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## Level-2 networks from shortest and longest distances<sup>☆</sup>

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### ABSTRACT

Recently it was shown that a certain class of phylogenetic networks, called level-2 networks, cannot be reconstructed from their associated distance matrices. In this paper, we show that they can be reconstructed from their induced shortest and longest distance matrices. That is, if two level-2 networks induce the same shortest and longest distance matrices, then they must be isomorphic. We further show that level-2 networks are reconstructible from their shortest distance matrices if and only if they do not contain a subgraph from a family of graphs. A generator of a network is the graph obtained by deleting all pendant subtrees and suppressing degree-2 vertices. We also show that networks with a leaf on every generator side are reconstructible from their induced shortest distance matrix.

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## 1. Introduction

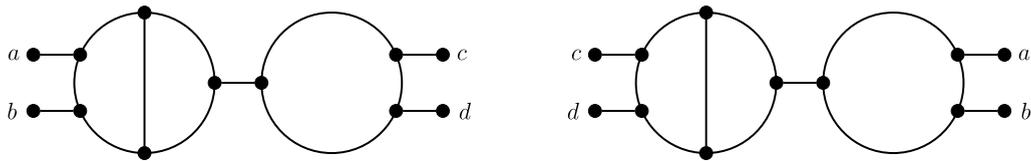
Finding a weighted undirected graph that realizes a distance matrix has applications in phylogenetics [12,15], psychology [8,16], electricity networks [10,11], information theory [9], and other areas. In their seminal paper, [11] showed that a necessary and sufficient condition for a distance matrix to be realizable on a graph is for it to be a metric space. While this gave existence for graph realizations on any metric spaces, such realizations were not necessarily unique. Many of the existing distance methods, including the one from this paper, take the following approach. Assuming a graph  $G$  realizes some distance matrix  $M$ , we first identify pendant structures of  $G$  from the information provided by  $M$ . The elements involved in such structures are clustered into one element in the newly updated distance matrix  $M'$ . This process is repeated until all structures of  $G$  have been identified, at which point we have essentially constructed  $G$  (should such a graph exist).

We consider a restriction of the distance matrix realizability problem in the context of phylogenetics, where graphs such as phylogenetic networks are used to elucidate the evolutionary histories of taxa. In recent years, phylogenetic networks have attracted increasing attention over phylogenetic trees, due to their generalized nature and ability to

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**Fig. 1.** Two level-2 networks with the same shortest distances between any pair of leaves. The shortest distance can be worked out by taking the length of the shortest path between a pair of leaves, where each edge is of length 1.

represent non-treelike evolutionary histories; this is suitable in visualizing complex reticulate events such as hybridization events and introgression, found to be rife within plants and bacteria [1,12]. In the context of phylogenetics, distances are defined between pairs of taxa to denote the number of character changes (in terms of the nucleotide bases in DNA) or the evolutionary/genetic distance between them. These distances are generally obtained from multiple sequence alignments. In this paper, we study the *reconstructibility* of phylogenetic networks from certain distance matrices. We say that a network is *reconstructible* from its induced distance matrix if it is the unique network that realizes the distance matrix.

Because networks contain undirected cycles, there can be many paths between two leaves (leaves are labeled by unique taxa, so leaves and taxa will be used interchangeably). This is in contrast to trees which contain only one path between each leaf pair. So while a tree induces only one metric, networks may induce many.<sup>1</sup> To date, different matrices have been considered for phylogenetic network reconstruction. These include the shortest distances (the traditional distance matrix), the sets of distances [5], and the multisets of distances [3,17], where the latter two are not distance matrices in the traditional sense of the term, however, they contain information on the inter-leaf distances. In particular, an element of the multisets of distances is a multiset of all distances between a pair of leaves, together with the multiplicities associated to each length. The set of distances can be obtained from the multisets of distances by ignoring the multiplicities.<sup>2</sup>

Both the sets and multisets of distances were first introduced to prove reconstructibility results for distance matrices induced by particular phylogenetic network classes [3,5]; shortest distances have also been used to prove reconstructibility results [6,18]. Recent results have shown unique realizability from sets and multisets of distances for certain rooted networks (tree-child and normal networks<sup>3</sup>) [2,4] and for certain unrooted networks [17]. In particular, the results of [17] showed that unweighted binary level-2 networks are reconstructible from their multisets of distances. Binary means that each leaf is of degree-1 and every other vertex is of degree-3; the level of a network refers to the number of edges needed to be removed from every biconnected component to obtain a tree (described more in detail below). They also showed that level-1 networks are reconstructible from their shortest distances, but that level-2 networks were not reconstructible in general from their shortest distances (Fig. 1).

It is interesting to know which level-2 networks are reconstructible from their shortest distances, or what additional information is needed to be able to do so. Therefore, motivated by the results in [17], we answer three open problems for binary networks from the paper on unique realizability of certain distance matrices.

1. Networks with a leaf on every generator side are reconstructible from their induced shortest distance matrix (Theorem 1);
2. Level-2 networks are reconstructible from their induced shortest and longest distance matrix (sl-distance matrix) (Theorem 3);
3. We characterize subgraphs of level-2 networks that are responsible for the class to not be reconstructible from their induced shortest distance matrix (Theorem 4).

**Structure of the paper.** In Section 2, we give formal definitions of phylogenetic terms. In Section 3, we show that networks with a leaf on every generator side (i.e., every vertex on the network is at most shortest distance-2 away from a leaf) are reconstructible from their shortest distances (Theorem 1). In Section 4, we show that level-2 networks are reconstructible from their sl-distance matrices (Theorem 3). This is proven by first showing that the splits of the network (cut-edges that induce a partition on the labeled leaves) are determined by the shortest distances that they realize (Theorem 2). In Section 5, we show a construction for obtaining pairs of distinct level-2 networks from a binary tree that realize the

<sup>1</sup> A matrix consisting of inter-leaf shortest distances, and a matrix consisting of inter-leaf longest distances are two examples of a metric induced by a network.

<sup>2</sup> The motivation for considering sets and multisets of distances is mostly combinatorial. It is not clear how such distances can be obtained from a multiple sequence alignment. A possibility is to divide the alignment into *blocks* depending on the parts of the chromosome responsible for encoding a particular gene, or by optimizing constraints such as the homoplasy score [13]. Treating each of these blocks as an alignment yields a distance matrix for each block, which can be collated to give multisets of distances between pairs of taxa. The fundamental flaw in this technique would be that every multiset of distances between leaf pairs would be of the same size (in particular the number of blocks), which is not always the case in the results where these multisets are used.

<sup>3</sup> Tree-child networks are directed networks with the property that every non-leaf vertex has a child that is a tree vertex or a leaf. Normal networks are tree-child networks with the additional constraint that given an edge  $uv$ , there cannot be another path from  $u$  to  $v$ .

same shortest distance matrix. We show that having such a network as a subgraph renders a level-2 network to be non-reconstructible from their shortest distances, thereby characterizing the family of subgraphs that are responsible for the non-reconstructibility (Theorem 4). We close with a discussion in Section 6, presenting ideas for possible future directions.

## 2. Preliminaries

An (*unrooted binary phylogenetic*) network on  $X$  (where  $|X| \geq 2$ ) is a simple connected undirected graph with at least two leaves where the leaves are labeled bijectively by  $X$  and are of degree-1. All internal vertices are of degree-3. An (*unrooted binary phylogenetic*) tree on  $X$  is a network with no cycles.

### 2.1. Graph theoretic definitions

Let  $N$  be a network. A set of two leaves  $\{x, y\}$  of  $N$  forms a *cherry* if they share a common neighbor. Let  $a = (a_1, \dots, a_k)$  be an ordered sequence of  $k$  leaves, and let  $p_a = (v_1, \dots, v_k)$ , where  $v_i$  is the neighbor of  $a_i$  for each  $i \in [k] = \{1, \dots, k\}$ .<sup>4</sup> We allow for  $v_1 = v_2$  and  $v_{k-1} = v_k$ . If  $p_a$  is a path in  $N$  then  $a$  is called a *chain* of length  $k \geq 0$ . We call chains of length 0 an empty chain. Assume that all chains are non-empty unless stated otherwise. Letting chains be of empty length is to generalize some statements later on in the paper. We say that  $a$  is a *maximal chain* if  $a$  does not form a subsequence for some other chain. We assume all chains to be maximal, unless stated otherwise. If  $a$  is a chain, then the vertices of  $p_a$  are called the *spine vertices*, and the path  $p_a$  is called a *spine*. The vertices  $a_1, a_k$  are called the *end-leaves* of the chain  $a$ , and the vertices  $v_1, v_k$  are called the *end-spine vertices* of the chain. For brevity, given a set  $S$ , we shall write  $S \cup a$  to denote the set  $S \cup \{a_1, a_2, \dots, a_k\}$ .

A *blob* of a network is a maximal 2-connected subgraph with at least three vertices. A network is a *level- $k$  network*, with  $k \geq 0$ , if at most  $k$  edges must be deleted from every blob to obtain a tree. We denote an edge between  $u$  and  $v$  by  $uv$ . We call a cut-edge *trivial* if the edge is incident to a leaf, and *non-trivial* otherwise. Given a cut-edge  $uv$  we say that a leaf  $x$  can be *reached from  $u$*  (via  $uv$ ) if, upon deleting the edge  $uv$  without suppressing degree-2 vertices,  $x$  is in the same component as  $v$  in the resulting subgraph. We say that a leaf is *contained* in a blob if the neighbor of the leaf is a vertex of the blob. We say that a chain is *contained* in a blob if any of the leaves of the chain are contained in the blob (and therefore all leaves of the chain are contained in the blob). An edge is *incident* to a blob if exactly one of the endpoints of the edge is a vertex of the blob. A blob is *pendant* if there is exactly one non-trivial cut-edge that is incident to the blob. We say that a leaf  $x$  can be *reached* from a blob  $B$  via a cut-edge  $uv$  if  $u$  is a vertex of  $B$  and  $x$  can be reached from  $u$  via  $uv$ . In this case, we also say that  $uv$  or  $u$  *separates  $x$*  from  $B$ .

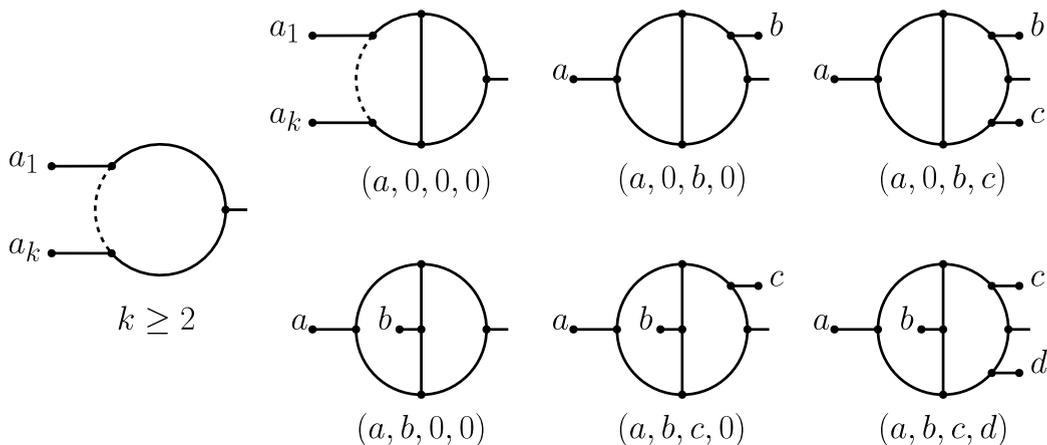
Letting  $X$  be a set of taxa, a *split* on  $X$  is a partition  $\{A, B\}$  of  $X$ . We denote a split which induces the partition  $\{A, B\}$  of  $X$  by  $A|B$  where the order in which we list  $A$  and  $B$  does not matter. Observe that some cut-edges of a network on  $X$  naturally induce a split as there are exactly two parts of the network separated by the edge. We call this a *cut-edge induced split*. We call a split  $A|B$  *non-trivial* if both  $A$  and  $B$  contain at least two elements. Otherwise we call a split *trivial*. Observe that non-trivial cut-edges induce non-trivial splits, and that trivial cut-edges induce trivial splits.

In this paper, we assume the restriction that every cut-edge must induce a unique split. Firstly, such a restriction eliminates the possibility for networks to contain *redundant* blobs, which are pendant blobs that contain no leaves. Secondly, the restriction removes all blobs that do not contain leaves, that are incident only to two non-trivial cut-edges. Such blobs can be interpreted as higher-level analogues of parallel edges.

The *generator*  $G(N)$  of a network  $N$  is the multi-graph obtained by deleting all pendant subtrees (i.e., deleting all leaves from  $N$ ) and suppressing degree-2 vertices. The generator may contain loops and parallel edges. A vertex of  $N$  that is not deleted or suppressed in the process of obtaining  $G(N)$  is called a *generator vertex*. We call the edges of  $G(N)$  the *sides* of  $N$ . Observe that the sides of  $N$  correspond to paths of  $N$ . Let  $s$  be a side of  $N$ , and let  $e_0 v_1 v_2 \dots v_k e_1$  with  $k \geq 0$  denote the path in  $N$  corresponding to  $s$ , where  $e_0$  and  $e_1$  are vertices of the generator. If  $k = 0$ , then the path is simply the edge  $e_0 e_1$ . We call  $e_0$  and  $e_1$  the *boundary vertices* of side  $s$ . We say that a leaf  $x$  is *on side  $s$*  if  $x$  is a neighbor of  $v_i$  for some  $i \in [k]$ . We say that a chain is *on side  $s$*  if all leaves of the chain are on the side  $s$ . Observe that a leaf of a chain is on a side if and only if the chain is on the side. Observe also that  $v_1 \dots v_k$  is a spine of some chain on  $s$ . We say that a side is *empty* if no leaves are on the side. A *side of a blob  $B$*  is an edge of  $G(N)$  which corresponds to a path in  $B$ . Observe that level-2 blobs contain exactly two vertices that are not cut-vertices. We call these the *poles* of the blob. There are exactly three edge-disjoint paths between the two poles. We call these three paths in  $N$  the *main paths* of  $B$ . The vertices in a main path  $s$  of  $B$  that are adjacent to the endpoints of  $s$  are called the *main end-spine vertices*.

We adopt the following notation for pendant level-2 blobs from [17]. Let  $B$  be a pendant level-2 blob, and let  $a, b, c, d$  denote the four chains contained in  $B$  of lengths  $k, \ell, m, n \geq 0$ , respectively, such that chains  $c$  and  $d$  are on the same main path of  $B$  as the non-trivial cut-edge. Then we say that  $B$  is of the form  $(a, b, c, d)$  (see Fig. 2). The order of the first two elements  $a, b$ , and the order of the last two elements  $c, d$  do not matter. For ease of notation, a side without leaves is seen as a length-0 chain. Note that since every cut-edge induces a unique split, it is not possible to obtain the pendant blob of the form  $(1, 0, 0, 0)$ .

<sup>4</sup> For consistency later on the section, we let  $[0] = \emptyset$ , the empty set.



**Fig. 2.** The seven possible pendant blobs in a level-2 network. The leftmost pendant blob is level-1, and the other pendant blobs are all level-2. Observe that for the pendant level-1 blob and the pendant level-2 blob of the form  $(a, 0, 0, 0)$ , the length of the chain  $a$  must be of length at least 2. This is due to the fact that networks do not contain parallel edges nor level-2 blobs with only two cut-edges incident to it. The dashed edges in these two blobs indicate that the chain can be longer than 2. For the five other pendant blobs, each of the leaves  $a, b, c, d$  indicates a chain.

### 2.2. Distances

For a network  $N$  on  $X$ , we let  $d_m^N(x, y)$  and  $d_l^N(x, y)$  denote the length of a shortest and a longest path between two vertices  $x, y$  in  $N$ , respectively. We exclude the superscript  $N$  when there is no ambiguity on the network at hand. Let  $a = \{a_1, \dots, a_k\}$  be a set of vertices in  $N$ , and let  $u$  be a vertex in  $N$  that is not in  $a$ . Then we define the shortest distance from  $u$  to  $a$  as the shortest distance from  $u$  to any of the vertices in  $a$ , that is,  $d_m^N(a, u) = \min\{d_m(a_i, u) : i \in [k] = \{1, \dots, k\}\}$ . Similarly, define the longest distance from  $u$  to  $a$  as the longest distance from  $u$  to any of the vertices in  $a$ , that is,  $d_l^N(a, u) = \max\{d_l(a_i, u) : i \in [k]\}$ .

The *shortest distance matrix*  $\mathcal{D}_m(N)$  of  $N$  is the  $|X| \times |X|$  matrix, where the rows and columns are indexed by the leaves of the network, whose  $(x, y)$ -th entry is  $d_m^N(x, y)$ . A network  $N$  realizes the shortest distance matrix  $\mathcal{D}_m$  if  $\mathcal{D}_m(N) = \mathcal{D}_m$ . We say that a network  $N$  is *reconstructible* from its shortest distance matrix if  $N$  is the only network, up to isomorphism, that realizes  $\mathcal{D}_m(N)$ . Here, we say that two networks  $N$  and  $N'$  on  $X$  are *isomorphic* if there exists a bijection  $f$  from the vertices of  $N$  to the vertices of  $N'$ , such that  $uv$  is an edge of  $N$  if and only if  $f(u)f(v)$  is an edge of  $N'$ , and the leaves of  $N$  are mapped to leaves of  $N'$  of the same label. Similarly, we define the *sl-distance matrix* (*shortest longest-distance matrix*)  $\mathcal{D}(N)$  as the  $|X| \times |X|$  matrix, where the rows and columns are indexed by the leaves of the network, whose  $(x, y)$ -th entry is  $d^N(x, y) = \{d_m^N(x, y), d_l^N(x, y)\}$  (see Fig. 3). We say that a network  $N$  realizes the sl-distance matrix  $\mathcal{D}$  if  $\mathcal{D}(N) = \mathcal{D}$ . A network  $N$  is *reconstructible* from its sl-distance matrix if  $N$  is the only network, up to isomorphism, that realizes  $\mathcal{D}(N)$ .

