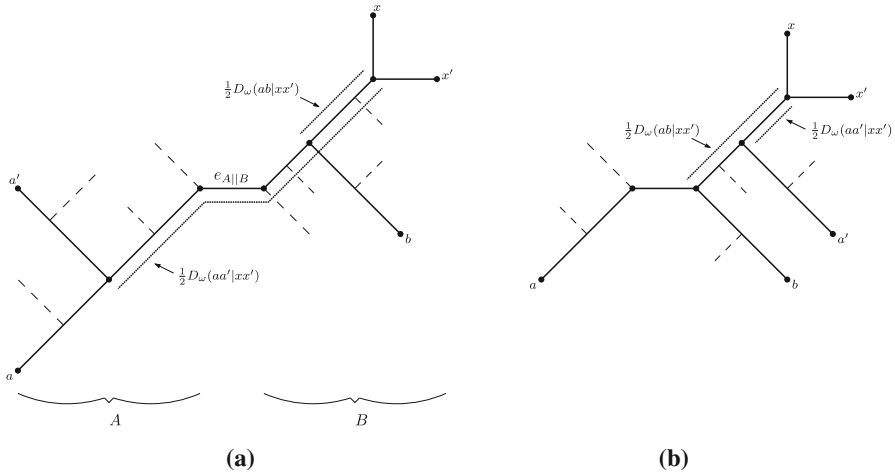
Fig. 3 a When A, B forms a T-split and $x, x' \in B$, then $D_\omega(aa'|xx') > D_\omega(ab|xx')$ holds for all $a, a' \in A$ and $b \in B$. **b** If A, B does not form a T-split, there exists, for all $a \in A$ and $x, x' \in B$, some $a' \in A$ and $b \in B$ with $D_\omega(aa'|xx') \leq D_\omega(ab|xx')$ (see *text* for details)

2.3.8 Finally, it is also well known (see e.g. Semple and Steel 2003) that, given two X-trees T and T', one has

$$T \simeq T' \iff \mathcal{Q}(T) = \mathcal{Q}(T') \iff \mathcal{S}(T) = \mathcal{S}(T') \iff \mathcal{S}_{nt}(T) = \mathcal{S}_{nt}(T')$$

or, more generally,

$$T \leq T' \iff \mathcal{Q}(T) \subseteq \mathcal{Q}(T') \iff \mathcal{S}(T) \subseteq \mathcal{S}(T') \iff \mathcal{S}_{nt}(T) \subseteq \mathcal{S}_{nt}(T').$$

3 Contents and outlook

Our series of papers devoted to a rather detailed study of edge-weight, topological, weak, and strong lassos is organized as follows: In the next section (Sect. 4), we will present some elementary properties and some instructive examples of lasso sets. In Sect. 5, we will present and apply some results that are helpful for investigating lassos in a recursive fashion. In Sect. 6, we will introduce and discuss a useful concept for recognizing strong lassos—the concept of '$\mathcal{L}$-shellability',—and, finally, we will study two particular types of lassos called *e-covers* and *t-covers*, respectively, in Sect. 7—lassos that show up naturally in our context and have, to some extent, already been recognized in previous work (cf. Barthélemy and Guéoche 1991; Chaiken et al. 1983) as exhibiting some particularly attractive and useful properties.

In particular, for any bipartition A, B of X, the set $\mathcal{L} = A \vee B := \{\{a, b\} : a \in A, b \in B\}$ is a topological lasso for an X-tree T if and only if $A \vee B$ is a *t-cover* of T if and only if A, B is incompatible with every non-trivial virtual T-split (Theorem 8).

In a subsequent paper Dress et al. (2011a), we will discuss various classes of examples and 'counter-examples'. In particular, we will present a full characterization of topological lassos for X-trees with at most two interior vertices, we will show that every t-cover of such an X-tree T is a weak lasso for T provided both of its two interior vertices have degree at least 4, and we will classify all edge-weight and all topological lassos for X-trees with at most five leaves. That paper will also show, in particular, that all edge-weight lassos for such a tree are strong lassos and that there are minimal topological lassos for every binary X-tree (V, E) with exactly five leaves (there is 'essentially' only one such tree) that have cardinality $|E| = 7$ while most such lassos are bipartite and have cardinality 6. And, using our recursive approach, we will draw some consequences that are of general interest for lassos for arbitrary X-trees.

In addition, noting that the minimal edge-weight lassos for an X-tree T form the set of bases of a certain matroid with point set $\binom{X}{2}$ denoted by $\mathbb{M}(T)$, we will study this matroid in yet another paper. In particular, we will show that T is determined, up to equivalence, by $\mathbb{M}(T)$, i.e., "$T \simeq T' \iff \mathbb{M}(T) = \mathbb{M}(T')$" holds for any two X-trees T, T'. We will also show that

(i) a binary X-tree T is a caterpillar tree if and only if the matroid $\mathbb{M}(T)$ is a binary matroid,

(ii) a subset $\mathcal{L}$ of $\binom{X}{2}$ is a strong lasso for some X-tree T if and only if it is a non-bipartite topological lasso for T—more generally, the co-rank of some connected subset $\mathcal{L}$ of $\binom{X}{2}$ in $\mathbb{M}(T)$ that is a weak lasso for T never exceeds 1, and it coincides with 1 if and only if $\mathcal{L}$ is bipartite which can happen for T only if every T-cherry is a proper T-cherry, and

(iii) the edge set $\mathcal{L}$ of a complete bipartite graph with vertex set X is a topological lasso if and only if $\mathcal{L}$ has co-rank 1 in $\mathbb{M}(T)$.

We will not deal here with the corresponding 'existence question': Given a subset $\mathcal{L}$ of $\binom{X}{2}$ and some map $D : \mathcal{L} \to X$, when does D extend to a tree metric on X? The computational complexity of this existence question has been settled, as it is nothing but the 'Matrix Completion to Additive' problem that—not unexpectedly—was shown to be NP-complete (Farach et al. 1995, Theorem 6), and algorithmic approaches to special instances of this problem have already been explored in Guénoche and Leclerc (2001), Guénoche et al. (2004), and Willson (2004).

Also, our focus here is on the mathematical, rather than the algorithmic, aspects of the uniqueness question, as the mathematical structure underlying that question appears to be intricate enough already compared with the case settled long ago in which all distances are known. As such, it seems to deserve especially dedicated attention.

4 Some basic properties and some instructive examples of lassos

Assume throughout this section that $T = (V, E)$ is an X-tree and that $\mathcal{L}$ is a subset of $\binom{X}{2}$. Recall that we will often write xy as a shorthand for $\{x, y\}$.

We begin by noting that edge-weight lassos can be characterized in terms of the linear forms their cords induce on the real vector space $\mathbb{R}^E$:

Theorem 1 *The set $\mathcal{L}$ is an edge-weight lasso for T if and only if $X = \bigcup \mathcal{L}$ and there is no non-zero map $\omega_0 \in \mathbb{R}^E$ such that the linear maps*

$$\lambda_{xy}^T : \mathbb{R}^E \to \mathbb{R} : \omega \mapsto \omega_+ (E_T(x|y)) \ (= D_\omega(x, y)) \ \left(xy \in \binom{X}{2} \right) \tag{9}$$

vanish on ω_0 for all $xy \in \mathcal{L}$.

In particular, $|\mathcal{L}| \geq |E|$ must hold for every edge-weight lasso $\mathcal{L}$ for T, and $|\mathcal{L}| = |E|$ must hold for every minimal edge-weight lasso $\mathcal{L}$ for T.

Proof If $(T, \omega) \stackrel{\mathcal{L}}{\equiv} (T, \omega')$ would hold for two distinct proper edge weightings $\omega, \omega' \in \Omega_T$, we would have $\lambda_{xy}^T(\omega_0) = 0$ for all $xy \in \mathcal{L}$ for the map $\omega_0 := \omega - \omega'$. And if, conversely, $\lambda_{xy}^T(\omega_0) = 0$ holds, for all $xy \in \mathcal{L}$, for some non-zero map $\omega_0 \in \mathbb{R}^E$, adding a sufficiently small multiple of ω_0 to any proper edge weighting ω of T would yield a proper edge weighting $\omega' \neq \omega$ of T with $(T, \omega) \stackrel{\mathcal{L}}{\equiv} (T, \omega')$. The last claim follows by applying some basic linear algebra to the bilinear pairing

$$\langle \cdots | \cdots \rangle_T : \mathbb{R}^{\mathcal{L}} \times \mathbb{R}^E \to \mathbb{R} : (\rho, \omega) \mapsto \langle \rho | \omega \rangle_T := \sum_{xy \in \mathcal{L}} \rho(xy) \, \lambda_{xy}^T(\omega).$$

$\square$

We will say that an edge-weight (or a strong) lasso $\mathcal{L}$ for T is *tight* if the number of cords in $\mathcal{L}$ coincides with the number $|E|$ of edges of T or, equivalently, if the bilinear map '$\langle \cdots | \cdots \rangle_T$' defines a proper non-degenerate pairing between $\mathbb{R}^{\mathcal{L}}$ and $\mathbb{R}^E$, i.e., it identifies each of these two vector spaces with the dual of the other.