### 2.3. Reducing cherries

By definition, we may identify cherries from shortest distance matrices.

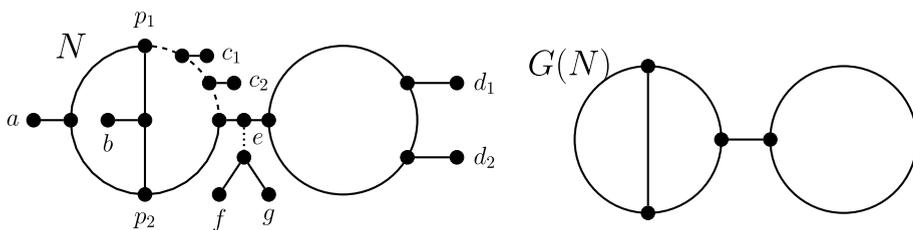
**Observation 1.** Let  $\mathcal{D}_m$  be a shortest distance matrix. A network  $N$  on  $X$  that realizes  $\mathcal{D}_m$  contains a cherry  $\{x, y\}$  if and only if  $d_m(x, y) = 2$ .

Reducing a cherry  $\{x, y\}$  to a leaf  $z$  from  $N$  is the action of deleting both leaves  $x, y$  and labeling the remaining unlabeled degree-1 vertex as  $z$ , assuming that  $z \notin X$  (this vertex was the neighbor of  $x$  and  $y$  in  $N$ ). As a result of reducing the cherry  $\{x, y\}$ , observe that the shortest distance between two leaves that are both not  $z$  are unchanged; the shortest distance between  $z$  and another leaf  $l \in X - \{x, y\}$  is exactly one less than that of  $x$  and  $l$  in  $N$ .

**Observation 2.** Let  $N$  be a network on  $X$  containing a cherry  $\{x, y\}$ . Upon reducing the cherry to a leaf  $z$ , we obtain a network  $N'$  on  $X' = X \cup \{z\} - \{x, y\}$  such that the shortest distance matrix for  $N'$  contains the elements

$$d_m^{N'}(a, b) = \begin{cases} d_m^N(a, b) & \text{if } a, b \in X - \{x, y\} \\ d_m^N(a, x) - 1 & \text{if } a \in X - \{x, y\} \text{ and } b = z. \end{cases}$$

In the setting of Observation 2, one may obtain a network that is isomorphic to  $N$  from  $N'$  by adding two labeled vertices  $x$  and  $y$ , adding the edges  $zx$  and  $zy$ , and unlabelling the vertex  $z$ . We call this *replacing  $z$  by a cherry  $\{x, y\}$* .



	<i>a</i>	<i>b</i>	<i>c</i> <sub>1</sub>	<i>c</i> <sub>2</sub>	<i>d</i> <sub>1</sub>	<i>d</i> <sub>2</sub>	<i>f</i>	<i>g</i>
<i>a</i>		(4, 8)	(4, 8)	(5, 7)	(7, 12)	(7, 12)	(6, 10)	(6, 10)
<i>b</i>			(4, 8)	(5, 7)	(7, 12)	(7, 12)	(6, 10)	(6, 10)
<i>c</i> <sub>1</sub>				(3, 7)	(7, 10)	(7, 10)	(6, 8)	(6, 8)
<i>c</i> <sub>2</sub>					(6, 11)	(6, 11)	(5, 9)	(5, 9)
<i>d</i> <sub>1</sub>						(3, 4)	(5, 6)	(5, 6)
<i>d</i> <sub>2</sub>							(5, 6)	(5, 6)
<i>f</i>								(2, 2)
<i>g</i>								

**Fig. 3.** A level-2 network  $N$  on the taxa set  $\{a, b, c_1, c_2, d_1, d_2, f, g\}$ , its generator  $G(N)$ , and its sl-distance matrix.  $N$  contains a cherry  $\{f, g\}$  and four chains  $(a), (b), (c_1, c_2)$  and  $(d_1, d_2)$ .  $N$  contains two pendant blobs: the leftmost is a level-2 blob of the form  $((a), (b), (c_1, c_2), \emptyset)$ , and the rightmost is a level-1 blob containing the leaves  $d_1$  and  $d_2$ . The poles of the pendant level-2 blob are labeled by  $p_1$  and  $p_2$ . The dotted cut-edge  $e$  induces the non-trivial split  $\{a, b, c_1, c_2, d_1, d_2\} | \{f, g\}$ . The blob side indicated by the dashed path contains the chain  $(c_1, c_2)$ . The chains  $(a)$  and  $(c_1, c_2)$  are adjacent once. The chains  $(a)$  and  $(b)$  are adjacent twice. The sl-matrix has  $ij$ -th elements of the form  $(x, y)$ , where  $x$  and  $y$  denote the shortest and longest distances between  $i$  and  $j$  in  $N$ . The diagonal elements, which are all  $(0, 0)$ , and the lower triangular elements are omitted as the matrix is symmetric.

**Observation 3.** Let  $N$  be a network on  $X$ , and let  $z$  be a leaf in  $N$ . Let  $x, y \notin X$  be leaf labels that do not appear in  $N$ . Then upon replacing  $z$  by a cherry  $\{x, y\}$ , we obtain a network  $M$  on  $Y = X \cup \{x, y\} - \{z\}$  that realizes the shortest distance matrix with entries

$$d_m^M(a, b) = \begin{cases} d_m^N(a, b) & \text{if } a, b \in Y - \{x, y\} \\ d_m^N(a, z) + 1 & \text{if } a \in Y - \{x, y\} \text{ and } b \in \{x, y\} \\ 2 & \text{if } a = x \text{ and } b = y. \end{cases}$$

It is easy to see that replacing a leaf by a cherry and reducing a cherry are inverse operations of one another.

**Lemma 1.** Let  $N$  be a network with a cherry  $\{x, y\}$ , and let  $N'$  denote the network obtained by reducing the cherry from  $N$  to a leaf  $z$ . Then  $N$  is reconstructible from its shortest distance matrix if and only if  $N'$  is reconstructible from its shortest distance matrix.

**Proof.** Suppose first that the network  $N$  is reconstructible from its shortest distance matrix. Suppose for a contradiction that the shortest distance matrix  $\mathcal{D}_m(N')$  of  $N'$  is also realized by a network  $N''$  that is not isomorphic to  $N'$ . Consider the networks  $M'$  and  $M''$  obtained from  $N'$  and  $N''$ , respectively, by replacing  $z$  by a cherry  $\{x, y\}$ . By **Observation 3**, the two distinct networks  $M'$  and  $M''$  realize the same shortest distance matrix. However, this shortest distance matrix is precisely  $\mathcal{D}_m(N)$ , since  $M'$  is isomorphic to  $N$ . This contradicts the fact that  $N$  is reconstructible from its shortest distance matrix. Therefore  $N'$  must be reconstructible from its shortest distance matrix.

Now suppose that the network  $N'$  is reconstructible from its shortest distance matrix. If there were two distinct networks  $N$  and  $M$  realizing  $\mathcal{D}_m(N)$ , then these networks must both contain the cherry  $\{x, y\}$ . Reducing this cherry to a leaf  $z$ , we see by **Observation 2** that both reduced networks, which are distinct, realize the same shortest distance matrix, which is exactly  $\mathcal{D}_m(N')$ . However, this is not possible, as  $N'$  is reconstructible from its shortest distance matrix. Therefore  $N$  is also reconstructible from its shortest distance matrix.  $\square$

Let  $N$  be a network. *Subtree reduction* refers to the action of reducing cherries of  $N$  until it is no longer possible to do so. We refer to the resulting network as the *subtree reduced version* of  $N$ . Note that the subtree reduced version of  $N$  is

unique, and the order in which the cherries are reduced does not matter. The following corollary follows immediately by applying Lemma 1 to every cherry that is reduced in the subtree reduction.

**Corollary 1.** *A network  $N$  is reconstructible from its shortest distance matrix if and only if the subtree reduced version of  $N$  is reconstructible from its shortest distance matrix.*

Note that Observations 2 and 3, Lemma 1, and Corollary 1 can naturally be extended to the sl-distances, with a single tweak for Observations 2 and 3, where the longest distances are adjusted exactly the same as done for the shortest distances (replace  $d_m$  by  $d_l$  wherever possible). This means we may assume for the rest of the paper, that all networks have undergone subtree reduction, and therefore that all networks contain no cherries.

#### 2.4. Chains

Upon reducing all cherries from our networks, we may identify unique chains from shortest distance matrices. Recall that chains are written as sequences  $a = (a_1, \dots, a_k)$  for some  $k \geq 1$ . We shall sometimes write these as  $(a, k)$ . In what follows, we will often require a way of referring to leaves of the network that are not in a particular chain. So while  $a$  is a sequence of leaves, we shall sometimes treat  $a$  as a set of leaves, e.g.,  $X - a = \{l \in X : l \neq a_i \text{ for } i \in [k]\}$ .

**Observation 4.** *Let  $\mathcal{D}_m$  be a shortest distance matrix. A network  $N$  on  $X$  that realizes  $\mathcal{D}_m$  contains a chain  $a = (a_1, \dots, a_k)$  where  $k \geq 1$  if and only if  $d_m(a_i, a_{i+1}) = 3$  for all  $i \in [k - 1]$  and there exists no leaf  $l \in X - a$  such that  $d_m(a, l) = 3$ .*

Observation 4 implies that the leaves in a network without cherries can be partitioned into chains. Indeed, no leaf can be contained in two distinct chains, as otherwise the chains would be non-maximal. Let  $(a, k)$  and  $(b, \ell)$  be two distinct chains. We say that  $(a, k)$  and  $(b, \ell)$  are *adjacent* if  $d_m(a_i, b_j) = 4$  for some combination of  $i \in \{1, k\}$  and  $j \in \{1, \ell\}$ . Observe that adjacent chains of a network  $N$  can be identified from shortest distance matrices, by first partitioning the leaf set of  $N$  into chains and then checking for chain end-leaves that are distance-4 apart. We say that two chains  $(a, k)$  and  $(b, \ell)$  are *adjacent once* if exactly one distinct pair of  $(a, k)$  and  $(b, \ell)$  is distance-4 apart. We say that the chains  $(a, k)$  and  $(b, \ell)$  are *adjacent twice* if two distinct pairs of  $(a, k)$  and  $(b, \ell)$  end-leaves are distance-4 apart. Since we assume networks to be binary, two chains may be adjacent at most twice. In the special case where  $k = \ell = 1$ , we can only tell whether the chains are adjacent from the shortest distances. We cannot tell whether they are adjacent twice. This can however be inferred from the sl-distance matrix.

#### 2.5. Known results

The following results appeared in [17].

**Lemma 2** (Theorem 4.2; Lemma 4.4; Lemma 5.3 of [17]). *Let  $N$  be a level-2 network on  $|X|$ . Then  $N$  is reconstructible from its shortest distance matrix if  $N$  is also level-1, if  $|X| < 4$ , or if  $N$  contains only one blob.*

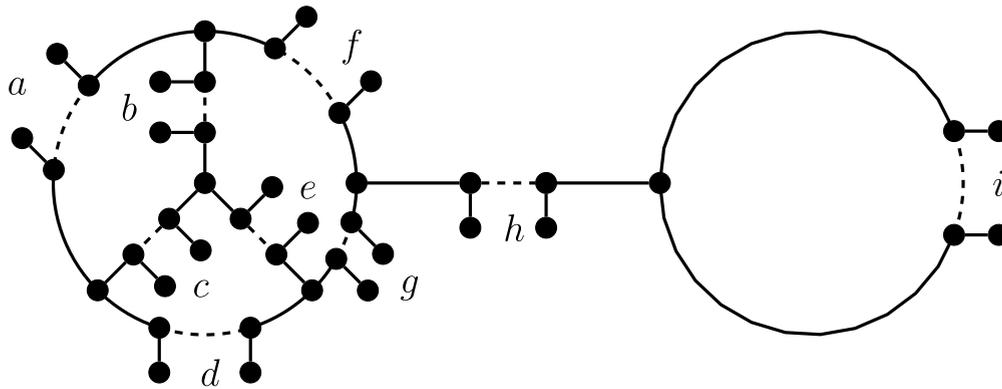
Therefore we may assume that the networks we consider are always at least level-2 on at least four leaves, and that the network contains at least two blobs. Furthermore, from Section 2.3, we may assume that the networks contain no cherries.

### 3. Leaf on each generator side

In this section, we consider networks with at least one leaf on each generator side, and show that such networks are reconstructible from their shortest distance matrices, regardless of level. Let  $N$  be one such network. Since we may assume that  $N$  has no cherries, each side of  $N$  can be determined by the chain contained therein. Furthermore, two sides are adjacent (i.e., the sides share a common endpoint in  $G(N)$ ) if and only if the chains on the sides are adjacent. Since chains partition the leaf set of  $N$ , this implies that the structure of the generator  $G(N)$ , and therefore the structure of the network  $N$  is determined by the chains of  $N$  and their adjacency in  $N$ .

Every vertex in  $N$  is either a leaf, a spine vertex of some chain, or a generator vertex. Since networks considered here are binary, exactly two or three generator sides may be incident to the same vertex in  $G(N)$  (as per conventional graph theory, we say that an edge is *incident* to its endpoints). If a vertex is incident to exactly two sides in  $G(N)$ , then one of these sides must be a loop. Loops in  $G(N)$  correspond to pendant level-1 blobs in  $N$ . Suppose that  $(a, k)$  is a chain (recall that this is a chain of length  $k$ ) and is adjacent to exactly one chain  $(b, \ell)$  twice, and that  $(a, k)$  is not adjacent to any other chains. Then  $(a, k)$  is contained in a pendant level-1 blob, since we may assume that  $N$  is a level-2 network with at least two blobs. Note that  $k \geq 2$  as  $N$  contains no parallel edges. In such a case, we call the pair  $(a, b)$  the *bulb* of  $a$  and  $b$ . We say that  $a$  is contained in the bulb as the *petal*. We say that  $N$  contains the petal  $(a, b)$ .

If a generator vertex is incident to three sides, then the three distinct chains in the network, corresponding to these three sides must be pairwise adjacent. Now consider three pairwise adjacent distinct chains  $(a, k)$ ,  $(b, \ell)$ ,  $(c, m)$  in  $N$ . Since we may assume  $N$  is not a level-2 network with a single blob (as we know such networks are reconstructible



**Fig. 4.** A level-3 network with leaves on every generator side. Each letter represents a chain on a side of the network. The network contains the pairwise adjacent triples  $(a, b, f)$ ,  $(a, c, d)$ ,  $(b, c, e)$ ,  $(d, e, g)$ ,  $(f, g, h)$  and the bulb  $(i, h)$  with  $i$  as the petal. The dashed edges indicate how each of the nine chains is of length at least 1.

from their shortest distances by Lemma 2), any three chains may be pairwise adjacent at most once. In particular, the end-leaves of  $a, b, c$  that are adjacent are unique. In this case, we say that  $(a, b, c)$  forms a *pairwise adjacent triple* (see Fig. 4 for examples of pairwise adjacent triples and petals). Therefore, if  $(a, b, c)$  is a pairwise adjacent triple, then there is a generator vertex that is incident to three sides such that one side contains chain  $a$ , one chain  $b$  and one chain  $c$ . We say that  $N$  contains the pairwise adjacent triple  $(a, b, c)$ .

Note that bulbs and pairwise adjacent triples both consist of three leaves. In what follows, the notion of a *median* vertex will be important. Given three vertices  $a, b, c$  of a network, a median of  $a, b, c$  is a vertex that belongs to a shortest path between each pair of  $a, b, c$ . A median may not always exist for any three vertices (consider, for example, a cycle on three vertices). However, for our purposes, we shall consider medians of three leaves, which will always exist. Moreover, a median of three vertices is not necessarily unique, as there may be more than one shortest path between a pair of vertices in a network.

**Lemma 3.** Let  $\mathcal{D}_m$  be a shortest distance matrix. Then  $\mathcal{D}_m$  can only be realized by a network  $N$  with leaves on each side of the generator, where  $N$  is not a single level-2 blob if and only if each chain of  $\mathcal{D}_m$  is contained in either

- (i) two distinct pairwise adjacent triples; or
- (ii) one pairwise adjacent triple and one bulb as a non-petal; or
- (iii) one bulb as the petal; or
- (iv) two bulbs as non-petals.

**Proof.** Let  $N$  be a network with leaves on each generator side and suppose that  $N$  realizes  $\mathcal{D}_m$ . Then each generator vertex of  $N$  is the median of three end-leaves of (not necessarily distinct) chains, such that these end-leaves are pairwise shortest distance-4 apart. Any three chains may be pairwise adjacent at most once (unless  $N$  is a network with a single level-2 blob, but we have specifically excluded this case in the statement of the lemma), and a chain contained in a pendant level-1 blob is adjacent twice to exactly one other chain. As  $N$  is binary, these median vertices encode either pairwise adjacent triples or bulbs. By *encode*, we mean that for every three end-leaves that are pairwise distance-4 apart, the median vertex corresponding to it is unique. Each chain is contained in exactly two of such constructs, where being contained in a bulb as the petal counts as two, since each side has two boundary vertices (except for the loop). The result follows immediately.