We now show that $\mathcal{L}$ is connected if $\mathcal{L}$ is a topological lasso for T, and that it is 'strongly non-bipartite'—i.e., every connected component of the graph $\Gamma(\mathcal{L})$ is not bipartite—if $\mathcal{L}$ is an edge-weight lasso for T:

Theorem 2 (i) *If $n \geq 4$ holds and $\mathcal{L}$ is a topological lasso for T, then $\mathcal{L}$ must be connected.*
 (ii) *If $\mathcal{L}$ is an edge-weight lasso for T, then $\mathcal{L}$ must be strongly non-bipartite.*
 (iii) *In particular, $\mathcal{L}$ must be connected and non-bipartite if $\mathcal{L}$ is a strong lasso for T.*

Proof (i) Suppose there exists a bipartition of X into two non-empty disjoint subsets A and B such that $\mathcal{L}$ contains no cord of the form ab with $a \in A$ and $b \in B$. Consider any proper edge weighting ω of T, the two trees $T|_A$ and $T|_B$ obtained by restricting T to A and B, respectively, and the associated edge weightings $\omega|_A$ and $\omega|_B$ of $T|_A$ and $T|_B$. Obviously, we can always form an X-tree T' with a proper edge weighting ω' such that T' is not equivalent to T while $T|_A = T'|_A$ and $T|_B = T'|_B$ as well as $\omega|_A = \omega'|_A$ and $\omega|_B = \omega'|_B$ and, therefore, also $(T, \omega) \stackrel{\mathcal{L}}{\equiv} (T', \omega')$ holds, for example by 'fusing' $T|_A$ and $T|_B$ via any appropriately chosen bridge.

(ii) Suppose that $\mathcal{L}$ contains a connected component that is bipartite relative to some bipartition of its vertex set Y into the two subsets Y^+ and Y^-. Then, the set $\mathcal{L}$ can never be an edge-weight lasso for T as, given any proper edge weighting of T with positive weights on all pendant edges, one can always add some small constant τ to the weights of all pendant edges containing a leaf from Y^+ and subtract the same amount from the weights of all pendant edges containing a leaf from Y^- without changing the distances between any two leaves $x, x' \in X$ with $xx' \in \mathcal{L}$.

(iii) The last assertion is a trivial consequence of the first two assertions. $\square$

Definition Given any cord $\mathfrak{c} = xx' \in \mathcal{L}$, let $\Gamma(\mathcal{L}, \mathfrak{c}) = (X - \mathfrak{c}, \mathcal{L}^{(\mathfrak{c})})$ denote the sub-graph of $\Gamma(\mathcal{L}) = (X, \mathcal{L})$ with vertex set $X - \mathfrak{c}$ and edge set

$$\mathcal{L}^{(\mathfrak{c})} := \{yy' \in \mathcal{L} : yy' \subseteq X - \mathfrak{c}, xx' \| yy' \in \mathcal{Q}(T), \quad \text{and} \quad xy, x'y' \in \mathcal{L} \text{ or } xy', x'y \in \mathcal{L}\}.$$

Clearly, given an edge-weighted X-tree (T', ω') with $(T, \omega) \overset{\mathcal{L}}{\equiv} (T', \omega')$, one has

$$D_\omega(xx'|yy') = D_{\omega'}(xx'|yy') \tag{10}$$

for any two distinct elements $y, y' \in X - \mathfrak{c}$ with $yy' \in \mathcal{L}^{(\mathfrak{c})}$ as if, say, $xy, x'y' \in \mathcal{L}$ holds, one has $D_{\omega'}(x, y) + D_{\omega'}(x', y') = D_\omega(x, y) + D_\omega(x', y') > D_\omega(x, x') + D_\omega(y, y') = D_{\omega'}(x, x') + D_{\omega'}(y, y')$. We claim:

Theorem 3 *Consider a subset $\mathcal{L}$ of $\binom{X}{2}$ with $X = \bigcup \mathcal{L}$ and a cord $\mathfrak{c} = xx' \in \mathcal{L}$, and assume that T is an X-tree. Assume further that the restriction $\Gamma(\mathcal{L}, \mathfrak{c})|_A$ of $\Gamma(\mathcal{L}, \mathfrak{c})$ to any subset A of $X - \mathfrak{c}$ for which $A, X - A$ is a virtual T-split is connected, that ω is a proper edge weighting of T, and that T' is another X-tree with a proper edge weighting ω' such that $(T, \omega) \overset{\mathcal{L}}{\equiv} (T', \omega')$ holds. Then, $D_\omega(xx'|yy') = D_{\omega'}(xx'|yy')$ must hold for any two distinct elements $y, y' \in X - \mathfrak{c}$ with $xx' \| yy' \in \mathcal{Q}(T)$.*

In particular, the subset $\mathcal{L}$ of $\binom{X}{2}$ must be a topological lasso for T if the two elements x, x' in $\mathfrak{c}$ form a proper T-cherry and $\Gamma(\mathcal{L}, \mathfrak{c})|_A$ is connected for any subset A of $X - \mathfrak{c}$ for which $A, X - A$ is a virtual T-split.

Proof Consider two distinct elements $y, y' \in X - \mathfrak{c}$ with $xx' \| yy' \in \mathcal{Q}(T)$. To show that $D_\omega(xx'|yy') = D_{\omega'}(xx'|yy')$ holds, we will use induction relative to the cardinality of the union A of the two disjoint and non-empty subsets $A(y|y'x)$ and $A(y'|yx)$ for which, according to 2.3.7, the split $A, X - A$ is a virtual T-split implying that, in view of our assumptions, the restriction $\Gamma(\mathcal{L}, \mathfrak{c})|_A$ of $\Gamma(\mathcal{L}, \mathfrak{c})$ to $A \subset X - \mathfrak{c}$ is connected. If $|A| = 2$ holds, this implies that $yy' \in \mathcal{L}^{(\mathfrak{c})}$ and, therefore, also $D_\omega(xx'|yy') = D_{\omega'}(xx'|yy')$ must hold.

Otherwise, our induction hypothesis implies that $D_\omega(xx'|ya) = D_{\omega'}(xx'|ya)$ holds for all $a \in X - \{x, x', y, y'\}$ with $ya \| xy' \in \mathcal{Q}(T)$, and that $D_\omega(xx'|y'a') = D_{\omega'}(xx'|y'a')$ holds for all $a' \in X - \{x, x', y, y'\}$ with $y'a' \| xy \in \mathcal{Q}(T)$. Furthermore, our assumption that $\Gamma(\mathcal{L}, \mathfrak{c})|_A$ is connected now implies that there must exist some cord $aa' \in \mathcal{L}^{(\mathfrak{c})}$ and, therefore, $D_\omega(xx'|aa') = D_{\omega'}(xx'|aa')$ with $a \in A(y|y'x)$ and $a' \in A(y'|yx)$. So, our claim holds in case $a = y$ and $a' = y'$. If, say, $a \neq y$ and $a' = y'$ holds, our induction hypothesis implies $D_{\omega'}(xx'|ya) = D_\omega(xx'|ya) > D_\omega(xx'|ay') =$

$D_{\omega'}(xx'|ay')$ and, therefore, $D_\omega(xx'|yy') = D_\omega(xx'|ay') = D_{\omega'}(xx'|ay') = D_{\omega'}(xx'|yy')$ in view of (7). And if $a \neq y$ and $a' \neq y'$ holds, our induction hypothesis implies $D_{\omega'}(xx'|ya) = D_\omega(xx'|ya) > D_\omega(xx'|aa') = D_{\omega'}(xx'|aa')$ and $D_{\omega'}(xx'|y'a') = D_\omega(xx'|y'a') > D_\omega(xx'|aa') = D_{\omega'}(xx'|aa')$ and, therefore, $D_\omega(xx'|yy') = D_\omega(xx'|aa') = D_{\omega'}(xx'|aa') = D_{\omega'}(xx'|yy')$ in view of (8), as claimed.

In particular, if the two elements x, x' in $\mathfrak{c}$ form a proper T-cherry, they must also form one in T', and a bipartition A, B of X with, say, $x \in B$ forms a non-trivial T-split if and only if B contains also x' and $D_\omega(xx'|aa') > D_\omega(xx'|ab)$ or, equivalently, $D_{\omega'}(xx'|aa') > D_{\omega'}(xx'|ab)$ holds for all $a, a' \in A$ and $b \in B$, that is, if and only if A, B forms a non-trivial T'-split. So, $T \simeq T'$ must clearly hold in this case in view of the last remark in 2.3.7. Remarkably, requiring only that $\Gamma(\mathcal{L}, \mathfrak{c})|_A$ is connected in case A, $X - A$ is a T-split, does not even imply that $\mathcal{L}$ is a weak lasso for T. $\qquad\square$

To conclude this section, we now discuss two instructive examples: We have seen above that there exist topological lassos for X-trees (e.g., the tree T_4) that are not edge-weight lassos. To show that, conversely, there exist edge-weight lassos for X-trees that are not topological lassos, consider the 'star tree'

$$T^* = \left(V^* := X \cup \{*\}, E^* := \{\{*, x\} : x \in X\}\right)$$

with leaf set X and exactly one 'central' vertex '$*$' of degree $n \geq 3$ adjacent to all leaves of T^*. While it is obvious that any subset of $\binom{X}{2}$, even the empty set, is a topological lasso for the star tree T^* in case $n = 3$, there is only one topological lasso in case $n \geq 4$, viz., the set $\binom{X}{2}$: Indeed, if ω is, e.g., the 'all-one' map $\mathbf{1}^{E^*}$ and if some cord $ab \in \binom{X}{2}$ is not contained in a subset $\mathcal{L}$ of $\binom{X}{2}$, we may "extract" the two leaves in that cord to form a proper cherry that is attached to a vertex v of degree 3 that in turn is attached to the central vertex $*$ of T^* and adjust the edge length accordingly by putting, say, $\omega'(\{a, v\}) = \omega'(\{b, v\}) = \omega'(\{v, *\}) = 0.5$ and $\omega'(\{x, *\}) = 1$ for all $x \in X - \{a, b\}$ to obtain an X-tree T' with an edge weighting ω' for which $(T^*, \omega) \stackrel{\mathcal{L}}{\equiv} (T', \omega')$ holds. So, no proper subset of $\binom{X}{2}$ can be a topological lasso—and, hence, even less a strong lasso—for T^*.

In contrast, it is easy to see that a subset $\mathcal{L}$ of $\binom{X}{2}$ with $X = \bigcup \mathcal{L}$ is an edge-weight lasso for T^* if and only if it is strongly non-bipartite implying that—in accordance with Theorem 1—any edge-weight lasso for T^* contains at least n cords and that all minimal edge-weight lassos for T^* are tight, i.e., they contain exactly n cords: Indeed, it follows from Theorem 2 (ii) that any edge-weight lasso for any X-tree must be strongly non-bipartite. And, conversely, if a subset $\mathcal{L}$ of $\binom{X}{2}$ is strongly non-bipartite, there exists, for every $x \in X$, some sequence $x_0 := x, x_1, x_2 \ldots, x_{2k}, x_{2k+1} := x, k \geq 0$, consisting of elements from X such that $x_i x_{i+1} \in \mathcal{L}$ holds for all $i = 0, \ldots, 2k$. Thus, if ω, ω' are any two edge weightings of T^* with $(T^*, \omega) \stackrel{\mathcal{L}}{\equiv} (T^*, \omega')$, the sum $\sum_{i=0}^{2k} (-1)^i D_\omega(x_i, x_{i+1}) = \sum_{i=0}^{2k} (-1)^i (\omega(e_{x_i}) + \omega(e_{x_{i+1}})) = 2\omega(e_x)$ must coincide with the sum $\sum_{i=0}^{2k} (-1)^i D_{\omega'}(x_i, x_{i+1}) = 2\omega'(e_x)$ implying that ω and ω' must coincide on all edges of T^*.

Fig. 4 The binary
$\{a, b, c, a', b', c'\}$-tree T_6 for
which $\mathcal{L}_6$ as defined in (11) is an
edge-weight, but not a
topological lasso
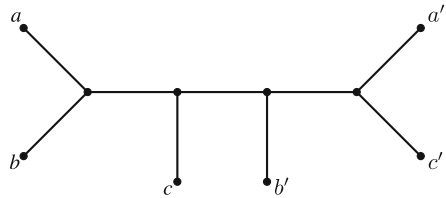
It follows in particular that, in contrast to Assertion (i) in Theorem 2, $\mathcal{L}$ can be disconnected if $\mathcal{L}$ is merely an edge-weight lasso for a (non-binary) X-tree. An example is provided by the star tree with the leaf set $X_6 := \{a, b, c, d, e, f\}$ and the set $\mathcal{L} := \binom{\{a,b,c\}}{2} \cup \binom{\{d,e,f\}}{2}$ which, consisting of two disjoint triangles, is clearly strongly non-bipartite. However, we will see shortly (Corollary 3) that $\mathcal{L}$ must be connected whenever $\mathcal{L}$ is an edge-weight lasso for a binary X-tree.

Finally, we show that there exist edge-weight lassos also for binary X-trees that are not topological lassos: Consider the set $X_6' := \{a, b, c, a', b', c'\}$, the binary X_6'-tree T_6 depicted in Fig. 4, and the subset

$$\mathcal{L}_6 := \binom{\{a, b, c\}}{2} \cup \binom{\{a', b', c'\}}{2} \cup \{aa', bb', cc'\} \tag{11}$$

of $\binom{X_6'}{2}$. $\mathcal{L}_6$ is an edge-weight lasso for T_6, since we can determine, for any proper edge weighting ω of T_6, the values of $D(x, y)$ for the metric $D := D_\omega$ for the six 'missing' cords xy in $\binom{X_6'}{2} - \mathcal{L}_6$ starting from the D-values of the cords in $\mathcal{L}_6$. For example, we have $D(a, b') = D(a, c) + D(b, b') - D(b, c)$, from which we can compute $D(b, a')$ as $D(b, a') = D(a, a') + D(b, b') - D(a, b')$. By symmetry, we can also compute $D(c, a')$ directly from the data and, then, $D(a, c')$ which, finally, allows us to also compute $D(b, c') = D(b, a') + D(a, c') - D(a, a')$ and $D(c, b') = D(c, a') + D(a, b') - D(a, a')$.

However, the example in Fig. 5 shows that $\mathcal{L}_6$ does not lasso the shape of T_6 and, so, is not a strong lasso for T_6.

5 Towards a recursive analysis of lasso sets

In this section, we will establish a result that can be used to analyse lassos recursively: Given an X-tree $T = (V, E)$, we define a non-empty subset U of V to be a T-core if the induced subgraph $T_U := (U, E_U := \{e \in E : e \subseteq U\})$ of T with vertex set U is connected (and, hence, a tree) and the degree $\deg_{T_U}(v)$ of any vertex v in T_U is either 1 or coincides with the degree $\deg_T(v)$ of v in T. Clearly, putting $E_v = E_v^T := \{e \in E : v \in e\}$ and $N_v = N_v^T := \bigcup_{e \in E_v} e$ for every vertex v of T, N_v is a T-core for every $v \in V$, and so is $\bigcup_{v \in U} N_v$ for every subset U of V for which T_U is connected.

It is also obvious that T_U must be an X_U-tree for $X_U := \{y \in U : \deg_{T_U}(y) = 1\}$ for every T-core $U \subseteq V$ as X_U is the leaf set of T_U.
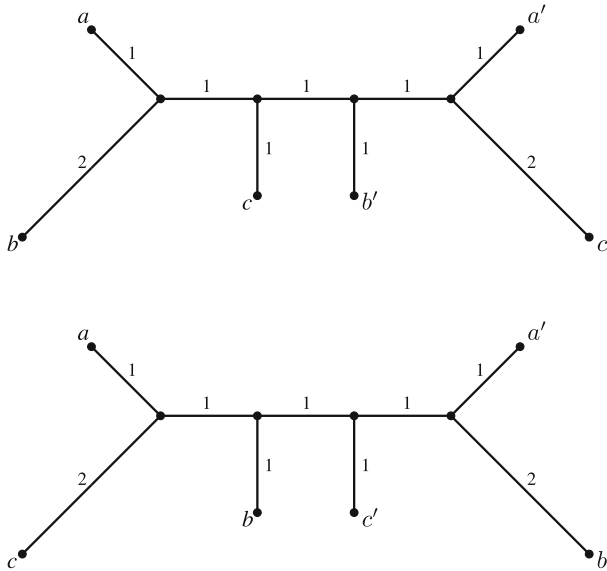
Fig. 5 Although $\mathcal{L}_6$ is an edge-weight lasso for T_6, it fails to be a strong lasso since both of the two edge-weighted trees depicted *above* induce the same distances on all cords in $\mathcal{L}_6$

Further, let x_U denote, for any leaf $x \in X$ of T and any T-core $U \subseteq V$, the *gate* of x in U, i.e., the unique vertex in U that is closest to x. Note that X_U must coincide with the set $gate_U(X) := \{x_U : x \in X\}$ of all gates of the elements of X in U.

Finally, for any subset $\mathcal{L}$ of $\binom{X}{2}$, let $\mathcal{L}_U$ denote the set consisting of all pairs of distinct elements y, y' in X_U for which there exists a cord $xx' \in \mathcal{L}$ with $x_U = y$ and $x'_U = y'$. Then, the following holds:

Theorem 4 *Given an X-tree $T = (V, E)$, a T-core $U \subseteq V$, and a subset $\mathcal{L}$ that is a weak, an edge-weight, a topological, or a strong lasso for T. Then, the set $\mathcal{L}_U$ is, respectively, a weak, an edge-weight, a topological, or a strong lasso for T_U. In particular, the graph $\Gamma(\mathcal{L}_U) = (X_U, \mathcal{L}_U)$ must be strongly non-bipartite for every T-core $U \subseteq V$ whenever $\mathcal{L}$ is an edge-weight lasso for T.*

Proof Indeed, this is a direct consequence of the following simple observation: Given any X_U-tree $T' = (U', F')$ with $U' \cap V = X_U$, the graph T^* with vertex set $V^* := (V - U) \cup U'$ and edge set $E^* := (E - E_U) \cup F'$ obtained by replacing the interior vertices and edges of T_U in T by those of T' is a well-defined X-tree. Furthermore, one has

$$E_{T_U}(x_U|y_U) \subseteq E_T(x|y), \quad E_{T'}(x_U|y_U) \subseteq E_{T^*}(x|y),$$

and

$$E_T(x|y) - E_{T_U}(x_U|y_U) = E_{T'}(x_U|y_U) - E_{T^*}(x|y),$$

for all $x, y \in X$. So, restricting any edge weighting ω of T to the edges of T_U induces an edge weighting ω_U of T_U, and extending any edge weighting ω' of T' to an edge weighting ω^* of T^* by putting $\omega^*(e) := \omega(e)$ for every $e \in E \cap E^* = E - E_U$ yields pairs of edge-weighted X- and X_U-trees such that $(T^*, \omega^*) \overset{\mathcal{L}}{\equiv} (T, \omega)$ if and only if $(T', \omega') \overset{\mathcal{L}_U}{\equiv} (T_U, \omega_U)$. $\qquad\qquad\square$

This theorem has a simple, yet useful consequence. To describe it, we define the following graph.