To show the other direction of the lemma, we prove the contrapositive. Let  $N$  be a network that has at least one empty generator side, and suppose that  $N$  realizes  $\mathcal{D}_m$ . We want to show that at least one chain of  $N$  does not satisfy any of the four properties (i) – (iv) as stated in the statement of the lemma. Find adjacent sides  $s_1$  and  $s_2$  of  $N$ , such that  $s_1$  contains a chain  $c$  while  $s_2$  is empty. Clearly,  $c$  cannot be contained in a bulb as its petal, since  $s_2$  contains no chains to which  $c$  can be adjacent twice (cannot satisfy (iii)). So we may assume that  $c$  is not contained in a pendant level-1 blob, and therefore that the boundary vertices  $e_0, e_1$  of  $s_1$  are distinct. We may assume without loss of generality that  $e_0$  is the boundary vertex of  $s_2$ . Since  $s_2$  is empty,  $e_0$  cannot be a median of three distinct end-leaves of chains. This implies that  $c$  can only be contained in exactly one pairwise adjacent triple, or in exactly one bulb as a non-petal (which is encoded by  $e_1$ ) (cannot satisfy (i), (ii), nor (iv)). □

**Lemma 4.** Let  $N$  and  $N'$  be networks with a leaf on each generator side, such that neither  $N$  nor  $N'$  are level-2 and contain precisely one level-2 blob. Then  $N$  and  $N'$  are isomorphic if and only if they contain the same chains, the same pairwise adjacent triples, and the same bulbs, where it is known which end-leaves of the chains are adjacent.

**Proof.** Suppose first that  $N$  and  $N'$  contain the same chains, the same pairwise adjacent triples, and the same bulbs. Then the networks must contain the same leaves and the same spine vertices (and also the edges therein). The remaining vertices in  $N$  and  $N'$  are their generator vertices, and the remaining edges are those incident on generator vertices and the end-spine vertices.

We show first that  $G(N) = G(N')$ . Every edge in the generator is a side that contains a chain. Since  $N$  and  $N'$  have the same chains, the number of edges in  $G(N)$  is the same as that in  $G(N')$ . Every vertex in the generator is a median of end-leaf vertices of three (not-necessarily distinct) chains. These generator vertices uniquely encode a pairwise adjacent triple or a bulb, since  $N$  and  $N'$  are not level-2 networks that contain precisely one level-2 blob. Since  $N$  and  $N'$  have the same pairwise adjacent triples and the same bulbs,  $G(N)$  and  $G(N')$  must have the same number of vertices. To see that  $G(N) = G(N')$ , observe that each generator vertex that encodes the pairwise adjacent triple  $(a, b, c)$  or a bulb  $(a, b)$  links the generator edges that contain the chains  $a, b, c$  or  $a, b$ , respectively. This means that two generator edges share a common endpoint if and only if the chains that they contain are in the same pairwise adjacent triple or bulb.

To see that  $N$  is isomorphic to  $N'$ , simply attach all chains to their corresponding generator sides, noting that the placement of the end-leaves are determined by the composition of the pairwise adjacent triples. Because we know which end-leaves of the chains are adjacent, the orientation of the chains are also determined. Since  $N$  and  $N'$  contain the same pairwise adjacent triples and bulbs, they must be isomorphic.

Conversely, if two networks are isomorphic, then they must have the same chains, the same pairwise adjacent triples, and the same bulbs.  $\square$

**Theorem 1.** *Networks with a leaf on each generator side are reconstructible from its shortest distances.*

**Proof.** If  $N$  is a level-2 network with a single blob, then  $N$  is reconstructible from its shortest distances by Lemma 2. Therefore we may assume  $N$  is not a level-2 network on a single blob, and therefore we may call Lemmas 3 and 4.

Let  $N$  be a network with a leaf on each generator side. This means that every chain in  $N$  satisfies one of properties (i)–(iv) of Lemma 3. As before, let  $\mathcal{D}_m(N)$  be the shortest distance matrix of  $N$ . Suppose that  $N'$  is another network that realizes  $\mathcal{D}_m(N)$ . Because each chain of  $\mathcal{D}_m(N)$  satisfies one of the four properties (i) – (iv) of Lemma 3,  $N'$  must be a network with a leaf on each generator side. Furthermore, any network realizing  $\mathcal{D}_m(N)$  must contain the same chains as  $N$ , by Observation 4. Therefore  $N$  and  $N'$  have the same chains. To see that  $N$  and  $N'$  also have the same generator vertices, observe that  $N$  and  $N'$  contain the same pairwise adjacent triples and the same bulbs; these can indeed be inferred from chain adjacencies, which can be inferred from  $\mathcal{D}_m(N)$  by definition of adjacent chains. It follows by Lemma 4 that  $N$  and  $N'$  must be isomorphic.  $\square$

#### 4. Level-2 reconstructibility from sl-distance matrix

As was pointed out in [17], level-2 networks are in general not reconstructible from their induced shortest distance matrix. Fig. 1 illustrates two distinct level-2 networks on four leaves with the same shortest distance matrices (Figure 2 of [17]). In this section, we show that level-2 networks are reconstructible from their sl-distance matrix.

##### 4.1. Cut-edges

First, we show that for a level-2 network, we may obtain all the cut-edge induced splits from its shortest distance matrix. Though the section is concerned with sl-distance reconstructibility, we show that the shortest distance matrix suffices in obtaining the cut-edge induced splits.

**Theorem 2.** *All cut-edge induced splits of a level-2 network  $N$  may be obtained from its shortest distance matrix  $\mathcal{D}_m(N)$ . A split  $A|B$  is induced by a cut-edge of  $N$  if and only if for all  $a, a' \in A$  and  $b, b' \in B$ ,*

- (i)  $d_m(a, b) + d_m(a', b') = d_m(a, b') + d_m(a', b)$ ; and
- (ii)  $d_m(a, a') + d_m(b, b') \leq d_m(a, b) + d_m(a', b') - 2$ .

**Proof.** The first statement of the theorem follows from the second statement of the theorem. Here, we prove the second statement.

Let  $N$  be a level-2 network on  $X$ . Suppose first that  $A|B$  is a split induced by some cut-edge  $uv$  in  $N$ . Let  $a, a' \in A$  and  $b, b' \in B$  be arbitrarily chosen. Since every shortest path from a leaf of  $A$  to a leaf of  $B$  contains the edge  $uv$ , we must have that

$$\begin{aligned} d_m(a, b) + d_m(a', b') &= d_m(a, u) + d_m(u, b) + d_m(a', u) + d_m(u, b') \\ &= d_m(a, b') + d_m(a', b). \end{aligned}$$

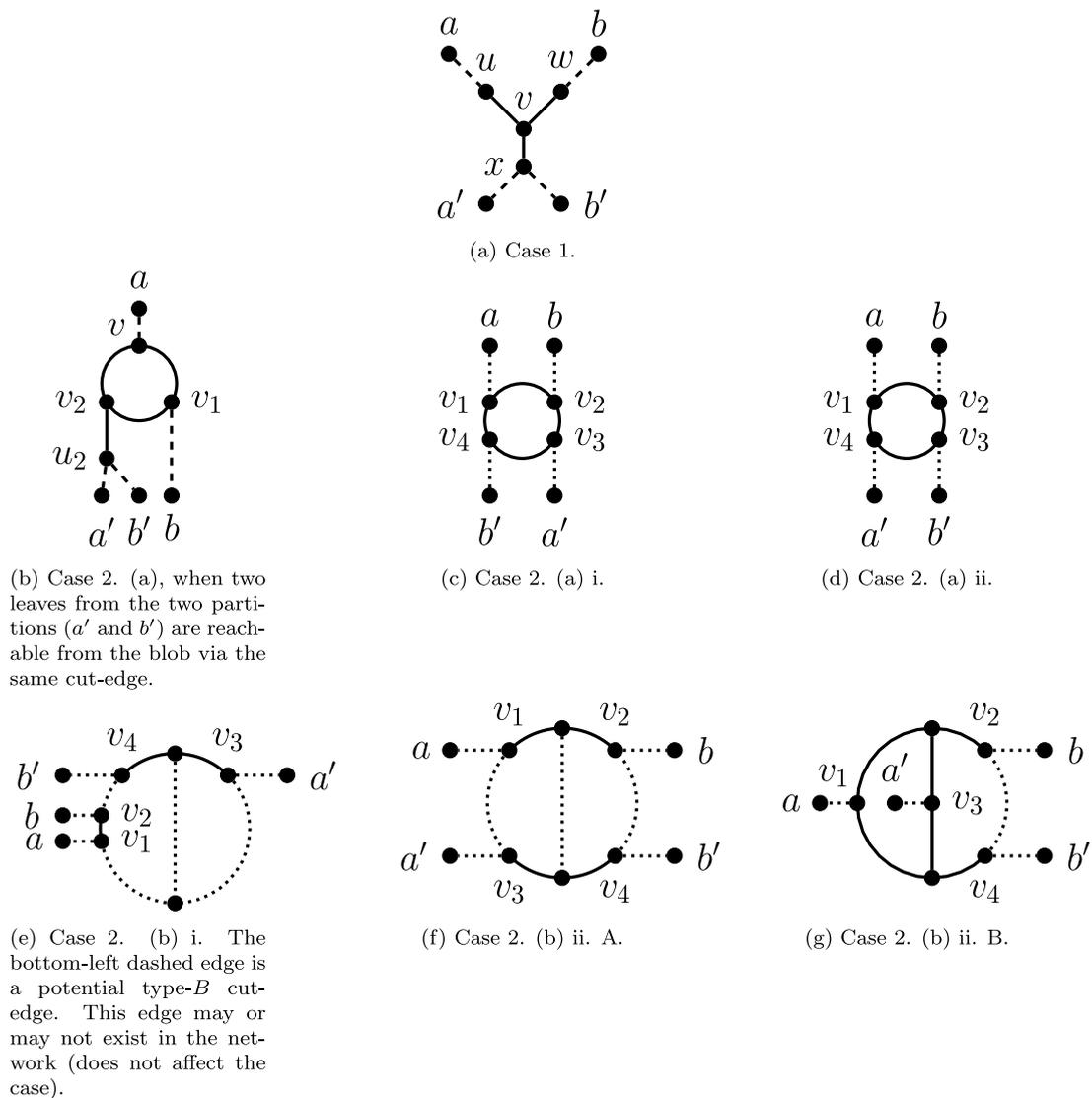


Fig. 5. All cases examined in the proof of Theorem 2. The dotted edges represent a path between the two vertices.

So property (i) holds. Since the length of the edge  $uv$  is 1, property (ii) also holds because

$$d_m(a, b) + d_m(a', b') = d_m(a, u) + 1 + d_m(v, b) + d_m(a', u) + 1 + d_m(v, b') \geq d_m(a, a') + d_m(b, b') + 2,$$

where in particular, we obtain equality if there exist a shortest path between  $a$  and  $a'$  and a shortest path between  $b$  and  $b'$  containing the vertices  $u$  and  $v$ , respectively.

Now suppose that  $A|B$  is a partition of the leaf-set of  $N$ , such that properties (i) and (ii) hold. Let  $a \in A$ , and let  $e = uv$  be a cut-edge in  $N$  that is farthest from  $a$ , such that  $e$  induces a split which separates  $a$  from  $B$ . If  $e$  induces the split  $A|B$ , then we are done. So suppose that there exists an  $a' \in A$  such that  $e$  induces a split that separates  $a$  from  $B \cup \{a'\}$  (in particular, we may assume that  $|A| \geq 2$  as every trivial split is clearly induced by a cut-edge). Without loss of generality, suppose that  $u$  is closer to  $a$  than to  $v$ . We consider several cases (see Fig. 5 for an illustration of the cases).

1.  **$v$  is not in a blob:** Let  $w, x$  denote the two neighbors of  $v$  that are not  $u$ . By our choice of  $e$ , there must be a leaf  $b \in B$  that can be reached from the edge  $vw$ , and a leaf  $b' \in B$  that can be reached from the edge  $vx$ . Without loss of generality, assume that  $a'$  can be reached from the edge  $vx$ . But this means that

$$d_m(a, b) + d_m(a', b') \leq d_m(a, v) + d_m(v, b) + d_m(a', x) + d_m(x, b') = [d_m(a, v) + d_m(v, x) + d_m(a', x)] - d_m(v, x)$$

$$\begin{aligned}
 &+ [d_m(b, v) + d_m(v, x) + d_m(x, b')] - d_m(v, x) \\
 &= d_m(a, a') - d_m(v, x) + d_m(b, b') - d_m(v, x) \\
 &= d_m(a, a') + d_m(b, b') - 2 \\
 &< d_m(a, a') + d_m(b, b'),
 \end{aligned}$$

where the first inequality may be strict since the shortest path between  $a'$  and  $b'$  may not pass through  $x$ . This contradicts the second condition of the claim.

2.  **$v$  is a vertex of a blob  $C$** : The blob  $C$  must be incident to at least two cut-edges  $e_1, e_2$  other than  $uv$ , for which there must be elements  $b$  and  $b'$  in  $B$  that are reachable from  $e_1$  and  $e_2$  respectively. Otherwise, as before, this would contradict our choice of a farthest  $uv$ . We claim that if  $a'$  can be reached from either  $e_1$  or  $e_2$ , then we would reach a contradiction. Without loss of generality, suppose that  $a'$  can be reached from  $e_2$ . Letting  $e_1 = u_1v_1$  and  $e_2 = u_2v_2$  where  $v_1$  and  $v_2$  are vertices on  $C$ , we have that

$$\begin{aligned}
 d_m(a, b) + d_m(a', b') &< d_m(a, v) + d_m(v, v_1) + d_m(v_1, b) + d_m(a', v_2) + d_m(v_2, b') \\
 &= d_m(a, a') - d_m(v, v_2) + d_m(b, b') - d_m(v_1, v_2) + d_m(v, v_1) \\
 &\leq d_m(a, a') + d_m(b, b'),
 \end{aligned}$$

where the first inequality follows as the shortest path between  $a'$  and  $b'$  does not contain  $v_2$ , and the final inequality follows from the triangle inequality. This contradicts the second condition of the claim. Therefore, we may assume from now that there are at least four cut-edges incident to the blob  $C$  and that no leaves from  $A$  and  $B$  can be reached from the same cut-edge incident to  $C$ . That is, every cut-edge incident to  $C$  induces a split that has either a subset of  $A$  or a subset of  $B$  as one of its parts. We refer to these as *type-A cut-edges* and *type-B cut-edges*, respectively.

We have another case that is common both for the instances when  $C$  is either a level-1 or a level-2 blob. Suppose first that there exist two pairs of cut-edges  $e_1, e_2$ , and  $e_3, e_4$  incident to  $C$ , whose endpoints are adjacent, respectively, such that all four edges are distinct and  $a, b, a', b'$  are reachable from  $e_1, e_2, e_3, e_4$  respectively. We let  $v_i$  denote the vertices of  $C$  that are endpoints of  $e_i$  for  $i = 1, 2, 3, 4$ , respectively. Then we have

$$\begin{aligned}
 d_m(a, b) + d_m(a', b') &= d_m(a, v_1) + d_m(v_1, v_2) + d_m(v_2, b) + d_m(a', v_3) \\
 &\quad + d_m(v_3, v_4) + d_m(v_4, b') \\
 &= d_m(a, a') + d_m(b, b') - d_m(v_1, v_3) - d_m(v_2, v_4) + 2 \\
 &\leq d_m(a, a') + d_m(b, b'),
 \end{aligned}$$

where the second equality follows as  $d_m(v_1, v_2) = d_m(v_3, v_4) = 1$ . This contradicts the second inequality of the claim.

If  $C$  is a level-1 blob, then the above case always applies. Indeed, there must be at least four cut-edges incident to  $C$ , of which at least two are type-A and the remaining edges are type-B. If there was only one type-B edge, then such a cut-edge induces the split  $A|B$ , and we are done. So this implies that there are always two distinct pairs of type-A and type-B edges, whose endpoints on  $C$  are adjacent. Thus we may assume that  $C$  is a level-2 blob.

We may assume that each main path of  $C$  contains only type-A cut-edges or only type-B cut-edges, or a combination of the two, for which such a main path contains one type of cut-edges, a single cut-edge of the other type, and possibly cut-edges of the first type. For example, a path corresponding to a main path of  $B$  may be  $e_0v_1 \cdots v_k e_1$  where  $k \geq 2$  and  $e_0, e_1$  are boundary vertices. For some integer  $j \leq k$ , we have  $v_1, v_2, \dots, v_{j-1}, v_{j+1}, \dots, v_k$  are incident to type-A cut-edges, and  $v_j$  is incident to a type-B cut-edge. We call such a main path a *combination side*. Observe that a combination side contains either one type-A or one type-B cut-edge. Also note that the blob  $C$  contains at most one combination side as otherwise there would be two distinct pairs of type-A and type-B edges, whose endpoints on  $C$  are adjacent.