Definition Given a non-empty subset $\mathcal{L}$ of $\binom{X}{2}$, an X-tree T, and a vertex v of T, let $G(\mathcal{L}, v)$ denote the graph with vertex set E_v and edge set $\mathcal{E}_{\mathcal{L},v}$ consisting of all pairs $\{e, e'\} \in \binom{E_v}{2}$ for which some cord xy in $\mathcal{L}$ with $e, e' \in E_T(x|y)$ exists.

Given any interior vertex $v \in V$, we can apply Theorem 4 to the T-core $U := N_v$ which, together with our results on star trees, yields:

Corollary 1 *Given any interior vertex $v \in V$ and any edge-weight lasso $\mathcal{L}$ for T, the graph $G(\mathcal{L}, v)$ is strongly non-bipartite and is therefore the complete graph with vertex set E_v if $\deg_T(v) = 3$. It is also the complete graph with vertex set E_v independently of the degree of v when $\mathcal{L}$ is a topological lasso for T.*

It follows that a necessary condition for a subset $\mathcal{L}$ of $\binom{X}{2}$ to lasso the edge weights or the shape of an X-tree T is that the graph $G(\mathcal{L}, v)$ is strongly non-bipartite or the complete graph with vertex set E_v, respectively, for every interior vertex v of T.

5.1 The case of a proper cherry a, b

Let us now suppose that a, b is a proper T-cherry for some X-tree $T = (V, E)$ and let $e_{ab} \in E$ denote the unique interior edge of T that is adjacent to $v := v_a = v_b$ so that $E_v = \{e_a, e_b, e_{ab}\}$ holds. Note that the set $U = U_{ab} := V - \{a, b\}$ obtained by deleting the two leaves a, b in the vertex set V of T is a T-core, and that the leaf set X_U of the associated tree T_U with vertex set U coincides with the set $(X - \{a, b\}) \cup \{v\}$. Note also that e_{ab} is the unique pendant edge $e_v^{T_U}$ of T_U containing its leaf v, and that $v = a_U = b_U$, $E_U = E - \{e_a, e_b\}$, and $|E_U| = |E| - 2$ holds.

We pause to introduce some further terminology. Given any non-empty subset $\mathcal{L}$ of $\binom{X}{2}$, put $\mathcal{L}^{ab} := \mathcal{L} - \{ab\}$ and, given in addition any two distinct elements $x, y \in X$, put

$$\delta_{xy \in \mathcal{L}} := \begin{cases} 1, & \text{if } xy \in \mathcal{L}; \\ 0, & \text{otherwise.} \end{cases}$$

Further, let $X(x, \mathcal{L})$ denote the set

$$X(x, \mathcal{L}) := \{y \in X : xy \in \mathcal{L}\}.$$

If ω_U denotes the restriction of an edge weighting $\omega \in \Omega_T$ to E_U, the linear maps λ_{xy}^T introduced above (Eq. 9) satisfy:

$$\lambda_{ax}^T(\omega) = \omega(e_a) + \lambda_{vx}^{T_U}(\omega_U) \quad \text{and} \quad \lambda_{bx}^T(\omega) = \omega(e_b) + \lambda_{vx}^{T_U}(\omega_U) \tag{12}$$

for all $x \in X - \{a, b\}$, and $\lambda_{xy}^T(\omega) = \lambda_{xy}^{T_U}(\omega_U)$ for every cord $xy \in \binom{X - \{a,b\}}{2}$. We also have

$$\mathcal{L}_U = \left(\mathcal{L} \cap \binom{X - \{a, b\}}{2} \right) \cup \left\{ \{x, v\} : x \in X(a, \mathcal{L}^{ab}) \cup X(b, \mathcal{L}^{ab}) \right\}$$

and, therefore, also

$$|\mathcal{L}_U| = |\mathcal{L}| - \delta_{ab \in \mathcal{L}} - |X(a, \mathcal{L}^{ab}) \cap X(b, \mathcal{L}^{ab})| \tag{13}$$

for every subset $\mathcal{L}$ of $\binom{X}{2}$. Thus, if $\mathcal{L}$ is a tight edge-weight lasso for T, we must have

$$\begin{aligned}
|\mathcal{L}| = |E| &= |E_U| + 2 \\
&\le |\mathcal{L}_U| + 2 = |\mathcal{L}| - \delta_{ab \in \mathcal{L}} - |X(a, \mathcal{L}^{ab}) \cap X(b, \mathcal{L}^{ab})| + 2 \\
&= |\mathcal{L}| + 1 - |X(a, \mathcal{L}^{ab}) \cap X(b, \mathcal{L}^{ab})| \le |\mathcal{L}| + 1
\end{aligned}$$

because (i) $\mathcal{L}_U$ must be an edge-weight lasso for T_U according to Theorem 4 and (ii) $ab \in \mathcal{L}$ must hold in this case.

In consequence, the induced edge-weight lasso $\mathcal{L}_U$ for T_U is tight if and only if there exists some (necessarily unique!) leaf $x \in X - \{a, b\}$ with $xa, xb \in \mathcal{L}$. Otherwise, $X(a, \mathcal{L}^{ab}) \cap X(b, \mathcal{L}^{ab}) = \emptyset$ must hold and $\mathcal{L}_U$ has cardinality $|E_U| + 1$ in which case there must exist—up to scaling—exactly one non-zero map $\rho_U : \binom{X_U}{2} \to \mathbb{R}$ with support in $\mathcal{L}_U$ and

$$\sum_{xy \in \binom{X_U}{2}} \rho_U(x, y) \lambda_{xy}^{T_U} = 0.$$

Furthermore, we must have $\alpha := \sum_{x \in X(a, \mathcal{L}^{ab})} \rho_U(x, v) \neq 0$ and $\beta := \sum_{x \in X(b, \mathcal{L}^{ab})} \rho_U(x, v) \neq 0$ for every such non-zero map ρ_U: Indeed, put

$$\rho(x, y) := \begin{cases} \rho_U(x_U, y_U), & \text{if } xy \in \mathcal{L}; \\ 0, & \text{if } xy \in \binom{X}{2} - \mathcal{L}; \end{cases}$$

and note that ρ is a non-zero map with support in $\mathcal{L}$. Note also that—as $\mathcal{L}_U$ is, by assumption, the disjoint union of $\left\{ \{v, x\} : x \in X(a, \mathcal{L}^{ab}) \right\}$, $\left\{ \{v, x\} : x \in X(b, \mathcal{L}^{ab}) \right\}$,

and $\mathcal{L}_U \cap \binom{X-\{a,b\}}{2}$—also

$$\sum_{xy \in \binom{X}{2}} \rho(x, y) \lambda_{xy}^T(\omega)$$

$$= \sum_{xy \in \binom{X-\{a,b\}}{2}} \rho_U(x, y) \lambda_{xy}^{T_U}(\omega_U) + \sum_{x \in X(a, \mathcal{L}^{ab})} \rho(a, x) \left(\lambda_{xv}^{T_U}(\omega_U) + \omega(e_a) \right)$$

$$+ \sum_{x \in X(b, \mathcal{L}^{ab})} \rho(b, x) \left(\lambda_{xv}^{T_U}(\omega_U) + \omega(e_b) \right)$$

$$= \sum_{xy \in \binom{X_U}{2}} \rho_U(x, y) \lambda_{xy}^{T_U}(\omega_U) + \alpha \, \omega(e_a) + \beta \, \omega(e_b)$$

must hold for every map $\omega \in \mathbb{R}^E$. However, noting that $\sum_{xy \in \binom{X_U}{2}} \rho_U(x, y) \lambda_{xy}^{T_U}$ vanishes by our choice of ρ_U, we must (with $\delta_{e_{ab}}$ as defined by Eq. (5)) also have

$$0 = \sum_{xy \in \binom{X_U}{2}} \rho_U(x, y) \lambda_{xy}^{T_U}(\delta_{e_{ab}})$$

$$= \sum_{x \in X(a, \mathcal{L}^{ab})} \rho_U(x, v) + \sum_{x \in X(b, \mathcal{L}^{ab})} \rho_U(x, v)$$

$$= \alpha + \beta$$

So, $\alpha = 0$ would imply that also $\beta = 0$ must hold and, therefore, also

$$\sum_{xy \in \binom{X}{2}} \rho(x, y) \lambda_{xy}^T(\omega) = \sum_{xy \in \binom{X_U}{2}} \rho_U(x, y) \lambda_{xy}^{T_U}(\omega_U) = 0$$

for every map $\omega \in \mathbb{R}^E$, which is impossible if $\mathcal{L}$ is a tight lasso for T.

This yields a good part of the following result.

Theorem 5 *Continuing with the definitions and notations introduced at the start of Sect.* 5.1, *a subset $\mathcal{L}$ of $\binom{X}{2}$ is an edge-weight lasso for T if and only if:*

(U1) *$\mathcal{L}$ contains the cord ab;*

(U2) *$\mathcal{L}_U$ is an edge-weight lasso for T_U; and at least one of the following two assertions **(U3-a)** or **(U3-b)** holds:*

(U3-a) *The two subsets $X(a, \mathcal{L}^{ab})$ and $X(b, \mathcal{L}^{ab})$ of X have a non-empty intersection.*

(U3-b) *There exists some non-zero map $\rho_U : \binom{X_U}{2} \to \mathbb{R}$ with support in $\mathcal{L}_U$ and*

$$\sum_{xy \in \mathcal{L}_U} \rho_U(x, y) \lambda_{xy}^{T_U} = 0 \quad \text{as well as} \quad \sum_{x \in X(a, \mathcal{L}^{ab})} \rho_U(x, u) \neq 0.$$

In particular, a subset $\mathcal{L}$ *of* $\binom{X}{2}$ *is a tight edge-weight lasso for* T *if and only if it has cardinality* $|E|$, *and* **(U1)**, **(U2)**, *and either one of the following two assertions* **(U3-a$'$)** *or* **(U3-b$'$)** *holds:*

(U3-a$'$) $\mathcal{L}_U$ *is a tight edge-weight lasso for* T_U,

(U3-b$'$) $\mathcal{L}_U$ *has cardinality* $|E_U|+1 = |\mathcal{L}| - 1$ *and* $\sum_{x \in X(a, \mathcal{L}^{ab})} \rho_U(x, u) \neq 0$ *holds for every non-zero map* $\rho_U \; : \; \binom{X_U}{2} \to \mathbb{R}$ *with support in* $\mathcal{L}_U$ *for which* $\sum_{xy \in \mathcal{L}_U} \rho_U(x, y) \lambda_{xy}^{T_U} = 0$ *holds.*

Proof In view of our observations above applied to any tight lasso for $T = (V, E)$ contained in $\mathcal{L}$, it suffices to show that a subset $\mathcal{L}$ of $\binom{X}{2}$ is an edge-weight lasso for T if **(U1)**, **(U2)**, and at least one of the assertions **(U3-a)** or **(U3-b)** hold.

So, assume that, for some map $\eta \in \mathbb{R}^E$, one has $\lambda_{xy}^T(\eta) = 0$ for all cords $xy \in \mathcal{L}$. We have to show that $\eta(e) = 0$ must hold for every edge $e \in E$. To this end, note first that to establish our claim, it suffices, in view of (12), to show that, if **(U1)**, **(U2)**, and either **(U3-a)** or **(U3-b)** hold, then $\eta(e_a) = \eta(e_b) = 0$ must hold for every map $\eta \in \mathbb{R}^E$ as above.

Yet, if **(U3-a)** holds (i.e., if $xa, xb \in \mathcal{L}$ holds for some $x \in X - \{a, b\}$), the assumption that $\lambda_{xy}^T(\eta) = 0$ holds for some $\eta \in \mathbb{R}^E$ and for all cords $xy \in \mathcal{L}$ implies that the following hold:

$$0 = \lambda_{ab}^T(\eta) = \eta(e_a) + \eta(e_b),$$
$$0 = \lambda_{ax}^T(\eta) = \eta(e_a) + \lambda_{ux}^T(\eta_U),$$
$$0 = \lambda_{bx}^T(\eta) = \eta(e_b) + \lambda_{ux}^T(\eta_U).$$

This readily implies $\eta(e_a) = \eta(e_b) = 0$ in this case (since we may add the first equation to either the second or the third one, and subtract the other one).

Moreover, if **(U1)** and **(U2)** hold, if $\sum_{xy \in \binom{X_U}{2}} \rho_U(x, y) \lambda_{xy}^{T_U} = 0$ and also $\sum_{x \in X(a, \mathcal{L}^{ab})} \rho_U(x, u) \neq 0$ holds for some non-zero map $\rho_U : \binom{X_U}{2} \to \mathbb{R}$, and if $\lambda_{xy}^T(\eta) = 0$ holds for all $xy \in \mathcal{L}$ for some map $\eta \in \mathbb{R}^E$, we must have

$$\lambda_{ux}^{T_U}(\eta_U) = -\eta(e_a) \quad \text{for all } x \in X(a, \mathcal{L}^{ab}),$$
$$\lambda_{ux}^{T_U}(\eta_U) = -\eta(e_b) \quad \text{for all } x \in X(b, \mathcal{L}^{ab}),$$

and

$$\rho_U(x, y) \lambda_{xy}^{T_U}(\eta_U) = 0 \quad \text{for all } xy \in \binom{X - \{a, b\}}{2}.$$

Thus, evaluating the identity $\sum_{xy \in \mathcal{L}_U} \rho_U(x, y) \lambda_{xy}^{T_U} = 0$ on η_U and noting that $\mathcal{L}_U$ is, by assumption, the disjoint union of $\{\{v, x\} : x \in X(a, \mathcal{L}^{ab})\}$, $\{\{v, x\} : x \in X(b, \mathcal{L}^{ab})\}$,

and $\mathcal{L}_U \cap \binom{X-\{a,b\}}{2}$, we get:

$$0 = \sum_{x \in X(a, \mathcal{L}^{ab})} -\rho_U(v, x)\eta(e_a) + \sum_{x \in X(b, \mathcal{L}^{ab})} -\rho_U(v, x)\eta(e_b)$$

$$= -\eta(e_a) \left(\sum_{x \in X(a, \mathcal{L}^{ab})} \rho_U(v, x) \right) - \eta(e_b) \left(\sum_{x \in X(b, \mathcal{L}^{ab})} \rho_U(v, x) \right).$$

Furthermore, evaluating the identity $\sum_{xy \in \binom{X_U}{2}} \rho_U(x, y)\lambda_{xy}^{T_U} = 0$ on the map $\delta_{e_{ab}}$ (Eq. 5) also yields the following:

$$0 = \sum_{x \in X-\{a,b\}} \rho_U(v, x) = \sum_{x \in X(a, \mathcal{L}^{ab})} \rho_U(v, x) + \sum_{x \in X(b, \mathcal{L}^{ab})} \rho_U(v, x)$$

and, therefore, the following holds:

$$0 = (\eta(e_b) - \eta(e_a)) \sum_{x \in X(a, \mathcal{L}^{ab})} \rho_U(u, x).$$

So, our assumption $\sum_{x \in X(a, \mathcal{L}^{ab})} \rho_U(x, v) \neq 0$ implies $0 = \eta(e_b) - \eta(e_a)$ which, together with $0 = \lambda_{ab}^T(\eta) = \eta(e_a) + \eta(e_b)$, implies that also in this case $0 = \eta(e_a) = \eta(e_b)$ must hold, as claimed. $\qquad\square$

Our observations imply also that we can construct all the tight edge-weight lassos of T from the edge-weight lassos $\mathcal{L}'$ of T_U with $|\mathcal{L}'| \leq |E_U| + 1$ as follows:

Corollary 2 (i) *Given any tight edge-weight lasso $\mathcal{L}'$ of T_U, there is a canonical one-to-one correspondence between all tight edge-weight lassos $\mathcal{L}$ of T with $\mathcal{L}_U = \mathcal{L}'$ and all pairs of subsets A, B of $X_U(v, \mathcal{L}')$ with $|A \cap B| = 1$.*

(ii) *Furthermore, given any edge-weight lasso $\mathcal{L}'$ of T_U of cardinality $|E_U| + 1$, there is a canonical one-to-one correspondence between all tight edge-weight lassos $\mathcal{L}$ of T with $\mathcal{L}_U = \mathcal{L}'$ and all pairs of disjoint subsets A, B of $X_U(v, \mathcal{L}')$ for which $\sum_{x \in A} \rho_U(x, v) \neq 0$ holds for one (or, equivalently, every) non-zero map $\rho_U : \binom{X_U}{2} \to \mathbb{R}$ with support in $\mathcal{L}'$ for which $\sum_{xy \in \binom{X_U}{2}} \rho_U(x, y)\lambda_{xy}^{T_U} = 0$ holds.*

In both cases, the correspondence is given by associating to each pair A, B, the set:

$$\mathcal{L}'_{A,B} := \left(\mathcal{L}' \cap \binom{X - \{a, b\}}{2} \right) \cup \{ax : x \in A \cup \{b\}\} \cup \{bx : x \in B\}.$$

As a second consequence of Theorem 5, we have the following result already indicated in the remark at the end of Sect. 4.