- (a)  **$C$  contains one combination side  $s$** : Suppose without loss of generality that  $s$  is a combination side containing exactly one type-A cut-edge. Let  $v_1$  denote the endpoint of this cut-edge on  $C$ , and let  $v_2$  be an adjacent vertex on  $C$  that is incident to a type-B cut-edge. Since  $C$  is incident to at least two type-A cut-edges, there must be another main path  $s'$  of  $C$  that is incident to only type-A cut-edges. Similarly, since  $C$  is incident to at least two type-B cut-edges, there must be another type-B cut-edge  $e_4$  that is incident to  $C$ . We may assume in particular that an endpoint  $v_4$  of  $e_4$  is a main end-spine vertex incident either to  $s$  or to the third main path of  $C$ . Either way, there must exist an end-spine vertex  $v_3$  on  $s'$  such that  $d_m(v_3, v_4) = 2$ . Observing that  $v_3$  is an endpoint of a type-A cut-edge, we may assume that the leaves  $a, b, a', b'$  are separated from  $C$  by  $v_1, v_2, v_3, v_4$ , respectively. Then,

$$\begin{aligned}
 d_m(a, b) + d_m(a', b') - 2 &= d_m(a, v_1) + d_m(v_1, v_2) + d_m(v_2, b) + d_m(a', v_3) \\
 &\quad + d_m(v_3, v_4) + d_m(v_4, b') - 2 \\
 &= d_m(a, a') + d_m(b, b') + d_m(v_1, v_2) + d_m(v_3, v_4) \\
 &\quad - d_m(v_1, v_3) - d_m(v_2, v_4) - 2
 \end{aligned}$$

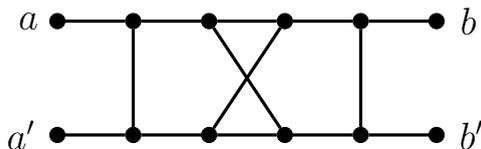


Fig. 6. A level-3 network on leaf-set  $\{a, a', b, b'\}$ . Observe that the conditions for Theorem 2 are satisfied for  $A = \{a, a'\}$  and  $B = \{b, b'\}$ , but there is no cut-edge that induces the split  $A|B$ .

$$\begin{aligned} &\leq d_m(a, a') + d_m(b, b') + 1 + 2 - 2 - d_m(v_1, v_3) \\ &\quad - d_m(v_2, v_4) \\ &< d_m(a, a') + d_m(b, b'), \end{aligned}$$

since  $d_m(v_1, v_3) \geq 1$  and  $d_m(v_2, v_4) \geq 1$ . This leads to a contradiction of the second condition.

- (b) **Each main path of C contain cut-edges of the same type:** Observe that at least one main path must contain at least two cut-edges, since there are at least four cut-edges incident to C and C has three main paths. Without loss of generality, suppose that there is a main path  $s$  with at least 2 type-B edges.

- i **There is another main path  $s'$  with at least two type-A edges:** Then choose  $v_1, v_3$  and  $v_2, v_4$  to be the main end-spine vertices of  $s'$  and  $s$ , respectively, such that  $d_m(v_1, v_2) = 2$  and  $d_m(v_3, v_4) = 2$ . Supposing that the leaves  $a, b, a', b'$  are separated from C by  $v_1, v_2, v_3, v_4$ , respectively, we have that

$$\begin{aligned} d_m(a, b) + d_m(a', b') &= d_m(a', b) + d_m(a, b') - d_m(v_1, v_4) - d_m(v_2, v_3) \\ &\quad + d_m(v_1, v_2) + d_m(v_3, v_4) \\ &\leq d_m(a', b) + d_m(a, b') - 3 - 3 + 2 + 2 \\ &< d_m(a', b) + d_m(a, b'), \end{aligned}$$

since  $d_m(v_1, v_4) \geq 3$  and  $d_m(v_2, v_3) \geq 3$ , where this inequality is strict when the third main path contains no cut-edges. This clearly contradicts the first condition of the claim.

- ii **The other two main paths contain exactly one type-A edge each:** Choose  $v_1, v_3$  to be the two possible vertices incident to the type-A cut-edges, and  $v_2, v_4$  to be the main end-spine vertices of  $s$ . Supposing that the leaves  $a, b, a', b'$  are separated from C by  $v_1, v_2, v_3, v_4$ , respectively, we have that

$$\begin{aligned} d_m(a, b) + d_m(a', b') &= d_m(a, a') + d_m(b, b') + d_m(v_1, v_2) + d_m(v_3, v_4) - d_m(v_1, v_3) - d_m(v_2, v_4) \\ &= d_m(a, a') + d_m(b, b') + 4 - 2 - d_m(v_2, v_4) \\ &< d_m(a, a') + d_m(b, b') + 2, \end{aligned}$$

which contradicts the second condition of the claim.

This covers all possible cases, for which we have obtained a contradiction in each case. Therefore  $A|B$  must be a cut-edge induced split of the network.  $\square$

Note that Theorem 2 does not hold for networks of level at least 3 (see Fig. 6). Let us call a split  $A|B$  *minimal* if there exists no non-trivial split  $A'|B'$  of the same network such that one of  $A'$  and  $B'$  is a proper subset of  $A$  or  $B$ . We say that  $A$  and  $B$  are *minimal parts* of  $A|B$ , respectively. Note that minimal parts of a split may not be unique as two pendant blobs may be connected by a non-trivial cut-edge  $e$ , for which both parts of the split are minimal parts.

**Lemma 5.** *Let  $N$  be a level-2 network on  $X$  with at least two pendant blobs. Then  $N$  contains a pendant blob containing the set of leaves  $A$  if and only if  $A|B$  is a minimal cut-edge induced non-trivial split where  $A$  is a minimal part.*

**Proof.** Suppose first that  $N$  contains a pendant blob  $C$  containing the set of leaves  $A$ . Then there exists exactly one non-trivial cut-edge  $e$  incident to  $C$ , which induces the non-trivial split  $A|B$  (where  $B = X - A$ ). To see that  $A$  is a minimal part, observe that for every cut-edge induced split  $A'|B'$  where  $A' \subseteq A$ , we have  $|A'| = 1$ , since every cut-edge incident to  $C$  other than  $e$  is trivial. Therefore,  $A|B$  is a minimal split, where  $A$  is a minimal part.

Suppose now that  $A|B$  is a minimal non-trivial split induced by  $e$ , where  $A$  is a minimal part. Suppose for a contradiction that  $N$  did not contain a pendant blob with the set of leaves  $A$ . Because we may assume  $N$  contains no cherries, the part of  $N$  corresponding to the split part  $A$  (i.e., the graph obtained by deleting  $e$  and taking the component with the leaves from  $A$ ) must contain a pendant blob  $C$ . Such a pendant blob contains the set of leaves  $A'$ , where  $A' \subseteq A$ . The non-trivial cut-edge incident to  $C$  induces the split  $A'|B'$ , where  $B' = X - A'$ . By definition,  $A'|B'$  must be a non-trivial split. But this contradicts the fact that  $A|B$  was minimal. Therefore,  $N$  must contain a pendant blob with the set of leaves  $A$ .  $\square$

#### 4.2. *sl*-distance reconstructibility

We show now that we can identify pendant blobs of level-2 networks from their *sl*-distance matrices.

**Lemma 6.** *Let  $N$  be a level-2 network on  $X$  with at least two blobs. Let  $A|B$  be a non-trivial split of  $N$  where  $A$  is the minimal part. Then  $N$  contains a pendant blob containing the set of leaves  $A$ , and if  $A$  contains*

- 1 chain  $(a, k)$ , then  $N$  contains
  - a pendant level-1 blob containing  $(a, k)$  if and only if
    - \*  $2 \leq k \leq 3$ ,  $d_m(a_1, a_k) = k + 1$ , and  $d_l(a_1, a_k) = 4$ .
    - \*  $k \geq 4$  and  $d_m(a_1, a_k) = 4$ .
  - a pendant level-2 blob of the form  $(a, 0, 0, 0)$  if and only if
    - \*  $2 \leq k \leq 3$ ,  $d_m(a_1, a_k) = k + 1$ , and  $d_l(a_1, a_k) = 6$ .
    - \*  $k \geq 4$  and  $d_m(a_1, a_k) = 5$ .
- 2 chains  $(a, k)$  and  $(b, \ell)$ , then  $N$  contains
  - a pendant level-2 blob of the form  $(a, b, 0, 0)$  if and only if for all  $x \in X - (a \cup b)$ , we have  $d_m(a, x) = d_m(b, x)$ .
  - a pendant level-2 blob of the form  $(a, 0, b, 0)$  if and only if for all  $x \in X - (a \cup b)$ , we have  $d_m(a, x) = d_m(b, x) + 1$ .
- 3 chains  $(a, k)$ ,  $(b, \ell)$ , and  $(c, m)$ , then  $N$  contains
  - a pendant level-2 blob of the form  $(a, b, c, 0)$  if and only if for all  $x \in X - (a \cup b \cup c)$ , we have  $d_m(a, x) = d_m(b, x) = d_m(c, x) + 1$ .
  - a pendant level-2 blob of the form  $(a, 0, b, c)$  if and only if for all  $x \in X - (a \cup b \cup c)$ , we have  $d_m(a, x) = d_m(b, x) + \min\{\ell, m\} + 1 = d_m(c, x) + \min\{\ell, m\} + 1$ .
- 4 chains  $(a, k)$ ,  $(b, \ell)$ ,  $(c, m)$ , and  $(d, n)$  then  $N$  contains a pendant level-2 blob of the form  $(a, b, c, d)$  if and only if  $(a, b, c)$  and  $(a, b, d)$  are both pairwise adjacent triples.

**Proof.** The fact that  $N$  contains a pendant blob containing the set of leaves  $A$  follows from Lemma 5.

Suppose first that  $N$  contains either a pendant level-1 blob or a pendant level-2 blob of the form  $(a, b, c, d)$ , where  $a, b, c, d$  could be empty chains. Then it is easy to see by inspection that these distances hold and also that the pairwise adjacent triple statement holds in the case of 4 chains (see Fig. 2).

To show the other direction, note that within a level-2 network, there is one level-1 pendant blob, and there are six possible level-2 pendant blobs. We know that  $N$  contains a pendant blob with the leaves of  $A$ ; it remains to show that if the conditions on the distances are satisfied, then  $N$  must contain the corresponding pendant blob. From the *sl*-distance matrix, we can infer the number of distinct chains contained in  $A$ , as well as their adjacencies. Then, we can infer the type of this pendant blob by looking at the distance from the leaves of  $A$  to some leaf that is not in  $A$ . We give one example here for the case when  $A$  consists of exactly three chains. The proof for the other cases follows in an analogous fashion.

We give a proof for the case when  $A$  contains 3 chains  $(a, k)$ ,  $(b, \ell)$ , and  $(c, m)$ . Pendant level-1 blobs contain exactly 1 chain; thus the pendant blob must be level-2. Level-2 pendant blobs have three main paths, one of which contains the endpoint of the incident non-trivial cut-edge. This main path, say  $s$ , contains at least 1 chain and at most 2 chains, whilst the other two main paths contain at most 1 chain. Let  $x \in X - a \cup b \cup c$  be an arbitrary leaf. Two of the chains, say  $a$  and  $b$ , have the same minimal distance to  $x$ , and the other chain  $c$  has different minimal distance. If the distance between  $c$  and  $x$  is shorter than that between  $a$  and  $x$ , then we know that  $c$  must be contained in the main path  $s$  of  $B$ , and we have a pendant level-2 blob of the form  $(a, b, c, 0)$ . On the other hand, if the distance between  $c$  and  $x$  is longer than that between  $a$  and  $x$ , then we know that  $a$  and  $b$  must be contained in the main path  $s$  of  $B$ , and we have a pendant level-2 blob of the form  $(c, 0, a, b)$ . □

Observe that in the proof of Lemma 6, the longest distance information was used only to distinguish the pendant level-1 blob with a chain  $(a, k)$  and the pendant level-2 blob of the form  $(a, 0, 0, 0)$  for  $k \in \{2, 3\}$ . In other words, using only the shortest distances, the pendant level-1 blob containing 2 leaves cannot be distinguished from the pendant level-2 blob also containing 2 leaves on the same side; the pendant level-1 blob containing 3 leaves cannot be distinguished from the pendant level-2 blob of containing the same leaves on the same side. We shall denote these four subgraph structures as *bad blobs*. That is, we say that a level-1 blob is *bad* if it is incident to exactly three or four cut-edges. We say that a level-2 blob  $B$  is *bad* if, of the three main paths  $s_1, s_2, s_3$  of  $B$ , the main side  $s_1$  is incident to a single cut-edge,  $s_2$  is incident to no cut-edges, and  $s_3$  is incident to exactly two or three cut-edges.

The reason why we cannot discern these bad blobs is because the shortest distance between the end-leaves of the chain uses the path containing the spine of the chain, which is the same length for both pendant level-1 and pendant level-2 blobs. Whenever these chains contain at least 4 leaves, a shortest path no longer contains the spine; since such

paths differ in distance for pendant level-1 and pendant level-2 blobs with a single chain, we are able to identify such pendant blobs. We later show that level-2 networks that do not contain bad blobs are reconstructible from their shortest distances (Corollary 2).

The following lemma states that if we can identify certain structures within level-2 networks, then we may replace them by a leaf, and we may obtain the distance matrix of the reduced network.

**Lemma 7.** *Let  $N$  be a level-2 network on  $X$  with a pendant blob  $B$ , and replace  $B$  by a leaf  $z \notin X$  to obtain the network  $N'$ . Letting  $Y$  denote the set of leaves contained in  $B$ , we have that the sl-distance matrix of  $N'$  contains the elements*

$$d^{N'}(p, q) = d^N(p, q)$$

for all pair of leaves  $p, q \in X - Y$ . Now, for all  $p \in X - Y$ , we have the following.

- **$B$  is a pendant level-1 blob with the chain  $(a, k)$ :**

$$d^{N'}(p, z) = \{d_m^N(p, a) - 2, d_l^N(p, a) - (k + 1)\}$$

- **$B$  is a pendant level-2 blob of the form  $F$ :**

$$d^{N'}(p, z) = \begin{cases} \{d_m^N(p, a) - 3, d_l^N(p, a) - (k + 3)\} & \text{if } F = (a, 0, 0, 0) \\ \{d_m^N(p, a) - 3, d_l^N(p, a) - (k + \ell + 3)\} & \text{if } F = (a, b, 0, 0) \\ \{d_m^N(p, c) - 2, d_l^N(p, c) - (k + m + 3)\} & \text{if } F = (a, 0, c, 0) \\ \{d_m^N(p, c) - 2, d_l^N(p, c) - (\max\{k, \ell\} + m + 3)\} & \text{if } F = (a, b, c, 0) \\ \{d_m^N(p, c) - 2, d_l^N(p, c) - (k + m + n + 3)\} & \text{if } F = (a, 0, c, d) \\ \{d_m^N(p, c) - 2, d_l^N(p, c) - (\max\{k, \ell\} + m + n + 3)\} & \text{if } F = (a, b, c, d) \end{cases}$$

**Proof.** To obtain the inter-taxa distances for  $N'$ , it suffices to simply subtract the shortest/longest distances from the vertex of the pendant blob incident to the non-trivial cut-edge to an end-spine leaf of a chain. These distances are easy to obtain as we know exactly what the pendant blobs are in all cases, due to Lemma 6. □

The above two lemmas will now be combined to prove the following result.

**Theorem 3.** *Level-2 networks are reconstructible from their sl-distance matrix.*

**Proof.** We prove by induction on the size of the network. For the base case, a network on a single edge has two leaves, which is trivially reconstructible from its shortest distances. In fact, we know by Lemma 2 that a network on a single blob is reconstructible from its shortest distances. So suppose that we are given a level-2 network  $N$  with  $|E(N)|$  edges, and that the result holds for all level-2 networks with at most  $|E(N)| - 1$  edges.

We may assume that  $N$  contains at least two pendant blobs. By the results in Section 2.4, we can partition the leaves into chains, and adjacency between chains can be obtained from sl-distance matrices. By Theorem 2, we can obtain all cut-edge induced splits of  $N$  from its shortest distance matrix; by Lemma 6, we can identify all pendant blobs from these splits, by using the sl distance matrix. We can also replace one of these pendant blobs by a leaf  $z$  to obtain a smaller level-2 network  $N'$ , for which its shortest and longest inter-taxa distances can be obtained by Lemma 7. By induction hypothesis,  $N'$  is reconstructible. Then, we can obtain a network isomorphic to  $N$  by replacing the leaf  $z$  with the pendant blob that was originally present.

To see that this network is unique, consider another network  $M$  that is not isomorphic to  $N$  such that  $M$  induces the same sl-distance matrix as  $N$ . Note that  $M$  must also contain a pendant blob  $P$ , and upon replacing  $P$  in  $M$  by a leaf  $z$ , we get by the induction hypothesis that the resulting network  $M'$  must be isomorphic to  $N'$ . We obtain a network isomorphic to  $M$  by replacing the leaf  $z$  by  $P$  in  $M'$ : but this operation yields a network that is also isomorphic to  $N$ . It follows that  $N$  and  $M$  must be isomorphic.

Therefore, level-2 networks are reconstructible from their sl-distance matrices. □

As stated before, it is possible to distinguish all pendant blobs from the shortest distances matrices if the networks do not contain the bad blobs. It follows then that the proof of Theorem 3 can be adapted to prove the following corollary, when we look at restricted level-2 networks.

**Corollary 2.** *Let  $N$  be a level-2 network containing no bad blobs. Then  $N$  is reconstructible from its shortest distance matrix.*

A direct consequence of Theorem 3 and Corollary 2, for restricted level-2 networks, is that by iteratively reducing pendant subtrees and pendant blobs from a network, it is possible to reconstruct the network from its sl-distance matrix and shortest distance matrix, respectively. Note that subtree reduction may be necessary after a few iterations of reducing pendant blobs from a network, as it is possible to obtain cherries from such reductions. Therefore the above results implicitly give an algorithm for reconstructing level-2 networks from their sl-distance matrices.

Completely excluding all bad blobs is quite restrictive. There can indeed exist networks that contain bad blobs that are still reconstructible from their shortest distances. For example, take a network in which there is exactly one bad blob. By reducing all cherries and all other pendant blobs before we reduce the bad blob, we are able to obtain a network on a single blob (which is necessarily the bad blob). Since networks on single blobs are reconstructible by Lemma 2, it follows then that the original network is also reconstructible. Therefore, in an effort to weaken the restriction of completely disallowing bad blobs, we next aim to characterize level-2 networks that are not reconstructible from their shortest distances.

## 5. Characterization of level-2 networks that cannot be reconstructed from their shortest distances

In this section we show that level-2 networks that cannot be reconstructed from their shortest distances can be categorized by a type of subgraph that they must contain. We only consider shortest distances in this section; we use  $d^N(x, y)$  to denote the shortest distance between two vertices  $x$  and  $y$  in a network  $N$ .

### 5.1. Alt-path structures

Let  $T$  be any binary tree with labeled leaves. Two-color the vertices of  $T$  with colors black and red. Let  $G$  denote a graph obtained by

- replacing each black internal vertex by a certain level-2 blob. That is, for each internal vertex  $v$  with neighbors  $u_i$  for  $i \in [3]$ , delete  $v$ , add vertices  $v_i, n_v, s_v$  and edges  $u_i v_i, n_v v_i, s_v v_i$  for  $i \in [3]$ ;
- replacing each black leaf by a pendant level-2 blob of the form  $(2, 0, 0, 0)$  or  $(3, 0, 0, 0)$ ; and
- replacing each red leaf by a pendant level-1 blob with two or three leaves.

The leaves of  $G$  are unlabeled. We call  $G$  an *alt-path structure* of  $T$ . We may obtain another alt-path structure  $H$  of  $T$  by swapping the roles of the red and black vertices in the blob replacement step. We say that  $H$  is *similar* to  $G$  if every pendant blob of  $H$  that replaces a leaf  $l$  of  $T$  contains the same number  $s$  of leaves as that of  $G$  that replaces  $l$ . See Fig. 7 for an example of obtaining two similar alt-path structures from the same binary tree. Note that every binary tree  $T$  on at least two leaves gives rise to exactly two alt-path structures, and these are similar to each other.

We say that a network *contains* an alt-path structure of some tree if the alt-path structure is a subgraph of the network up to deleting leaf labels. Suppose that  $N$  contains an alt-path structure  $G$  of some tree  $T$ . Let  $H$  be the similar alt-path structure of  $G$ . The operation of *replacing*  $G$  by its similar alt-path structure is the action of replacing the subgraph  $G$  by  $H$  in  $N$ .

**Lemma 8.** *Similar alt-path structures of a given binary tree realize the same shortest distance matrix.*

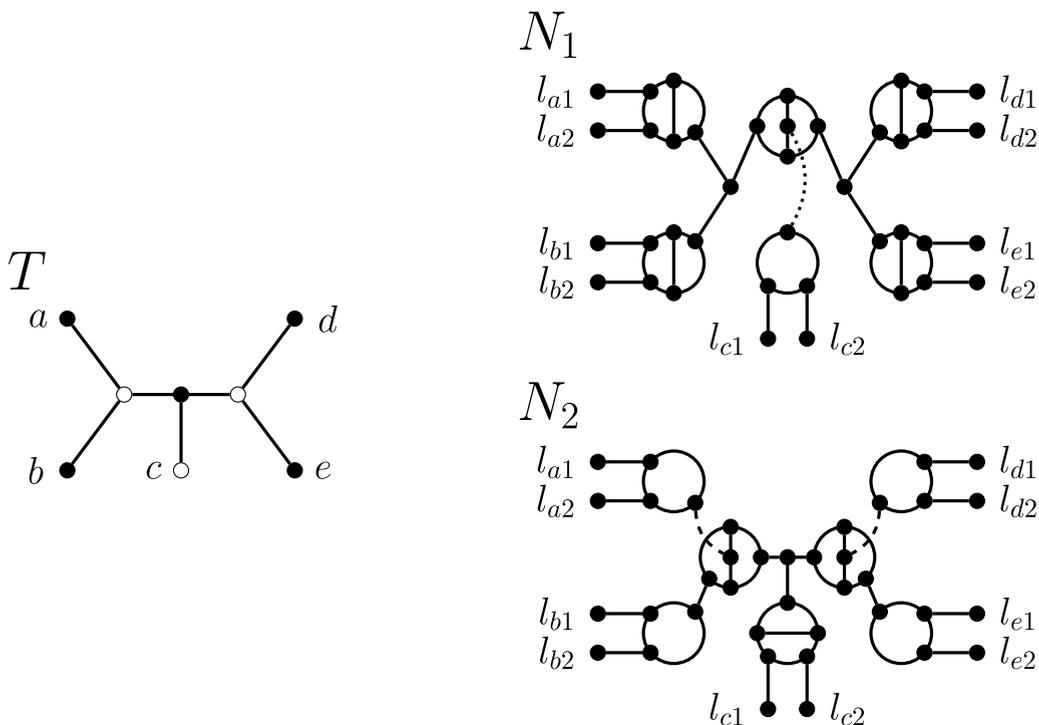
**Proof.** Let  $N$  be a level-2 network that is an alt-path structure  $G$  of some binary tree  $T$ . Let  $N'$  be a network obtained from  $N$  by replacing  $G$  by its similar alt-path structure.

Let  $x$  and  $y$  denote two leaves in  $N$ . The two networks  $N$  and  $N'$  both contain the same chains by construction. Furthermore, each chain is of length at most 3. Thus we have that  $d^N(x, y) = d^{N'}(x, y)$  if  $x$  and  $y$  are contained in the same chains. So we may assume that  $x$  and  $y$  are contained in different chains. We wish to show that  $d^N(x, y) = d^{N'}(x, y)$ . Consider the leaves  $l_x$  and  $l_y$  of  $T$  that were replaced by the pendant blobs containing  $x$  and  $y$ , respectively. If  $d_T(l_x, l_y)$  is odd, then there is an even number of internal vertices in the path between  $l_x$  and  $l_y$  in  $T$ . This means that  $N$  and  $N'$  contain the same number of non-pendant level-2 blobs and the same number of non-leaf vertices not contained in blobs in the shortest path between  $x$  and  $y$ . Moreover, due to parity, exactly one of the two leaves will be contained in a pendant level-1 blob in  $N$  and the other leaf in a pendant level-2 blob. The reverse is true for  $N'$ . Thus it follows that if  $d_T(l_x, l_y)$  is odd, then  $d^N(x, y) = d^{N'}(x, y)$ . Now if  $d_T(l_x, l_y)$  is even, the number of non-pendant level-2 blobs in the shortest path between  $x$  and  $y$  will be greater by one in either  $N$  or in  $N'$ . Without loss of generality, suppose that  $N$  has this property. But this difference is offset by the fact that the pendant blobs in this path are both level-1 in  $N$ , whereas they are both level-2 in  $N'$ . Therefore  $d^N(x, y) = d^{N'}(x, y)$ .  $\square$

**Corollary 3.** *Let  $N$  be a level-2 network containing an alt-path structure  $G$  of some binary tree  $T$  as a subgraph. Then  $N$  is not reconstructible from its shortest distance matrix.*

**Proof.** Let  $N'$  denote the network obtained from  $N$  by replacing  $G$  by its similar alt-path structure. We claim that the distinct networks  $N$  and  $N'$  must realize the same shortest distance matrix, thereby proving that  $N$  is not reconstructible from its shortest distance matrix. Consider any two leaves  $x$  and  $y$  of  $N$ , and let  $P$  denote a shortest path between  $x$  and  $y$  in  $N$ . If  $P$  does not contain any edges of  $G$ , then a path between  $x$  and  $y$  on the same length must exist in  $N'$ , since only the subgraph  $G$  of  $N$  was changed to obtain  $N'$ . On the other hand, if  $P$  contains an edge of  $G$ , then  $P$  must contain exactly one path of  $G$  that starts and ends at two leaves  $l_1, l_2$  of  $G$ . Since only the subgraph  $G$  of  $N$  was changed to obtain  $N'$ , we have that  $d^N(x, l_1) = d^{N'}(x, l_1)$ , and that  $d^N(l_2, y) = d^{N'}(l_2, y)$ . By Lemma 8, we have that  $d^N(l_1, l_2) = d^{N'}(l_1, l_2)$ . So a path between  $x$  and  $y$  on the same length must also exist in  $N'$ . It follows that  $d^N(x, y) \leq d^{N'}(x, y)$ .

Now consider a shortest path  $Q$  between  $x$  and  $y$  in  $N'$ . By applying the same arguments to  $Q$ , but with the alt-path structure that is similar to  $G$ , we conclude that  $d^N(x, y) \leq d^{N'}(x, y)$ . This proves that  $d^N(x, y) = d^{N'}(x, y)$ .  $\square$



**Fig. 7.** An example of obtaining two alt-path structures from a binary tree  $T$ . The network  $N_1$  is obtained by replacing all filled internal vertices by a level-2 blob with each cut-edge subdividing the three different sides, filled leaf vertices by a pendant level-2 blob of the form  $(k, 0, 0, 0)$  for  $k = 2$  (note that this can also be  $k = 3$ ), and unfilled leaf vertices by a pendant level-1 blob of 2 or 3 leaves. The similar alt-path structure  $N_2$  is obtained by the same construction, with the roles of filled and unfilled vertices reversed. Observe that  $N_1$  and  $N_2$  have the same shortest distance matrix, as stated in [Lemma 8](#).

It is now easy to explain why the two networks in [Fig. 1](#) realize the same shortest distance matrix; they contain similar alt-path structures of a binary tree on two leaves. We show in the next subsection that the converse of [Corollary 3](#), that a level-2 network containing no alt-path structure is reconstructible, is also true.

5.2. Level-2 networks without alt-path structures are reconstructible

We introduce some more terminology. Let  $N$  be a level-2 network. A *blob tree* of  $N$  is the graph obtained by contracting all edges of blobs, deleting all labeled leaves, and suppressing all degree-2 vertices. A vertex of a blob-tree is called a *blob-vertex*. We define the *connection* of a pendant blob as the endpoint of the non-trivial cut-edge incident to the blob that is not on the blob. We say that a blob  $B$  contains a pendant blob  $C$  if the connection of  $C$  is a vertex of  $B$ . For any blob  $B$  in  $N$ , we let  $l(B)$  denote the level of  $B$ .

Let  $P_1$  be a bad pendant blob on two leaves  $l_1, l_2$ , and let  $u$  be a vertex of  $N$  that is not a neighbor of  $l_1$  nor  $l_2$ . We let  $d^N(P_1, u) = d^N(l_1, u)$  denote the shortest distance between  $P_1$  and  $u$ . This is well-defined for all bad pendant blobs containing exactly two leaves, since the shortest distance from either of the two leaves to any other vertex in the network is the same. Let  $P_2$  be another bad pendant blob on two leaves  $l'_1, l'_2$ . Then we may similarly define the shortest distance between  $P_1$  and  $P_2$  by  $d^N(P_1, P_2) = d^N(l_1, l'_1)$ . This again is well-defined as the two bad pendant blobs both contain two leaves.

Let  $P_1$  and  $P_2$  be two pendant blobs that are contained in the same blob  $B$ . Let  $p_1$  and  $p_2$  be the connections of  $P_1$  and  $P_2$ , respectively. We say that  $P_1$  and  $P_2$  are *adjacent* if  $p_1$  and  $p_2$  are adjacent. Let  $l$  be a leaf that is not contained in  $P_1$ . We say that  $l$  and  $P_1$  are *adjacent* if the neighbor of  $l$  is adjacent to  $p_1$ . We say that  $P_1$  is *adjacent* to a chain of leaves  $(a, k)$  if  $P_1$  is adjacent to an end-leaf of  $(a, k)$ .

**Lemma 9.** Let  $N$  be a level-2 network on  $X$  containing a bad pendant blob with 3 leaves  $(a_1, a_2, a_3)$ , and let  $N'$  denote the network obtained by deleting  $a_2$  from  $N$ . Then the shortest distance matrix realized by  $N'$  is given by

$$d^{N'}(x, y) = \begin{cases} d^N(x, y) & \text{if } x, y \in X - \{a_2\} \text{ and } \{x, y\} \neq \{a_1, a_3\}; \\ 3 & \text{if } \{x, y\} = \{a_1, a_3\}. \end{cases}$$

**Proof.** The only shortest paths containing the edges incident to the neighbor of  $a_2$  in  $N$  were those involving  $a_2$ , or a path between  $a_1$  and  $a_3$ . Since  $a_2$  is no longer a leaf in  $N'$ , the only path that is affected in the leaf deletion is the shortest path between  $a_1$  and  $a_3$ , which is now of length 3 in  $N'$ .  $\square$

We are now ready to prove the main theorem of the section. Because the proof exhaustively checks for contradictions within each case, it is rather long, and so we split the three main cases of the proof into subsubsections. In each subsubsection, a short summary will be given to clarify the proof steps.

**Theorem 4.** *A level-2 network containing no alt-path structure is reconstructible from its shortest distances.*

**Proof.** Suppose for a contradiction that there exist distinct networks  $N$  and  $N'$  with no alt-path structures that realize the same shortest distance matrix. In particular, choose  $N$  and  $N'$  to be minimal counter-examples with respect to the size of the networks. This means that every pendant blob of  $N$  and  $N'$  must be a bad blob; indeed, all other pendant blobs are identifiable from the shortest distance matrix by Lemma 7, and thus can be reduced otherwise, allowing for smaller counter-examples to exist. We may further assume that all pendant bad blobs contain exactly two leaves, as otherwise we can find a smaller counter-example by calling Lemma 9. Finally, observe that if  $N$  contains a pendant level-1 blob with some leaves  $l_1, l_2$ , then  $N'$  must contain a pendant level-2 blob of the form  $(2, 0, 0, 0)$  containing the leaves  $l_1, l_2$ , as again we would be able to obtain a smaller counter-example otherwise. Similarly, if  $N$  contains a pendant level-2 blob of the form  $(2, 0, 0, 0)$  with leaves  $l_1, l_2$  then  $N'$  must contain a pendant level-1 blob with leaves  $l_1, l_2$ . If  $N$  contains a pendant blob  $P_i$ , we say that  $N'$  contains the *corresponding* pendant blob  $P'_i$  on the same leaves such that  $l(P_i) \neq l(P'_i)$ . For each pendant blob  $P_i, P'_i$  in  $N, N'$ , we let  $p_i, p'_i$  denote their connections, respectively.

Since  $N$  and  $N'$  realize the same shortest distance matrix, the two networks have the same cut-edge induced splits by Theorem 2. Since each cut-edge in our networks induces a unique split, this implies that their blob-trees must be identical. This follows as every edge of the blob tree is a cut-edge of the network, and because trees are uniquely determined by their induced splits [7]. Note that the blob-vertices of the blob-trees correspond to either a degree-3 vertex, a level-1 blob, or a level-2 blob of the network. Observe that the blob-tree of  $N$  must contain at least 3 blob-vertices, as otherwise  $N$  would be a level-2 network with a single blob – which is reconstructible from their shortest distances by Lemma 2 – or a level-2 network with two pendant blobs, which implies that  $N$  must contain an alt-path structure as  $N$  contains only bad pendant blobs, or  $N$  and  $N'$  cannot realize the same shortest distance matrix.

Consider the blob-vertex  $u$  whose neighbors are all leaves, except possibly for one neighbor; let  $uv$  denote the edge in the blob-tree to this one neighbor. Since every edge of the blob-tree corresponds to a non-trivial cut-edge in the network, the edge  $uv$  must be incident to a degree-3 vertex/blob which correspond to  $u$  in  $N$  and  $N'$ . Let  $B, B'$  denote the corresponding structures in  $N, N'$ , respectively. Then  $B$  contains at least one pendant blob, possibly some chain of leaves, and the cut-edge  $uv$  incident to it, with  $u$  as a vertex of  $B$ . The same can be said for  $B'$ , but we use  $u'$  instead of  $u$  to be the vertex of  $B'$  incident to the cut-edge for clarity. Note that it is possible for  $u$  and  $u'$  to be a connection of some pendant blob. Let  $\bar{B}$  be the graph obtained from  $N$  by deleting the edge  $uv$  and taking the component containing  $u$ . Similarly define  $\bar{B}'$  as the graph obtained from  $N'$  by deleting the edge  $u'v$  and taking the component containing  $u'$ . Since we have deleted the edges corresponding to the same edge in the blob-tree,  $\bar{B}$  and  $\bar{B}'$  contain the same chains, and  $\bar{B}$  contains a pendant blob if and only if  $\bar{B}'$  contains the corresponding pendant blob. Observe that  $\bar{B}$  and  $\bar{B}'$  are not networks because they contain a degree-2 vertex  $u$  and  $u'$ , respectively. However, to avoid having to introduce new notation, we shall still use terms defined for networks, such as blobs containing pendant blobs, pendant blobs being adjacent to one another in  $\bar{B}$  and  $\bar{B}'$ .

The rest of the proof will be as follows. We consider the cases where  $B$  is a degree-3 vertex, a level-1 blob, or a level-2 blob. Based on the graph  $\bar{B}$  in comparison with the graph  $\bar{B}'$ , we seek a contradiction with regard to the networks realizing the shortest distance matrix and the choice of the minimum counter-example. Because the results are symmetric, it is worth mentioning that once we have proven the case for when  $B$  is a degree-3 vertex, then we may assume that  $B'$  is also not a degree-3 vertex. After we prove the case for when  $B$  is a level-1 blob, then we may assume that  $B'$  is also not a level-1 blob.