Corollary 3 *If $\mathcal{L}$ is an edge-weight lasso for a binary X-tree, then $(X, \mathcal{L})$ is a connected graph.*

6 Shellability

In this section, we introduce a concept that relates to strong lassos and will apply in particular in the discussion of all edge-weight lassos for X-trees with $|X| = 5$ and other examples in Dress et al. (2011a): Given a subset $\mathcal{L}$ of $\binom{X}{2}$ with $X = \bigcup \mathcal{L}$, and an X-tree T, we say that $\binom{X}{2} - \mathcal{L}$ is T-*shellable* if there exists a labelling of the cords in $\binom{X}{2} - \mathcal{L}$ as, say, $a_1 b_1, a_2 b_2, \ldots, a_m b_m$ such that, for every $\mu \in \{1, 2, \ldots, m\}$, there exists a pair x_μ, y_μ of 'pivots' for $a_\mu b_\mu$, i.e., two distinct elements $x_\mu, y_\mu \in X - \{a_\mu, b_\mu\}$, for which the tree $T|_{Y_\mu}$ obtained from T by restriction to $Y_\mu := \{a_\mu, b_\mu, x_\mu, y_\mu\}$, is a quartet tree of type $a_\mu x_\mu \| y_\mu b_\mu$, and all cords in $\binom{Y_\mu}{2}$ except $a_\mu b_\mu$ are contained in $\mathcal{L}_\mu := \mathcal{L} \cup \{a_{\mu'} b_{\mu'} : \mu' \in \{1, 2, \ldots, \mu - 1\}\}$. Any such labelling of $\binom{X}{2} - \mathcal{L}$ will also be called a T-*shelling* of $\binom{X}{2} - \mathcal{L}$, and any subset $\mathcal{L}$ of $\binom{X}{2}$ for which a T-*shelling* of $\binom{X}{2} - \mathcal{L}$ exists will also be called an *s-lasso for T*.

6.1 Example

Consider the caterpillar tree T_5 on X_5 depicted in Fig. 2. We claim that the set $\mathcal{L} := \{ab, bc, cd, de, ea, ad, ac\}$, is an *s*-lasso for T_5: Indeed, labelling the elements in the cords in $\binom{X}{2} - \mathcal{L} = \{bd, be, ce\}$ as

$$a_1 := c, b_1 := e; \quad a_2 := b, b_2 := e; \quad \text{and} \quad a_3 := b, b_3 := d$$

yields a T_5-shelling of $\binom{X}{2} - \mathcal{L}$ because, choosing the elements

$$x_1 := a, y_1 := d; \quad x_2 := a, y_2 := c; \quad \text{and} \quad x_3 := a, y_3 := e$$

as pivots, the quartet trees $T_5|_{Y_\mu}$ are indeed quartet trees of type $a_\mu x_\mu \| b_\mu y_\mu$ for $Y_\mu = \{a_\mu, b_\mu, x_\mu, y_\mu\}$, $\mu = 1, 2, 3$, as required, and all cords in $\binom{Y_\mu}{2}$ except $a_\mu b_\mu$ are contained in $\mathcal{L}_\mu = \mathcal{L} \cup \{a_{\mu'} b_{\mu'} : \mu' \in \{1, 2, \ldots, \mu - 1\}\}$ for all $\mu = 1, 2, 3$. Thus, listing the cords in $\binom{X}{2} - \mathcal{L}$ 'anti-lexicographically' in the order ce, be, bd yields a T_5-shelling of $\binom{X}{2} - \mathcal{L}$, implying that $\mathcal{L}$ is an *s*-lasso for T_5 as claimed. □

We now establish the following simple, yet sometimes rather helpful result:

Theorem 6 *Every s-lasso* $\mathcal{L} \subseteq \binom{X}{2}$ *for an X-tree T is a strong lasso for T.*

Proof Given a T-shelling $a_1 b_1, a_2 b_2, \ldots, a_m b_m$ of $\binom{X}{2} - \mathcal{L}$ with corresponding pivots $x_1, y_1; x_2, y_2; \ldots; x_m, y_m$, we can compute, for every proper edge weighting ω of T, the distances $D_\omega(a_\mu, b_\mu)$ for all $\mu \in \{1, 2, \ldots, m\}$ recursively, because:

$$D_\omega(a_\mu, b_\mu) = D_\omega(a_\mu, y_\mu) + D_\omega(b_\mu, x_\mu) - D_\omega(x_\mu, y_\mu)$$

must hold in view of the fact that, by assumption,

$$D_\omega(a_\mu, x_\mu) + D_\omega(b_\mu, y_\mu) < D_\omega(a_\mu, b_\mu) + D_\omega(x_\mu, y_\mu)$$

must hold. □

The converse to Theorem 6 does not hold, that is, there exists an X-tree T and a strong lasso for T that is not an s-lasso for T, as the following example shows.

6.2 Example

Put $X_7 := \{a, b, c, d, e, f, g\}$, and let T_7 denote the binary X_7-tree with exactly two proper cherries a, b and f, g, and the three 'single' leaves c, d, e. Assume furthermore that the corresponding adjacent vertices v_c, v_d, v_e are passed in this order on the path connecting the cherry a, b with f, g. Then, the bipartite set

$$\mathcal{L}_7 := \{ab, ad, bc, be, cd, cf, de, dg, ef, fg\}$$

is a topological lasso for T_7 since any X_7-tree T' with $(T_7, \omega) \stackrel{\mathcal{L}_7}{\cong} (T', \omega')$ for some proper edge weightings $\omega \in \Omega_{T_7}$ and $\omega' \in \Omega_{T'}$ must display the quartets $ab\|cd$, $bc\|de$, $cd\|ef$, and $de\|fg$ which is well known to imply that T_7 and T' must be equivalent (see e.g. Böcker et al. 1999 or Dress et al. 2011b). It follows that adding the cord ag to $\mathcal{L}_7$ yields an edge-weight lasso for T_7, since the associated 11×11 incidence matrix of paths (one for each cord) and edges of T_7 has full rank. Thus $\mathcal{L} = \mathcal{L}_7 \cup \{ag\}$ is a strong lasso for T_7 which, however, is easily seen not to be an s-lasso for T_7 as there exists not even any 4-subset Y of X_7 with $|\binom{Y}{2} \cap \mathcal{L}| \geq 5$.

7 Covers of binary X-trees

Recall that, by Corollary 1, a necessary condition for a subset $\mathcal{L}$ of $\binom{X}{2}$ to lasso the edge weights (or, respectively, the shape) of a tree T is that, for every interior vertex v of T, the graph $G(\mathcal{L}, v)$ defined above is strongly non-bipartite (or, respectively, a complete graph). This suggests the following:

Definition A subset $\mathcal{L}$ of $\binom{X}{2}$ is an *e-cover* of T if X coincides with $\bigcup \mathcal{L}$ and $G(\mathcal{L}, v)$ is strongly non-bipartite for every interior vertex v of T, and it is called a *t-cover* of T if $X = \bigcup \mathcal{L}$ holds and $G(\mathcal{L}, v)$ is a complete graph for every interior vertex v of T—see Fig. 6(i) below for an illustration.

In the first part of this section, we restrict our attention to covers of binary X-trees. Clearly, e- and t-covers coincide for such trees—so, we will just call them covers in this case.

By definition (and Corollary 1), every edge-weight lasso for an X-tree T is an e-cover of T. The converse, however, does not hold, not even for binary X-trees. For example, the topological lasso $\mathcal{L}_4 = \{ab, ac, bd, cd\}$ for the quartet tree T_4 of type $ab\|cd$ depicted in Fig. 1 is clearly a cover for T_4, but—in view of $|\mathcal{L}| < |E|$—it does not lasso the edge weights of T.

Note also that, if $\mathcal{L}$ is a topological lasso for T, then $\mathcal{L}$ must also be a t-cover of T. However, once again, the converse does not hold; for example, the subset

$$\mathcal{L}'_6 := \{ab, ac, a'b', a'c', bb', cc'\} \tag{14}$$
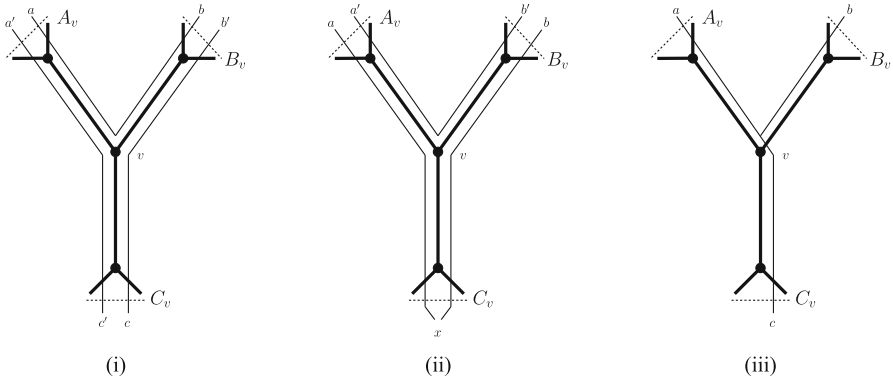
Fig. 6 **i** The three cords ab, $b'c$, and $c'a'$ provide a 'cover of the degree 3 vertex v'. **ii** The three cords ax, bx, and $a'b'$ provide a 'pointed cover of v'. **iii** The three cords ab, bc, and ca provide a 'triplet cover of v'. It is possible for $a = a'$ or $b = b'$ (in cases **i** and **ii**) and also $c = c'$ (in case **i**) (see *text* for details)

of $\mathcal{L}_6$ as defined in (11) is a cover for the two non-equivalent binary X'_6-trees depicted in Fig. 5.

More strikingly, $\mathcal{L}_6$ itself is, thus, both an edge-weight lasso and a t-cover for T_6, yet $\mathcal{L}_6$ fails to lasso the shape of this tree.