The following claim will be used extensively throughout the proof.

**Claim 1.** *Let  $x, y$  be leaves in  $\bar{B}$ . Then*

$$d^N(x, u) - d^{N'}(x, u') = d^N(y, u) - d^{N'}(y, u').$$

**Proof.** Let  $z$  be a leaf of  $N$  that is not in  $\bar{B}$ . Such a leaf must exist by our choice of  $B$ , and in particular,  $z$  must be reachable from  $B$  via  $uv$ . Then we have

$$\begin{aligned} d^N(z, x) &= d^N(z, u) + d^N(u, x) \\ d^N(z, y) &= d^N(z, u) + d^N(u, y), \end{aligned}$$

which gives

$$d^N(z, x) - d^N(z, y) = d^N(x, u) - d^N(y, u).$$

Similarly we have

$$d^{N'}(z, x) - d^{N'}(z, y) = d^{N'}(x, u') - d^{N'}(y, u').$$

Since the shortest distance matrices of  $N$  and  $N'$  are the same, we have

$$d^N(x, u) - d^{N'}(x, u') = d^N(y, u) - d^{N'}(y, u'). \quad \square$$

5.2.1.  **$B$  is a degree-3 vertex in  $N$**

Suppose first that a leaf  $l$  is a neighbor of  $u$  in  $\bar{B}$ , and let  $P_1$  be a pendant blob in  $\bar{B}$  whose connection is  $u$ . Since  $N'$  has the same cut-edge induced splits,  $\bar{B}'$  must either be a degree-3 vertex or a blob that contains  $l$  and the corresponding pendant blob  $P'_1$ . But then

$$d^N(P_1, l) = 4,$$

whereas

$$d^{N'}(P'_1, l) \geq 5,$$

which contradicts the fact that  $N$  and  $N'$  must realize the same shortest distance matrix.

So now suppose that  $u$  is the connection of two pendant blobs  $P_1$  and  $P_2$  in  $\bar{B}$ . We check the three possible scenarios with regard to the levels of  $P_1$  and  $P_2$ .

1.  **$l(P_1) = 1$  and  $l(P_2) = 1$** : Then we have  $d^N(P_1, P_2) = 6$ . But since  $l(P'_1) = l(P'_2) = 2$ , we must have that  $d^{N'}(P'_1, P'_2) \geq 8$ . This contradicts the fact that  $N$  and  $N'$  realize the same shortest distance matrix.
2.  **$l(P_1) = 1$  and  $l(P_2) = 2$** : Then we have  $d^N(P_1, P_2) = 7$ . Since  $l(P'_1) = 2$  and  $l(P'_2) = 1$ , we have that  $d^{N'}(P'_1, P'_2) \geq 7$ , where equality is achieved whenever  $u'$  is a degree-3 vertex. But this would mean that

$$d^N(P_1, u) - d^{N'}(P'_1, u') = -1,$$

whereas

$$d^N(P_2, u) - d^{N'}(P'_2, u') = 1,$$

which contradicts [Claim 1](#).

3.  **$l(P_1) = 2$  and  $l(P_2) = 2$  (see [Fig. 8 for an illustration of the cases](#))**: Then  $d^N(P_1, P_2) = 8$ . Since  $l(P'_1) = l(P'_2) = 1$ , and because  $N'$  contains a split with one of the sets containing exactly the leaves of  $P'_1$  and  $P'_2$ ,  $\bar{B}'$  must be a level-2 blob.

In particular,  $P'_1$  and  $P'_2$  cannot be adjacent. There are two possibilities for this –  $u'$  is a neighbor of one of  $p'_1$  or  $p'_2$  but not the other, or all three vertices  $u', p'_1, p'_2$  are pairwise non-adjacent (i.e., they all lie on different main paths of  $\bar{B}'$ ). In the former case, we have that, assuming without loss of generality that  $u'$  is adjacent to  $p'_1$ ,

$$d^N(P_1, u) - d^{N'}(P'_1, u') = 4 - 4 = 0,$$

whereas

$$d^N(P_2, u) - d^{N'}(P'_2, u') = 4 - 5 = -1,$$

which contradicts [Claim 1](#). For the latter case, we claim that there is a smaller counter-example. We replace  $\bar{B}$  in  $N$  by a pendant level-1 blob  $P_3$  containing two leaves  $l_1, l_2$ . We replace  $\bar{B}'$  in  $N'$  by a pendant level-2 blob  $P'_3$  of the form  $(2, 0, 0, 0)$  with the same leaves  $l_1, l_2$ . Then, we may adjust the shortest distance matrix by first deleting elements containing the leaves of  $P_1$  and  $P_2$ . And for all other leaves  $z$  in the network, we add the elements

$$d^N(l_i, z) = d^N(P_1, z) - 2,$$

and

$$d^{N'}(l_i, z) = d^{N'}(P'_1, z) - 2$$

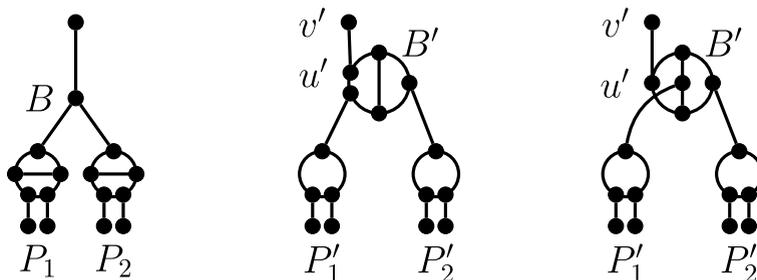
for  $i = 1, 2$ . All other matrix elements remain the same. Note that before the replacement of the blobs,

$$d^N(P_1, u) = d^N(P_2, u) = 4,$$

and

$$d^{N'}(P'_1, u') = d^{N'}(P'_2, u') = 5.$$

The replacement of  $\bar{B}$  and  $\bar{B}'$  by pendant level-1 and level-2 blobs, respectively ensures that the distance differences are preserved. Therefore the modified networks both must satisfy this new reduced shortest distance matrix. These modified networks  $N$  and  $N'$  still contain no alt-path structures, as otherwise the original networks also must have contained alt-path structures; all other parts of the networks remain unchanged, and the two leaves  $l_1$  and  $l_2$  are contained in pendant blobs of different level in  $N$  and  $N'$ . Therefore, this gives a counter-example on fewer leaves than that of  $N$  and  $N'$ , contradicting our original choice of  $N$  and  $N'$ .



**Fig. 8.** Section 5.2.1 case 3 in the proof of Theorem 4. The left figure is the part of the network  $N$  containing the internal vertex  $B$  and its neighboring pendant blobs. The middle and the right figures are the two subcases for what  $N'$  could look like. In the middle network, two cut-edges are incident to the same side; in the right network, the three cut-edges are incident to distinct sides of  $B'$ .

5.2.2.  $B$  is a level-1 blob in  $N$ :

We may now also assume that  $B'$  is either a level-1 or a level-2 blob. Note that either  $\bar{B}$  or  $\bar{B}'$  must contain a pendant level-1 blob, and that we shall obtain a contradiction in each of those cases. Before we do so, we prove a claim that will be used in many of the arguments to come. In the following claim, we assume that  $B$  is either a level-1 or a level-2 blob.

**Claim 2.** Suppose  $l(B), l(B') \in \{1, 2\}$ , and suppose that  $\bar{B}$  contains a pendant level-1 blob  $P_1$ . Then,

- (i)  $P_1$  cannot be adjacent to a chain of leaves  $(a, k)$  in  $\bar{B}$ ;
- (ii)  $P_1$  cannot be adjacent to another pendant level-1 blob in  $\bar{B}$ ;
- (iii)  $P_1$  is adjacent to a pendant level-2 blob  $P_2$  in  $\bar{B}$  if and only if  $P'_1$  and  $P'_2$  are adjacent in  $\bar{B}'$ ;
- (iv)  $P_1$  is adjacent to at most one pendant level-2 blob in  $\bar{B}$ . In particular, this means that every pendant level-2 blob in  $\bar{B}$  is adjacent to at most one pendant level-1 blob.
- (v)  $P_1$  can be shortest distance 6 away from at most two end-leaves of distinct chains in  $\bar{B}$ .

**Proof.**

- (i) If  $P_1$  is adjacent to a chain of leaves  $(a, k)$ , then one of the end-leaves of  $(a, k)$  must be shortest distance 5 away from  $P_1$ . Without loss of generality, suppose that  $d^N(P_1, a_1) = 5$ . In  $B'$ , since  $l(B') = 2$ , we must have that  $d^{N'}(P'_1, a_1) \geq 6$ , which contradicts the fact that  $N$  and  $N'$  must realize the same shortest distance matrix.
- (ii) If  $P_1$  is adjacent to another pendant level-1 blob  $P_2$ , then  $d^N(P_1, P_2) = 7$ . In  $\bar{B}'$ , both corresponding pendant blobs are of level-2. This means that  $d^{N'}(P'_1, P'_2) \geq 8$ , which contradicts the fact that  $N$  and  $N'$  must satisfy the same shortest distance matrix.
- (iii) If  $P_1$  is adjacent to  $P_2$ , then we have  $d^N(P_1, P_2) = 8$ . Since  $N$  and  $N'$  satisfy the same shortest distance matrix, one must also have  $d^{N'}(P'_1, P'_2) = 8$ . The shortest distance from  $P'_1$  to its connection  $p'_1$ , and that from  $P'_2$  to its connection  $p'_2$  is 3 and 4, respectively. Since  $l(B') \in \{1, 2\}$ , the vertices  $p'_1$  and  $p'_2$  cannot be the same. Therefore to satisfy  $P'_1$  and  $P'_2$  being shortest distance 8 from one another in  $\bar{B}'$ , one must have that  $p'_1$  and  $p'_2$  are adjacent, which means that  $P'_1$  and  $P'_2$  must be adjacent. The converse follows by symmetry.
- (iv) Suppose for a contradiction that  $P_1$  is adjacent to two pendant level-2 blobs  $P_2$  and  $P_3$  in  $\bar{B}$ . Then  $d^N(P_2, P_3) = 10$ . By 3., we know that  $P'_1$  must be adjacent to both  $P'_2$  and  $P'_3$  in  $\bar{B}'$ . We also know that  $l(P'_2) = l(P'_3) = 1$ . It follows that  $d^{N'}(P'_2, P'_3) = 8$ . But this contradicts the fact that  $N$  and  $N'$  must realize the same shortest distance matrix. If a pendant level-2 blob is adjacent to two pendant level-1 blobs, then the corresponding pendant level-1 blob in  $\bar{B}'$  is adjacent to two pendant level-2 blobs, which we have just shown cannot be true.
- (v) Suppose  $l$  is an end-leaf of a chain such that  $d^N(P_1, l) = 6$ . Since  $l(B') = 2$ , and since  $N$  and  $N'$  realize the same shortest distance matrix, the leaf  $l$  must be adjacent to  $P'_1$  in  $\bar{B}'$ . So every leaf that is shortest distance 6 away from  $P_1$  in  $\bar{B}$  must be adjacent to  $P'_1$  in  $\bar{B}'$ . Note that  $P'_1$  can be adjacent to at most two chains. These chains must be distinct in  $\bar{B}'$ , since  $u'$  is contained in  $\bar{B}'$ . This implies that in  $\bar{B}$ ,  $P_1$  can be shortest distance 6 away from at most two end-leaves of distinct chains.  $\square$

It follows that each main path of  $\bar{B}$  (and  $\bar{B}'$ ) may contain at most two pendant level-1 blobs. Either  $\bar{B}$  or  $\bar{B}'$  must contain a pendant level-1 blob.

1.  $\bar{B}$  has a pendant level-1 blob  $P_1$ : Since  $N$  contains no parallel edges, and since leaves cannot be adjacent to pendant level-1 blobs,  $P_1$  must be adjacent to a pendant level-2 blob  $P_2$  in  $\bar{B}$ . By Claim 2 (iv),  $P_1$  can be adjacent to at most one pendant level-2 blob in  $\bar{B}$ . This implies that  $p_1$  must be adjacent to  $u$ . In  $N'$ , the corresponding pendant blobs  $P'_1$  and  $P'_2$  are adjacent by Claim 2 (iii). Then we have that

$$d^N(P_1, u) - d^N(P_2, u) \leq 4 - 5 = -1.$$

Observe that  $d^{N'}(P'_1, p'_1) = 4$  and  $d^{N'}(P'_2, p'_1) = 4$  since  $l(P'_1) = 2$  and  $l(P'_2) = 1$ . This implies that

$$\begin{aligned} d^{N'}(P'_1, u') - d^{N'}(P'_2, u') &\geq d^{N'}(P'_1, p'_1) + d^{N'}(p'_1, u') - d^{N'}(P'_2, p'_1) - d^{N'}(p'_1, u') \\ &= 4 - 4 \\ &= 0, \end{aligned}$$

which is a contradiction to [Claim 1](#).

2.  **$\bar{B}'$  has a pendant level-1 blob  $P'_1$** : If  $l(B') = 1$ , then we are done by symmetry via case 1. So suppose that  $l(B') = 2$ , and suppose in addition that  $\bar{B}$  contains no pendant level-1 blobs. This implies that  $\bar{B}'$  contains no pendant level-2 blobs. We claim that  $\bar{B}'$  also contains no pendant level-1 blobs other than  $P'_1$ . Suppose for a contradiction that it did, so that  $\bar{B}'$  contains another pendant level-1 blob  $P'_2$ . Because  $\bar{B}'$  contains no pendant level-2 blobs, and since leaves cannot be adjacent to pendant level-1 blobs by [Claim 2](#), we must have that  $p'_1$  and  $p'_2$  are adjacent to the same pole, or that they must both be adjacent to  $u'$ . In any case, we must have  $d^{N'}(P'_1, P'_2) = 8$ . But  $l(P_1) = l(P_2) = 2$ , and therefore  $d^N(P_1, P_2) \geq 9$ , which is a contradiction. So  $P'_1$  is the only pendant blob in  $\bar{B}'$ .

We now consider two possible cases: either  $p'_1$  is or is not adjacent to  $u'$ . Either way, at least one main path of  $B'$  that does not contain  $p'_1$  must contain a chain of leaves, as otherwise  $B'$  contains parallel edges, or  $B'$  is a level-2 blob with only two cut-edges incident to it.

- (a)  **$p'_1$  is adjacent to  $u'$** : One of the main paths of  $\bar{B}'$  must contain a chain, since  $N'$  does not contain parallel edges. So there must exist a leaf  $l$  that is shortest distance 6 away from  $P'_1$ . Then

$$d^{N'}(P'_1, u') - d^{N'}(l, u') \leq 4 - 3 = 1.$$

On the other hand, in  $\bar{B}$ , the leaf  $l$  is adjacent to  $P_1$ ; then  $d^N(P_1, p_1) = 4$  and  $d^N(l, p_1) = 2$ . It follows that

$$\begin{aligned} d^N(P_1, u) - d^N(l, u) &\geq d^N(P_1, p_1) + d^N(p_1, u) - d^N(l, p_1) - d^N(p_1, u) \\ &= 2, \end{aligned}$$

which contradicts [Claim 1](#).

- (b)  **$p'_1$  is not adjacent to  $u'$** : Observe that  $\bar{B}'$  has five sides: two sides  $s'_1, s'_2$  which have  $p'_1$  as one of their boundary vertices; two sides  $s'_3, s'_4$  which have  $u'$  as one of their boundary vertices; and one side  $s'_5$  that has neither  $p'_1$  nor  $u'$  as a boundary vertex. By [Claim 2 \(i\)](#) and (v), the sides  $s'_1$  and  $s'_2$  are empty, and at most two of the three remaining sides of  $\bar{B}'$  may contain chains. In particular, at least one of these remaining three sides must contain a chain. We first show that  $s'_5$  must be empty. Suppose not, and let  $(a, k)$  denote the chain contained in  $s'_5$ . Note that both end-leaves of  $(a, k)$  are shortest distance 6 away from  $P'_1$ , and so by [Claim 2 \(v\)](#), this chain must be of length  $k = 1$ . Since either  $s'_3$  or  $s'_4$  must be empty,

$$d^{N'}(a_1, u') - d^{N'}(P'_1, u') = 3 - 5 = -2.$$

In  $\bar{B}$ , the blob  $P_1$  and the leaf  $a_1$  must be adjacent. The vertex  $u$  must be adjacent to the neighbor of  $a_1$ , since  $\bar{B}$  contains no other pendant blobs. So we have

$$d^N(a_1, u) - d^N(P_1, u) \leq 2 - 5 = -3,$$

which contradicts [Claim 1](#). So  $s'_5$  is empty.

Now suppose that  $s'_3$  and  $s'_4$  contain the chains  $(b, \ell)$  and  $(c, m)$ , respectively, where at least one of  $\ell \geq 1$  or  $m \geq 1$  holds. If  $\ell = 1$  and  $m = 0$ , then  $\bar{B}'$ , together with the edge incident to  $u'$  is an alt-path structure of a binary tree on two leaves. This contradicts our choice of  $N'$ . By symmetry, the case  $m = 1$  and  $\ell = 0$  is also not possible. So we may assume that  $\ell \geq 1$  and  $m \geq 1$ . Suppose the chains are arranged such that

$$d^{N'}(b_1, u') = d^{N'}(c_1, u') = 2.$$

If  $\ell > 1$  or  $m > 1$ , then  $d^{N'}(b_\ell, c_m) = 5$ , whereas  $d^N(b_\ell, c_m) = 4$ . This contradicts the fact that  $N$  and  $N'$  realize the same shortest distance matrix. So we must have  $\ell = m = 1$ . But then  $\bar{B}'$ , together with the edge incident to  $u'$  is an alt-path structure of a binary tree on two leaves. This contradicts our choice of  $N'$ .

### 5.2.3. $B$ is a level-2 blob in $N$ :

Our only remaining case is if  $B$  and  $B'$  are both level-2 blobs. The proofs of [Claims 3–5](#) are given in the appendix.

**Claim 3.** *Two pendant level-2 blobs cannot be adjacent to one another in  $\bar{B}$  and in  $\bar{B}'$ .*

An immediate consequence of [Claim 3](#) is that distinct pendant level-1 blobs in  $\bar{B}$  or  $\bar{B}'$  must be distance at least 10 apart. In particular, they cannot be adjacent by [Claim 2](#) and they cannot be shortest distance-8 apart, since two pendant level-2 blobs are shortest distance at least 9 apart. The following claim dictates the placement of pendant blobs and leaves in  $\bar{B}$ .

**Claim 4.** A pendant level-2 blob may not be adjacent to both a pendant level-1 blob and a leaf simultaneously in  $\bar{B}$  and in  $\bar{B}'$ .

Pendant level-1 blobs may be adjacent to at most one pendant level-2 blob by Claim 2. Pendant level-2 blobs cannot be adjacent to other pendant level-2 blobs by Claim 3. Pendant level-1 blobs cannot be adjacent to a leaf by Claim 4. So the main path of  $\bar{B}$  (and  $\bar{B}'$ ) that contains  $u$  ( $u'$ ) contains at most two pendant level-1 blobs; the other two main paths of  $\bar{B}$  (and  $\bar{B}'$ ) contain at most one pendant level-1 blob.

**Claim 5.**  $\bar{B}$  and  $\bar{B}'$  contain at most one pendant level-1 blob.

We have now arrived at the two final cases for this proof. In summary, the current setting is as follows. Both  $\bar{B}$  and  $\bar{B}'$  are level-2 blobs, and they both contain at most one pendant level-1 blob. In fact, this implies that  $\bar{B}$  and  $\bar{B}'$  also contain at most one pendant level-2 blob. We split into the cases for when  $\bar{B}$  does not, or does contain a pendant level-2 blob.

1.  **$\bar{B}$  contains no pendant level-2 blob:** By assumption,  $\bar{B}$  must contain a pendant level-1 blob  $P_1$ . Let  $s$  denote the main path of  $B$  containing  $P_1$ . Note that  $s$  may contain at most one chain. Indeed,  $P_1$  cannot be adjacent to a chain of leaves by Claim 2 (i), so  $p_1$  must be adjacent to a pole of  $\bar{B}$ ; if  $p_1$  is adjacent to  $u$ , then  $s$  can contain a chain of leaves  $(a, k)$  such that an end-spine vertex of  $(a, k)$  is adjacent to  $u$ . The other two main paths of  $\bar{B}$  may contain at most one chain of leaves each. So in total,  $\bar{B}$  may contain at most three chains.

For each chain contained in  $\bar{B}$ , we have that one end-leaf of a chain is shortest distance-6 from  $P_1$ . This means that each chain contained in  $\bar{B}$  must be adjacent to  $P'_1$  in  $\bar{B}'$ . But  $P'_1$  may be adjacent to at most two chains. So  $\bar{B}$  may contain up to two chains. This also implies that  $\bar{B}'$  only contains leaves on the main path that contains  $p'_1$ . Since  $\bar{B}'$  contains no parallel edges, we must then have that  $u'$  lies on a main path that does not contain  $p'_1$ .

Note that  $\bar{B}$  must contain at least one chain, as otherwise  $B$  would be a level-2 blob incident only to two cut-edges. We now split into subcases depending on the location of  $u$ .

(a)  **$u$  is adjacent to  $p_1$ :** Then  $d^N(P_1, u) = 4$ . Since  $u'$  is not on the same main path as that containing  $P'_1$ , we have  $d^{N'}(P'_1, u') \geq 6$ . Now there exists a leaf  $l$  such that  $d^{N'}(l, u') = 3$ . Noting that  $d^N(l, u) \geq 2$ , we have

$$d^N(P_1, u) - d^N(l, u) \leq 2$$

and

$$d^{N'}(P'_1, u') - d^{N'}(l, u') \geq 3,$$

which contradicts Claim 1.

(b)  **$u$  is not adjacent to  $p_1$ :** We let  $s, s_1, s_2$  denote the three main paths of  $\bar{B}$  such that  $s$  contains  $p_1$ ,  $s_1$  contains  $u$ , and  $s_2$  contains neither  $p_1$  nor  $u$ . We claim first that  $s_2$  contains no chains. Suppose for a contradiction that it did contain some chain  $(a, k)$ . Note first that  $a_1$  and  $a_k$  are both shortest distance 6 from  $P_1$ ; this implies that  $P'_1$  is adjacent to both  $a_1$  and  $a_k$  in  $\bar{B}'$ , implying that  $a_1$  and  $a_k$  are in different chains in  $\bar{B}'$ . But this is not possible, so we require  $k = 1$ . Note also that since  $\bar{B}$  contains at most two chains,  $u$  must be adjacent to a pole; this implies that  $d^N(P_1, u) = 5$  and  $d^N(a_1, u) = 3$ . However in  $\bar{B}'$ , we have  $d^{N'}(P'_1, u') \geq 6$  and  $d^{N'}(a_1, u') = 3$ , which contradicts Claim 1 as

$$d^N(P_1, u) - d^N(a_1, u) = 5 - 3 = 2$$

whereas

$$d^{N'}(P'_1, u') - d^{N'}(a_1, u') \geq 6 - 3 = 3.$$

So the main path  $s_2$  contains no chains; this leaves only  $s_1$  to contain chains.

The main path  $s_1$  may contain two chains,  $(b, \ell)$  and  $(c, m)$ , such that  $\ell, m \geq 0$  and  $d^N(b_1, u) = d^N(c_1, u) = 2$ , whenever  $\ell > 0$  and  $m > 0$ , respectively. We require  $\ell + m \geq 3$ , as otherwise  $\bar{B}$  with the edge incident to  $u$  is an alt-path structure that can be obtained from a binary tree on two leaves. We fall into two subcases depending on the value of  $\ell$ .

i.  $\ell = 0$ : Then  $m \geq 3$ , and so

$$d^N(P_1, c_1) = 7,$$

whereas

$$d^{N'}(P'_1, c_1) = 8,$$

which contradicts the fact that  $N$  and  $N'$  realize the same shortest distance matrix.

ii.  $\ell \neq 0$ : By symmetry, we may assume  $m \neq 0$ . Now,

$$d^N(b_1, c_1) = 4,$$

whereas

$$d^{N'}(b_1, c_1) = 5,$$

since  $\ell + m \geq 3$ . This contradicts the fact that  $N$  and  $N'$  realize the same shortest distance matrix.

2.  **$\bar{B}$  contains one level-2 blob:** If  $\bar{B}$  did not contain a pendant level-1 blob, then we are done by applying the arguments from the previous case to  $\bar{B}'$ . So suppose that  $\bar{B}$  contains a pendant level-1 blob  $P_1$  and a pendant level-2 blob  $P_2$ . We first show that  $P_1$  and  $P_2$  cannot be adjacent in  $\bar{B}$ . Suppose that they were adjacent. Then the vertex on  $\bar{B}$  that is shortest distance-2 from  $p_1$  must be a pole of  $\bar{B}$  or  $u$ . Indeed, it cannot be a neighbor of some leaf  $l$ ; this would mean that  $d^N(P_1, l) = 6$ , implying that  $P'_1$  must be adjacent to  $l$ . But this is not possible by Claim 4. In particular, it cannot be a connection since  $\bar{B}$  contains only the pendant blobs  $P_1$  and  $P_2$ .

Now, if  $u$  was adjacent to  $p_2$ , then this would mean that the two main paths of  $\bar{B}$  would be empty, resulting in parallel edges in  $\bar{B}$ . So  $u$  must either be adjacent to  $p_1$  or  $u$  must be contained in one of the two other main sides of  $\bar{B}$ . Either way, we have

$$d^N(P_1, u) - d^N(P_2, u) \leq -1.$$

In  $\bar{B}'$ , we have  $d^{N'}(P'_1, p'_1) = d^{N'}(P'_2, p'_1) = 4$ . So

$$d^{N'}(P'_1, u') - d^{N'}(P'_2, u') \geq 0,$$

which contradicts Claim 1. So we may assume that  $P_1$  and  $P_2$  are not adjacent in  $\bar{B}$ . We split into cases depending on the position of  $u$  in  $\bar{B}$ .

- (a)  **$u$  is on the same main path as  $p_1$ :** Then  $u$  must be adjacent to  $p_1$ , since  $P_1$  cannot be adjacent to a chain by Claim 2, and since  $P_1$  is not adjacent to the only pendant level-2 blob in  $\bar{B}$ . Then  $d^N(P_1, u) = 4$  and  $d^N(P_2, u) \geq 5$ . We split into subcases depending on the position of  $u'$  in  $\bar{B}'$ .

- i.  **$u'$  is on the same main path as  $p'_2$ :** Then  $u'$  must be adjacent to  $p'_2$ . So we have  $d^{N'}(P'_2, u') = 4$  and  $d^{N'}(P'_1, u') \geq 5$ , which contradicts Claim 1.
- ii.  **$u'$  is not on the same main path as  $p'_2$ :** If  $u'$  is adjacent to an end-spine vertex of some chain, then there exists a leaf  $l$  such that  $d^{N'}(l, u') = 2$ . We also have  $d^{N'}(P'_1, u') \geq 5$ . But in  $\bar{B}$ , we have  $d^N(l, u) \geq 2$ . This contradicts Claim 1, as

$$d^N(P_1, u) - d^N(l, u) \leq 4 - 2 = 2,$$

whereas

$$d^{N'}(P'_1, u') - d^{N'}(l, u') \geq 5 - 2 = 3.$$

So  $u'$  cannot be adjacent to an end-spine vertex of some chain, which means that  $d^{N'}(P'_2, u') = 5$ . But  $d^N(P_2, u) \geq 5$ , and so

$$d^N(P_1, u) - d^N(P_2, u) \leq 4 - 5 = -1,$$

whereas

$$d^{N'}(P'_1, u') - d^{N'}(P'_2, u') \geq 0,$$

which contradicts Claim 1.

- (b)  **$u$  is not on the same main path as  $p_1$ :** We may assume that  $u'$  is not on the same main path as  $p'_2$  by symmetry (apply the previous case to  $\bar{B}'$ ).

- i.  **$u$  and  $p_2$  are not on the same main side:** We let  $s_u, s_1, s_2$  denote the three main paths of  $\bar{B}$  such that  $s_u$  contains  $u$  and  $s_i$  contains  $p_i$  for  $i = 1, 2$ .

Note that  $s_u$  may contain up to two chains: denote these chains as  $(a, k)$  and  $(b, \ell)$  where  $d^N(a_1, u) = d^N(b_1, u) = 2$ , if  $k > 0$  and  $\ell > 0$ , respectively. If  $k > 0$  and  $\ell > 0$ , then  $d^N(P_2, a) \geq 7$  and  $d^N(P_2, b) \geq 7$ . Since  $d^N(P_1, a_k) = d^N(P_1, b_\ell) = 6$ , the pendant blob  $P'_1$  must be adjacent to the two chains  $a$  and  $b$  in  $\bar{B}'$ . Depending on the placement of  $u'$ , at least one, and at most two of the chain endpoints  $a_1, b_1$  are shortest distance 6 away from  $P'_2$ . But this contradicts that  $N$  and  $N'$  realize the same shortest distance matrix. Therefore,  $s_u$  contains at most one chain; this means that  $d^N(P_1, u) = 5$ . We also have  $d^N(P_2, u) \geq 6$ .

The same argument can be used in the case when  $u'$  and  $p'_1$  are not on the same main path of  $\bar{B}'$ . In that case, the main path of  $\bar{B}'$  containing  $u'$  contains at most one chain. We now split into subcases depending on the position of  $u'$ .

A.  **$u'$  and  $p'_1$  are not on the same main path of  $\bar{B}'$** : Then, the main path of  $\bar{B}'$  that contains  $u'$  contains at most one chain. In particular, this means that  $u'$  must be adjacent to a pole in  $\bar{B}'$ . So  $d^{N'}(P'_2, u') = 5$ . Furthermore,  $d^{N'}(P'_1, u') \geq 6$ . But this contradicts Claim 1.

B.  **$u'$  and  $p'_1$  are on the same main path of  $\bar{B}'$** : Consider the generator side  $s'$  of  $B'$  that contains  $u'$  and a pole of  $\bar{B}'$  as its boundary vertices. We claim that  $s'$  is empty. If not, then  $s'$  contains a chain  $(a, k)$  such that  $d^{N'}(a_1, u') = 2$ . But then  $d^{N'}(P'_2, a_k) = 6$ , meaning that  $a_k$  must be adjacent to  $P_2$  in  $B$ . This further implies that  $d^N(P_1, a_1) = 6$ , which leads to a contradiction as  $a_1$  is clearly not adjacent to  $P'_1$  in  $B'$  (we have  $d^{N'}(P'_1, a_1) \geq 7$ ). Thus  $s'$  must be empty. But then

$$d^N(P_1, u) - d^N(P_2, u) \leq 5 - 6 = -1,$$

whereas

$$d^{N'}(P'_1, u') - d^{N'}(P'_2, u') \geq 5 - 5 = 0,$$

which contradicts Claim 1.

ii.  **$u$  and  $p_2$  are on the same main path of  $\bar{B}$** : We may assume also that  $u'$  and  $p'_1$  are on the same main path of  $\bar{B}'$ . Consider the main path  $s$  of  $\bar{B}$  that does not contain  $p_1$  nor  $p_2$ . We claim that  $s$  is empty. Suppose not, and suppose that  $s$  contains a chain  $(a, k)$ . In  $B'$ , we require  $P'_1$  to be adjacent to both  $a_1$  and to  $a_k$ . For this to be possible, since  $(a, k)$  must also be a chain in  $\bar{B}'$ , we require  $k = 1$ . Note that in  $\bar{B}'$ , the leaf  $a_1$  is contained in the side with boundary vertices  $p'_1$  and  $u'$ . If it had been contained in the other side of  $\bar{B}'$  with  $p'_1$  as its boundary vertex, then  $P_2$  must be adjacent to  $a_1$  in  $B$ , which is clearly not the case. Observe that a shortest path from  $P_1$  to  $u$  contains the same pole contained in a shortest path from  $a_1$  to  $u$ . Noting that the shortest distance from  $P_1$  to this pole, and the shortest distance from  $a_1$  to this pole are 4 and 2, respectively, it follows that

$$d^N(P_1, u) - d^N(a_1, u) = 4 - 2 = 2,$$

whereas

$$d^{N'}(P'_1, u') - d^{N'}(a_1, u') = 6 - 2 = 4,$$

which contradicts Claim 1. So  $s$  is empty, and we may assume that the main path of  $\bar{B}'$  that does not have  $p'_1$  nor  $p'_2$  is empty.

If all three other sides of  $B$  are empty, then  $B$  contains an alt-path structure formed by a binary tree on two leaves, and we get a contradiction on the choice of  $N$ . In particular, the three sides must contain at least two leaves. Let  $s_1, s_2, s_3$  denote the sides of  $B$  that has  $p_2$  but not  $u, p_2$  and  $u$ , and  $u$  but not  $p_2$  as its boundary vertices, respectively. Similarly let  $s'_1, s'_2, s'_3$  denote the sides of  $B'$  that has  $p'_1$  but not  $u', p'_1$  and  $u'$ , and  $u$  but not  $p'_1$  as its boundary vertices, respectively. It is easy to see that a chain contained in  $s_1$  must be contained in  $s'_1$ ; a chain contained in  $s_2$  must be contained in  $s'_3$ ; a chain contained in  $s_3$  must be contained in  $s'_2$ .

A. **the side  $s_1$  is non-empty**: Let  $(a, k)$  denote the chain contained in  $s_1$ , such that  $d^N(a_1, P_2) = d^N(a_k, P_1) = 6$ . We claim that  $s_2$  and  $s_3$  must both be empty. If  $s_2$  is non-empty, then it contains a chain  $(b, \ell)$ , such that  $d^N(b_1, P_2) = 6$ . So the chains  $(a, k)$  and  $(b, \ell)$  are adjacent. In  $\bar{B}'$ , the chain  $(b, \ell)$  is contained in the side  $s'_3$ . But then  $(a, k)$  and  $(b, \ell)$  cannot be adjacent in  $N'$ , which contradicts the fact that  $N$  and  $N'$  satisfy the same shortest distance matrix. So  $s_2$  must be empty. By applying the same argument to  $B'$ , we see that  $s'_2$  must also be empty; therefore, the side  $s_3$  must be empty. So  $s_2$  and  $s_3$  must both be empty.

We require  $k \geq 2$ , as otherwise  $B$  contains an alt-path structure obtained from a tree on two leaves. But then

$$d^N(a_1, u) - d^N(a_k, u) = 3 - 4 = -1,$$

whereas

$$d^{N'}(a_1, u') - d^{N'}(a_k, u') = 4 - 3 = 1,$$

since  $a_1$  is adjacent to  $P_2$  in  $\bar{B}$  and  $a_k$  is adjacent to  $P'_1$  in  $\bar{B}'$ . This contradicts Claim 1.