We now describe two particular types of covers: Given a binary X-tree $T = (V, E)$, we will say that a subset $\mathcal{L}$ of $\binom{X}{2}$ is a *triplet cover* of T if, for every interior vertex $v \in V$ of T, there exist three distinct leaves a, b, c with $ab, ac, bc \in \mathcal{L}$ and $v = \text{med}_T(a, b, c)$ (see Fig. 6(iii) for an illustration of this concept). Note that a triplet cover of a binary X-tree T can be represented as a collection $\mathcal{C}$ of 3-element subsets of X with $\bigcup \mathcal{C} = X$ and with the property that the function that assigns each triplet to its associated median vertex in T maps $\mathcal{C}$ surjectively onto the set of interior vertices of T. A combinatorial characterization of arbitrary collections $\mathcal{C}$ of 3-element subsets of X with $\bigcup \mathcal{C} = X$ for which this function is injective for some binary X-tree is simply, as described recently in Dress and Steel (2009), that $|\bigcup \mathcal{C}'| \geq |\mathcal{C}'| + 2$ holds for all non-empty subsets $\mathcal{C}'$ of $\mathcal{C}$.

Secondly, given an element $x \in X$, a subset $\mathcal{L}$ of $\binom{X}{2}$ is called a *pointed x-cover* of a binary phylogenetic X-tree T if it is a cover of T and there exist, for each interior vertex v of T, two distinct leaves $a, b \in X$ with $ax, bx \in \mathcal{L}$ and $v = \text{med}_T(a, b, x)$ (see Fig. 6(ii) for an illustration). Moreover, it is called just a pointed cover of T if there exists some $x \in X$ such that $\mathcal{L}$ is a pointed x-cover of T.

Clearly, every triplet and every pointed cover of T is, in particular, a cover of T. To present some examples of triplet and pointed covers, recall first that a *circular ordering* of (the leaf set X of) an X-tree T is a cyclic permutation σ of the elements in X for which there exists a planar embedding of T such that, for every $x \in X$, the leaf that follows the leaf x when one traverses the leaves of T in that embedding in, say, a clockwise fashion is the leaf $\sigma(x)$. An equivalent characterization is that each edge of T is covered only twice by the paths connecting the n pairs of leaves in the set $\{\{x, \sigma(x)\} : x \in X\}$. For example, there exist planar embeddings of the two X'_6-trees depicted in Fig. 5 such that the permutation (a, b, b', a', c', c) is a circular ordering
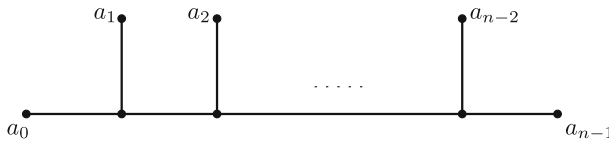
Fig. 7 A caterpillar tree for which $(a_0, a_1, \ldots, a_{n-2}, a_{n-1})$ is a circular ordering

for both of them, while the permutation (a, b, a', c', b', c) is a circular ordering for T_6 (under a different planar embedding), but not for the other X_6'-tree depicted in that figure under any planar embedding (as the three paths connecting the three pairs b and a', a' and c', and c' and b' share one edge). For more details on circular orderings, see Semple and Steel (2003).

Now, let $(a_0, a_1, \ldots, a_{n-2}, a_{n-1})$ be a circular ordering for a binary X-tree $T = (V, E)$, and put

$$\mathcal{L} := \{a_0 a_i : i = 1, \ldots, n-1\} \cup \{a_{i-1} a_i : i = 2, \ldots, n-1\}.$$

Then, $|\mathcal{L}| = |T| = 2n - 3$ holds and $\mathcal{L}$ is a triplet as well as a pointed a_0-cover of T, and it is a well-known fact that $\mathcal{L}$ lassos the edge weights of T (see Proposition 2.3 of Barthélemy and Guéoche 1991 or Chaiken et al. 1983 for the case where $\omega(e) = 1$ for all $e \in E$).

Further, if T is a caterpillar tree with the two cherries a_0, a_1 and a_{n-2}, a_{n-1} and $(a_0, a_1, \ldots, a_{n-2}, a_{n-1})$ is a circular ordering for T relative to the planar embedding of T that is indicated in Fig. 7, then the union $\mathcal{L}$ of the sets $\{a_0 x : x \in X, x \neq a_0\}$ and $\{a_{n-1} x : x \in X, x \neq a_{n-1}\}$ is a triplet as well as a pointed a_0-cover of T for which $|\mathcal{L}| = |E| = 2n - 3$ holds.

Theorem 5 implies the following result.

Proposition 1 *Every triplet cover $\mathcal{L}$ of a binary X-tree T lassos the edge weights for T. Furthermore, $(T, \omega) \equiv (T', \omega')$ must hold for every proper edge weighting ω of T and every pair (T', ω') that consists of an X-tree T' and an edge weighting ω' of T' such that $\mathcal{L}$ is also a triplet cover of T' and $(T, \omega) \stackrel{\mathcal{L}}{\equiv} (T', \omega')$ holds.*

Proof Choose any T-cherry a, b and note that, with $U = U_{ab} := V - \{a, b\}$ and all the notations and conventions introduced in the context of Theorem 5, the subset $\mathcal{L}_U$ of $\binom{X_U}{2}$ is a triplet cover of X_U whenever $\mathcal{L}$ is a triplet cover of T. Thus, we may assume that, by induction, $\mathcal{L}_U$ satisfies our claims for T_U. Moreover, every triplet cover $\mathcal{L}$ of T must contain the cord ab and there must exist some $c \in X - \{a, b\}$ with $ac, bc \in \mathcal{L}$. So, all the assertions **(U1)**, **(U2)**, and **(U3-a)** must hold for $\mathcal{L}$, implying that $\mathcal{L}$ is indeed an edge-weight lasso for T.

Furthermore, given any proper edge weighting ω of T, the pair a, b must form a T'-cherry in every X-tree T' for which $\mathcal{L}$ is also a triplet cover of T' and an edge weighting ω' of T' with $(T, \omega) \stackrel{\mathcal{L}}{\equiv} (T', \omega')$ exists. Indeed, it is obvious that, given any triple a', b', c' of distinct leaves with $a'b', a'c', b'c' \in \mathcal{L}$, the interior vertex $\text{med}_T(a', b', c')$
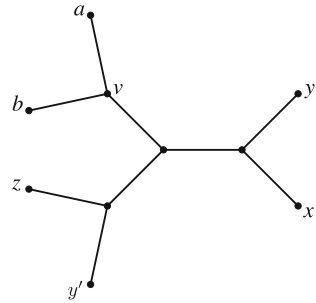
is adjacent to a' in T if and only if we have

$$D_\omega(a'a'|b'c') = \min(D_\omega(a'a'|yz) : y, z \in X - \{a'\}; a'y, a'z, yz \in \mathcal{L}),$$

(note that, by definition (cf. 2), $D_\omega(aa|bc) = D_\omega(a, b) + D_\omega(a, c) - D_\omega(b, c)$ holds for all $a, b, c \in X$). Thus, if $\text{med}_T(a', b', c')$ is adjacent to a' for some $a', b', c' \in X$ as above, this must also be true for the vertex $\text{med}_{T'}(a', b', c')$ in T', provided that $(T, \omega) \stackrel{\mathcal{L}}{\equiv} (T', \omega')$ holds. In particular, the pair a, b must form a T'-cherry if it forms a T-cherry and $(T, \omega) \stackrel{\mathcal{L}}{\equiv} (T', \omega')$ holds. It follows that $(T_U, \omega_U) \stackrel{\mathcal{L}_U}{\equiv} (T'_U, \omega'_U)$ must also hold and, by induction, therefore $(T_U, \omega_U) \equiv (T'_U, \omega'_U)$ also holds, which easily implies our claim $(T, \omega) \equiv (T', \omega')$. □

Regarding pointed covers, even a stronger result holds:

Theorem 7 *If a subset $\mathcal{L}$ of $\binom{X}{2}$ is a pointed cover of a binary X-tree T, then $\mathcal{L}$ is an s-lasso and, hence, a strong lasso for T. More specifically, if $\mathcal{L}$ is a pointed x-cover of T for some $x \in X$, then there exists an "x-shelling" $a_1b_1, a_2b_2, \ldots a_mb_m$ of $\binom{X}{2} - \mathcal{L}$, i.e., a shelling such that, for every $\mu = 1, \ldots, m$, one of the two pivots x_μ, y_μ for $a_\mu b_\mu$ can be chosen to coincide with x.*

Proof Clearly, we may assume, without loss of generality, that $n \geq 5$ holds. Consider a (necessarily proper) T-cherry a, b not containing x. As above, we put $U = U_{ab} := V - \{a, b\}$ and use all the notations and conventions introduced in the context of Theorem 5.

First note that, if we have any two distinct elements $y, z \in X - \{x, a, b\}$, the tree $T|_{\{a,b,x,y\}}$ obtained from T by restriction to $\{a, b, x, y\}$ is always a quartet tree of type $ab\|xy$. Moreover, the two trees $T|_{\{a,x,y,z\}}$ and $T|_{\{b,x,y,z\}}$ obtained from T by restriction to $\{a, x, y, z\}$ and $\{b, x, y, z\}$ are, respectively, quartet trees of type $xy\|az$ and $xy\|bz$ in case the tree $T_U|_{\{v,x,y,z\}}$ obtained from T_U by restriction to $\{v, x, y, z\}$ is a quartet tree of type $xy\|vz$, and these two trees are, respectively, quartet trees of type $xa\|yz$ and $xb\|yz$ in case $T_U|_{\{v,x,y,z\}}$ is a quartet tree of type $xv\|yz$—see Fig. 8 for an illustration.

Now assume that $\mathcal{L} \subseteq \binom{X}{2}$ is a pointed x-cover of T for some leaf $x \in X$. It is obvious that $\mathcal{L}_U$ is an pointed x-cover of T_U. So, by induction, there must exist a shelling $a_1b_1, a_2b_2, \ldots, a_mb_m$ of $\binom{X_U}{2} - \mathcal{L}_U$ such that, for every $\mu \in \{1, 2, \ldots, m\}$,

there exists some element y_μ in $X_U - \{x, a_\mu, b_\mu\}$ for which the tree $T_U|_{\{a_\mu, b_\mu, x, y_\mu\}}$ obtained from T_U by restriction to $\{a_\mu, b_\mu, x, y_\mu\}$ is a quartet tree of type $a_\mu x \| y_\mu b_\mu$ and all cords in $\binom{\{a_\mu, b_\mu, x, y_\mu\}}{2}$ except $a_\mu b_\mu$ are contained in $\mathcal{L}_{U,\mu} := \mathcal{L}_U \cup \{a_{\mu'} b_{\mu'} : \mu' \in \{1, 2, \ldots, \mu - 1\}\}$. So, to produce an x-shelling of $\binom{X}{2} - \mathcal{L}$, we may first take all cords in $\binom{X}{2} - \mathcal{L}$ of the form ay with $by \in \mathcal{L}$ and use b as their second pivot.

Noting that the tree $T|_{\{a, b, x, y\}}$ is a quartet tree of type $ab \| xy$ and that all cords in $\binom{\{a, b, x, y\}}{2}$ except for ay, are contained in $\mathcal{L}$, we can take these cords in any order.

Then, we take all cords in $\binom{X}{2} - \mathcal{L}$ of the form by with $ay \in \mathcal{L}$ in any order and use a as their second pivot, which works for the same reason. Then, for each $\mu = 1, 2, \ldots, m$ with $v \notin \{a_\mu, b_\mu, y_\mu\}$, we take the cord $a_\mu b_\mu$ and use y_μ as its second pivot. In case $y_\mu = v$, we take the cord $a_\mu b_\mu$ and use a or b as its second pivot. In case $a_\mu = v$, we take the cord ab_μ and use y_μ as the second pivot and then add the cord bb_μ, taking a as the second pivot. And finally, in case $b_\mu = v$, we switch a_μ and b_μ and, otherwise, proceed as above. Now, a simple inductive argument shows that this defines an x-shelling of $\binom{X}{2} - \mathcal{L}$ as required. $\qquad\square$

Our earlier Example 6.1 illustrates Theorem 7, as $\{ab, bc, cd, de, ea, ad, ac\}$ is obviously a pointed a-cover of T_5.

Let us finally return to the general setting of (not necessarily binary) X-trees and consider subsets $\mathcal{L}$ of $\binom{X}{2}$ that are of the form

$$\mathcal{L} = A \vee B := \{\{a, b\} : a \in A, b \in B\}$$

for some X-split A, B. For example (cf. Fig. 1), the topological lasso $\mathcal{L}_4$ for T_4 is of this form as it coincides with $\{a, d\} \vee \{b, c\}$.

It follows immediately from our definitions that, given any 2-subset $\mathfrak{c} = \{x, x'\}$ of X with $x \in A$ and $x' \in B$ and any subset Y of $X - \mathfrak{c}$, the restriction $\Gamma(\mathcal{L}, \mathfrak{c})|_Y$ of the graph $\Gamma(\mathcal{L}, \mathfrak{c})$ introduced in Sect. 4 is the complete bipartite graph with vertex set Y whose edge set is $(A \cap Y) \vee (B \cap Y)$. Thus, it is connected if and only if one has either $|Y| = 1$ or neither $A \cap Y$ nor $B \cap Y$ are empty. And it is also obvious that, whenever $\mathcal{L} = A \vee B$ is a t-cover of an X-tree T, one must have $A \cap \mathfrak{c} \neq \emptyset \neq B \cap \mathfrak{c}$ for every 2-subset $\mathfrak{c}$ of X whose elements form a T-cherry.

$\mathcal{L}$ can therefore only be a t-cover of an X-tree T if there exist no three distinct leaves a, b, c of T with $v_a = v_b = v_c$. Thus, Theorem 3 implies the following characterization of topological lassos $\mathcal{L}$ that are of the form $\mathcal{L} = A \vee B$ for some X-split A, B:

Theorem 8 *Given an X-tree T and an X-split A, B of X, the following four assertions are equivalent:*

(i) *The subset $A \vee B$ of $\binom{X}{2}$ is a topological lasso for T.*
(ii) *$A \vee B$ is a t-cover of T.*
(iii) *$A \cap \mathfrak{c} \neq \emptyset \neq B \cap \mathfrak{c}$ holds for every 2-subset $\mathfrak{c}$ of X whose elements form a T-cherry.*
(iv) *The bipartition A, B of X is incompatible with every non-trivial virtual T-split.*

Proof It is obvious from the definitions and previously recorded facts that "(i) $\Rightarrow$ (ii) $\Rightarrow$ (iii)" holds. The implication "(iii) $\Rightarrow$ (iv)" holds because any subset A' of X for which $A', X - A'$ is a non-trivial virtual T-split must contain two elements that form a T-cherry.

And "(iv) $\Rightarrow$ (i)" holds in view of Theorem 3: First observe that there exists always a 2-subset $\mathfrak{c}$ of X whose elements form a proper T-cherry.[2] Note next that, for any such 2-subset $\mathfrak{c}$, there must exist $x \in A$ and $x' \in B$ with $\mathfrak{c} = \{x, x'\}$ (as A, B is supposed to be incompatible with every non-trivial virtual T-split and, hence, in particular with the T-split $\mathfrak{c}, X - \mathfrak{c}$), and that (for the same reason) $A \cap Y \neq \emptyset \neq B \cap Y$ must hold for every subset Y of $X - \mathfrak{c}$ for which $Y, X - Y$ is a non-trivial virtual T-split implying that $\Gamma(\mathcal{L}, \mathfrak{c})|_Y$ must be connected (as required in Theorem 3). $\qquad\square$

8 Remarks and questions

Our results raise further questions concerning the properties of different types of lassos:

- Q1. Does there exist a triplet cover of a *binary* tree that is not a strong lasso?
- Q2. Can we characterize those covers of a binary X-tree T that are a tight edge-weight or strong lasso of T?

Regarding the second question, two necessary conditions for a cover of a binary X-tree T of cardinality $2n - 3$ to lasso the edge weights of T are as follows:

- For each subset Y of X of cardinality m, the cardinality of $\mathcal{L} \cap \binom{Y}{2}$ cannot exceed $2m - 3$ (to avoid over-determination at Y).
- If $ab, bc, cd, da \in \mathcal{L}$ holds for some four leaves $a, b, c, d \in X$, then no edge of T can separate a, c from b, d (as this would imply that $D(a, b) + D(c, d) = D(b, c) + D(d, a)$ would hold).

It may also be of interest to investigate further the properties of weak lassos. Note that if T is a binary X-tree, then $\mathcal{L}$ is a weak lasso for T if and only if $\mathcal{L}$ is a topological lasso for T; however, for non-binary trees, these are quite different concepts. For example, any subset of $\binom{X}{2}$ (including the empty set) is a weak lasso for the star tree T^* with leaf set X since any X-tree is a resolution of that tree, but it requires all of $\binom{X}{2}$ to lasso the shape of T^*.

Finally, we can view a triplet cover as a subset of $\binom{X}{2}$ that contains all the cords "induced" by a sufficiently large collection of subtrees each of which has three leaves. Thus, it is mathematically natural, and relevant to phylogenetic analysis (supertree reconstruction), to study the lasso properties of subsets of $\binom{X}{2}$ that are induced by collections of phylogenetic trees with three or more leaves. More precisely, given an

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[2] To see this, just take any leaf a of maximal distance to some other arbitrary vertex u. Then, a must be part of a cherry a, b whose elements a, b must be adjacent to an interior vertex $v = v_a = v_b$ that is incident with only one interior edge (by the maximal distance to u assumption) and with no other pendant edge (by the condition imposed in (iv)). So, a, b must necessarily be a proper cherry.

X-tree T and a collection $\mathcal{P} = \{X_1, \ldots, X_k\}$ of subsets of X, let

$$\mathcal{L}_\mathcal{P} := \bigcup_{i=1}^{k} \binom{X_i}{2}.$$

It would be of interest to determine conditions on $\mathcal{P}$ in order for $\mathcal{L}_\mathcal{P}$ to lasso T, at least in case T is binary. The quartet case (where all sets in $\mathcal{P}$ are 4-subsets of X) is an obvious candidate for analysis, in view of a range of combinatorial results from Böcker et al. (1999), Dress and Erdös (2003), Dress et al. (2011b), Grünewald et al. (2008) and Steel (1992).

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