B. **the side  $s_1$  is empty**: Let  $(b, \ell)$  and  $(c, m)$  denote the chains contained in  $s_2$  and  $s_3$ , respectively, such that  $d^N(P_2, b_1) = 6$  and  $d^N(b_\ell, c_m) = 4$ , whenever  $\ell > 0$  and  $m > 0$ , respectively. Note that  $\ell + m \geq 2$ , as otherwise  $\bar{B}$  together with the edge incident to  $u$  is an alt-path structure formed by a binary tree on two leaves. In particular, at least one of  $\ell$  or  $m$  must be non-zero. By symmetry, we may assume without loss of generality that  $m > 0$ . Then in  $\bar{B}'$ , the blob  $P'_1$  is adjacent to  $c_1$ . This means that

$$d^{N'}(P'_2, c_1) = 7.$$

In  $\bar{B}$ , there are three paths from  $c_1$  to  $P_2$ . One uses the empty main path and is of length 8. The second uses the main path with  $p_1$  and is of length 9. These two paths cannot be altered by deleting leaves. The third path contains the spine of the chain  $(b, \ell)$ , and is of length  $\ell + m + 6$ . Since  $m \geq 1$ , we only obtain  $d^N(P_2, c_1) = 7$  if and only if  $m = 1$  and  $\ell = 0$ . But this is not possible, since we require  $\ell + m \geq 2$ . So the networks  $N$  and  $N'$  cannot satisfy the same shortest distance matrix, which is a contradiction.

Therefore we reach a contradiction for the case when  $B$  and  $B'$  are both level-2 blobs.

□

The following corollary follows immediately from [Corollary 3](#) and [Theorem 4](#).

**Corollary 4.** *A level-2 network is reconstructible if and only if it does not contain an alt-path structure.*

## 6. Discussion

The results of this paper build on, and answer three open problems presented in the paper by van Iersel et al. [17]. We have shown that networks with a leaf on each generator side are reconstructible from their shortest distance matrix ([Theorem 1](#)). We have shown that level-2 networks are reconstructible from their sl-distance matrix ([Theorem 3](#)). We have characterized the family of subgraphs that prevent level-2 networks from being reconstructible from their shortest distances ([Theorem 4](#)).

Previously, it was only known that level-2 networks were reconstructible from their multisets of distances, the full collection of lengths of all inter-taxa distances together with their multiplicities. An algorithm based on this result was recently presented and implemented in the Bachelor Thesis of Riche Mol [14], where a major bottleneck originated from having to adjust the large multisets of distances upon identifying and reducing a particular pendant structure. As a result, the theoretical running time of the algorithm is exponential in the number of leaves in the network (though it is polynomial in the size of the input, the multisets of distances). The results presented in this paper point to a possibility of an alternative algorithm for constructing level-2 networks from their sl-distance matrix; since updating the sl-distance matrix can be done much quicker than for multisets of distances, we wonder if this could culminate in a polynomial time algorithm with respect to the number of leaves in the network. It would be of great interest to see the speed-up both theoretically and in practice.

In this paper, we have excluded all blobs incident to exactly two cut-edges. One of the consequences of excluding such blobs is that we never obtain pendant level-2 blobs of the form  $(1, 0, 0, 0)$  in our networks. Conditions for identifying and reducing such pendant blobs from level-2 networks are outlined in Lemmas 5.9 and 5.10 of [17]. In fact, such pendant blobs can be inferred from only the shortest distance matrix. This means that [Theorem 3](#), which says that level-2 networks are reconstructible from their sl-distance matrix, holds in general when this restriction is not imposed. On the other hand, allowing for such blobs introduces a new level of complexity within alt-path structures. Call a level-2 blob with two cut-edges a *macaron*, and consider an alt-path structure  $G$  obtained from some tree  $T$ , and replace every cut-edge in  $G$  by a path of arbitrary many macarons. Call this graph  $G'$ . Let  $H$  denote a similar alt-path structure to  $G$ , and let us replace the same cut-edges by paths consisting of the same number of macarons (where by the same cut-edge, we mean the cut-edge that induces the same split). Call this resulting graph  $H'$ . It is easy to see that  $G'$  and  $H'$  realize the same shortest distance matrix. The converse is not immediately obvious. In other words, it is not clear whether excluding these ‘macaron-added’ alt-path structures from level-2 networks guarantee reconstructibility from their shortest distances. Nevertheless, we make the following conjecture.

**Conjecture 1.** *A level-2 network is reconstructible from its shortest distance matrix if and only if after suppressing macarons and degree-2 vertices, it does not contain an alt-path structure.*

A potential shortcoming of our findings lies in the fact that the networks we consider are unweighted. In phylogenetic analysis, weighted edges are often used to indicate the extent on how two species may differ from one another – to depict the passage of time, or to indicate the amount of genetic divergence between two species. The major issue that arises from weighted edges is that the foundational structures such as cherries and chains can no longer be characterized by their distances. In the rooted weighted variant of the problem, this is overcome by simulating a ‘relative root’ by imposing ultrametric conditions and through the use of outgroups [4]. This makes it possible to locate cherries and the rooted analogue of chains (*reticulated cherries*), even when the network is weighted. While these techniques do not translate over to the unrooted setting, some additional conditions will almost certainly be required to obtain results for the weighted variant of the problem.

## Appendix. Proof of claims from section 5.2.3

To prove these claims, we will use the following observation.

**Observation 5.** Let  $P_1$  be a pendant level-1 blob contained in  $\bar{B}$ . Suppose that  $p'_2 p'_1 p'_3 p'_4$  is a path in  $\bar{B}'$ , such that each  $p'_i$  is a connection for a pendant blob  $P'_i$  for  $i \in [4]$ . Suppose also that  $l(P'_1) = l(P'_3) = 1$  and  $l(P'_2) = l(P'_4) = 2$ . A vertex  $p$  on the blob  $\bar{B}$  such that  $d^N(p_1, p) = 2$  must either be  $u$  or a pole of  $\bar{B}$ .

**Proof.** Suppose for a contradiction that  $p$  is either a neighbor of a leaf or a connection of some pendant blob. Suppose first that  $p$  is a neighbor of a leaf  $l$ . Then  $d^N(P_1, l) = 6$ . Since  $N$  and  $N'$  have the same shortest distance matrix, this means that  $P'_1$  must be adjacent to  $l$  in  $\bar{B}'$ . But this is not possible as  $P'_1$  is already adjacent to  $P'_2$  and  $P'_3$ . So suppose that  $p$  is a connection of a pendant blob  $P_5$ . Suppose first that  $l(P_5) = 1$ . Then  $d^N(P_1, P_5) = 8$ . Since  $l(P'_1) = l(P'_5) = 2$ , such a distance can be realized in  $N'$  if and only if  $p'_1 = p'_5$ . But this is impossible as  $B'$  is a level-2 blob. Finally suppose that  $l(P_5) = 2$ . Then since  $d^N(P_1, P_5) = 9$ , the corresponding blob  $P'_5$  must be adjacent to  $P'_2$  or to  $P'_4$ , which is not possible as pendant level-1 blobs cannot be adjacent to one another by Claim 2.  $\square$

**Claim 3.** Two pendant level-2 blobs cannot be adjacent to one another in  $\bar{B}$  (and in  $\bar{B}'$ ).

**Proof.** Suppose for a contradiction that  $\bar{B}$  contains two adjacent pendant level-2 blobs  $P_1$  and  $P_2$  on the main path  $s$ . Then  $B'$  contains two corresponding pendant level-1 blobs  $P'_1$  and  $P'_2$  on the same leaves. We split into cases depending on the locations of  $p'_1$  and  $p'_2$  in  $B'$  (see Fig. 9).

1.  **$p'_1$  and  $p'_2$  are on the same main path  $s'$  of  $B'$ :** Since the shortest distance between  $p'_1$  and  $p'_2$  must be exactly 3, there must be at least two vertices on the same main path in the path  $Q'$  between  $p'_1$  and  $p'_2$ . This path  $Q'$  may contain  $u'$  as a vertex; we split into cases again.

(a)  **$u'$  is a vertex of  $Q'$ :** Observe first that if both  $P'_1$  and  $P'_2$  are adjacent to level-2 blobs  $P'_3$  and  $P'_4$  respectively, then  $d^{N'}(P'_3, P'_4) \geq 10$ . However, the counterparts of these blobs in  $\bar{B}$  must be adjacent to  $P_1$  and  $P_2$ . Since  $P_1$  and  $P_2$  are adjacent, this implies that  $d^N(P_3, P_4) = 9$ , which contradicts the fact that  $N$  and  $N'$  satisfy the same shortest distance matrix. Therefore only one of  $P'_1$  or  $P'_2$  can be adjacent to a pendant level-2 blob. Note that at least one of  $P'_1$  or  $P'_2$  must be adjacent to a pendant level-2 blob, such that its connection is on the path  $Q'$ . So without loss of generality, suppose that  $P'_1$  is adjacent to a pendant level-2 blob  $P'_3$ , such that  $p'_3$  is a vertex in  $Q'$ . At this point, we have that  $P_3, P_1$  and  $P_1, P_2$  are adjacent in  $\bar{B}$ .

We claim that  $P'_3$  cannot be adjacent to a leaf or to pendant blobs other than  $P'_1$  in  $\bar{B}'$ . Firstly, if  $P'_3$  was adjacent to a leaf  $l$ , then  $d^{N'}(P'_1, l) \in \{5, 6\}$ . The distance  $d^{N'}(P'_1, l) = 5$  is impossible as  $l(B) = 2$ ; if  $d^{N'}(P'_1, l) = 6$ , then  $P_1$  must be adjacent to  $l$  in  $\bar{B}$ . But this is impossible as  $P_1$  is already adjacent to  $P_2$  and  $P_3$ . This is a contradiction. The blob  $P'_3$  cannot be adjacent to a pendant level-1 blob other than  $P'_1$ , as this would contradict Claim 2. Finally, we claim that  $P'_3$  cannot be adjacent to a pendant level-2 blob  $P'_4$ . Since this would mean that  $d^{N'}(P'_1, P'_4) = 9$ , we must in  $\bar{B}$  that either  $P_2$  or  $P_3$  is adjacent to  $P_4$ . The former is not possible as  $P'_2$  is not adjacent to  $P'_4$  in  $B'$ ; the latter is not possible as two pendant level-1 blobs cannot be adjacent by Claim 2. So  $P'_3$  cannot be adjacent to a leaf or to pendant blobs in  $\bar{B}'$ .

By Claim 2, the connection  $p'_1$  must be adjacent to a pole of  $B'$ . Since  $P'_2$  cannot be adjacent to a leaf or to a pendant level-1 blob by Claim 2, and it also cannot be adjacent to any pendant level-2 blobs by assumption,  $p'_2$  must also be adjacent to the other pole of  $B'$  and to  $u'$ . Since  $p'_3$  must be adjacent to  $u'$ , it follows that the main path  $s'$  is the path  $p'_1 p'_3 u' p'_2$ .

Now  $B'$  must contain another leaf on one of the other two main sides since they cannot contain parallel edges. We claim that such a leaf cannot exist, thereby reaching a contradiction. Let  $l$  denote such a leaf that is on one of these two main sides, whose neighbor (if  $l$  is not in a pendant blob) / connection (if  $l$  is in a pendant blob) is shortest distance-2 to  $p'_1$ . Suppose first that  $l$  is not in a pendant blob. Then

$$d^{N'}(P'_1, l) = 6,$$

and so  $P_1$  must be adjacent to  $l$  in  $\bar{B}$ , which is not possible as  $P_1$  is already adjacent to  $P_2$  and to  $P_3$ . So now suppose that  $l$  is contained in a pendant level-1 blob. Then

$$d^{N'}(P'_1, l) = 8.$$

But the level of the corresponding pendant blob in  $\bar{B}$  is 2, and since  $l(P_1) = 2$ , we must have that  $d^N(P'_1, l) \geq 9$ , which contradicts the fact that  $N$  and  $N'$  have the same shortest distance matrix. Finally, if  $l$  is contained in a pendant level-2 blob  $P'_4$ , then

$$d^{N'}(P'_1, l) = 9.$$

This means that in  $\bar{B}$ , the corresponding blob  $P_4$  must be adjacent either to  $P_2$  or  $P_3$ . The former is not possible as  $P'_2$  is not adjacent to  $P'_4$  in  $B'$ ; the latter is not possible as two pendant level-1 blobs cannot be adjacent by Claim 2.

(b)  **$u'$  is not a vertex of  $Q'$** : Let  $p'_3$  and  $p'_4$  denote the neighbors of  $p'_1$  and  $p'_2$  in this path  $Q'$ , respectively. Since  $l(P'_1) = l(P'_2) = 1$ , the vertices  $p'_3$  and  $p'_4$  must be connections of pendant level-2 blobs  $P'_3$  and  $P'_4$ , respectively. At this point, we have that  $P_3, P_1; P_1, P_2; P_2, P_4$  are adjacent in  $B$ . Now suppose that there is another vertex  $p'_5$  that is a neighbor of  $p'_3$  that is not  $p'_4$  in  $B'$ . By **Observation 5**, the vertex  $p'_5$  cannot be a neighbor of a leaf nor a connection of some pendant blob. By nature of  $B'$ ,  $p'_5$  must be the vertex  $u'$ , but this would contradict our assumption that the path  $Q'$  does not include  $u'$ . Therefore  $p'_3$  must be adjacent to  $p'_4$ . Thus,  $P'_1, P'_3; P'_3, P'_4$ ; and  $P'_4, P'_2$  are adjacent in  $B'$ .

By **Claim 2**, since pendant level-1 blobs may not be adjacent to leaves and they may be adjacent to at most one pendant level-2 blob, either  $p'_1$  or  $p'_2$  must be adjacent to a pole of  $B'$ . Suppose without loss of generality that  $p'_1$  is adjacent to a pole of  $B'$ . Consider the two main paths of  $B'$  that are not  $s'$ . Since  $N$  contains no parallel edges, one of the two main paths must contain a vertex. In particular, there must exist a vertex that is distance-2 away from  $p'_1$ . By **Observation 5**, such a vertex cannot be a neighbor of a leaf nor a connection of a pendant blob in  $B'$ . Then such a vertex must be  $u'$ . By invoking **Observation 5** again, for both  $p'_1$  and  $p'_2$ , it is easy to see that these two main paths cannot contain any leaves in  $\bar{B}'$ . So  $\bar{B}$  and  $B'$  must contain only the eight leaves of these four pendant blobs on the same main paths, with the vertices  $u$  and  $u'$  on a different main path, respectively. But we find that

$$d^N(P_1, u) - d^{N'}(P'_1, u') = 7 - 5 = 2,$$

whereas

$$d^N(P_3, u) - d^{N'}(P'_3, u') = 5 - 7 = -2,$$

which contradicts **Claim 1**.

2.  **$p'_1$  and  $p'_2$  are incident to different main paths of  $B'$** : Let  $s'_1, s'_2$  denote the main sides of  $\bar{B}'$  that contains  $p'_1, p'_2$ , respectively. Let  $s'_3$  denote the third main path of  $\bar{B}'$ . The vertex  $u'$  is contained either in  $s'_1, s'_2$ , or in  $s'_3$ . The first two cases are equivalent by symmetry, so we split into two cases.

(a)  **$u'$  is in  $s'_1$** : If  $P'_1$  and  $P'_2$  are both not adjacent to a pendant level-2 blob, then  $d^{N'}(P'_1, P'_2) = 8$  and we reach a contradiction as we have  $d^N(P_1, P_2) = 9$ . Therefore  $P'_1$  or  $P'_2$  must be adjacent to a pendant level-2 blob on this distance-8 path. If  $P'_1$  and  $P'_2$  are both adjacent to level-2 blob  $P'_3$  and  $P'_4$ , respectively, then  $d^{N'}(P'_3, P'_4) \geq 10$ . But since  $P_3, P_1; P_1, P_2$ ; and  $P_2, P_4$  would be adjacent in  $\bar{B}$ , we must have  $d^N(P_3, P_4) = 9$ , which contradicts the fact that  $N$  and  $N'$  satisfy the same shortest distance matrix. Therefore, exactly one of  $P'_1$  or  $P'_2$  must be adjacent to a pendant level-2 blob.

i.  **$P'_1$  is adjacent to a pendant level-2 blob  $P'_3$** : Note that  $p'_1$  is adjacent to  $u'$  and to  $p'_3$ . In particular,  $P'_1$  must be adjacent to  $u'$  to make sure that the shortest path between  $P'_1$  and  $P'_2$  is of length 9. Then we have

$$d^{N'}(P'_1, u') - d^{N'}(P'_3, u') = 4 - 6 = -2.$$

But in  $\bar{B}$ , we have that  $d^N(P_1, p_1) = d^N(P_3, p_1) = 4$ . This implies that

$$\begin{aligned} d^N(P_1, u) - d^N(P_3, u) &\geq d^N(P_1, p_1) + d^N(p_1, u) - d^N(P_3, p_1) - d^N(p_1, u) \\ &= 0, \end{aligned}$$

which contradicts **Claim 1**.

ii.  **$P'_2$  is adjacent to a pendant level-2 blob  $P'_4$** : Observe that  $p'_4$  must be placed on  $s'_2$  such that  $d^{N'}(p'_1, p'_4) = 2$ . Then we have that

$$d^{N'}(P'_4, u') - d^{N'}(P'_1, u') = 7 - 4 = 3.$$

In  $\bar{B}$ ,  $P_2$  must be adjacent to both  $P_1$  and  $P_4$ . Then  $d^N(P_1, p_1) = 4$ , whereas  $d^N(P_4, p_1) = 5$ . We have that

$$d^N(P_4, u) - d^N(P_1, u) \leq 1,$$

which contradicts **Claim 1**.

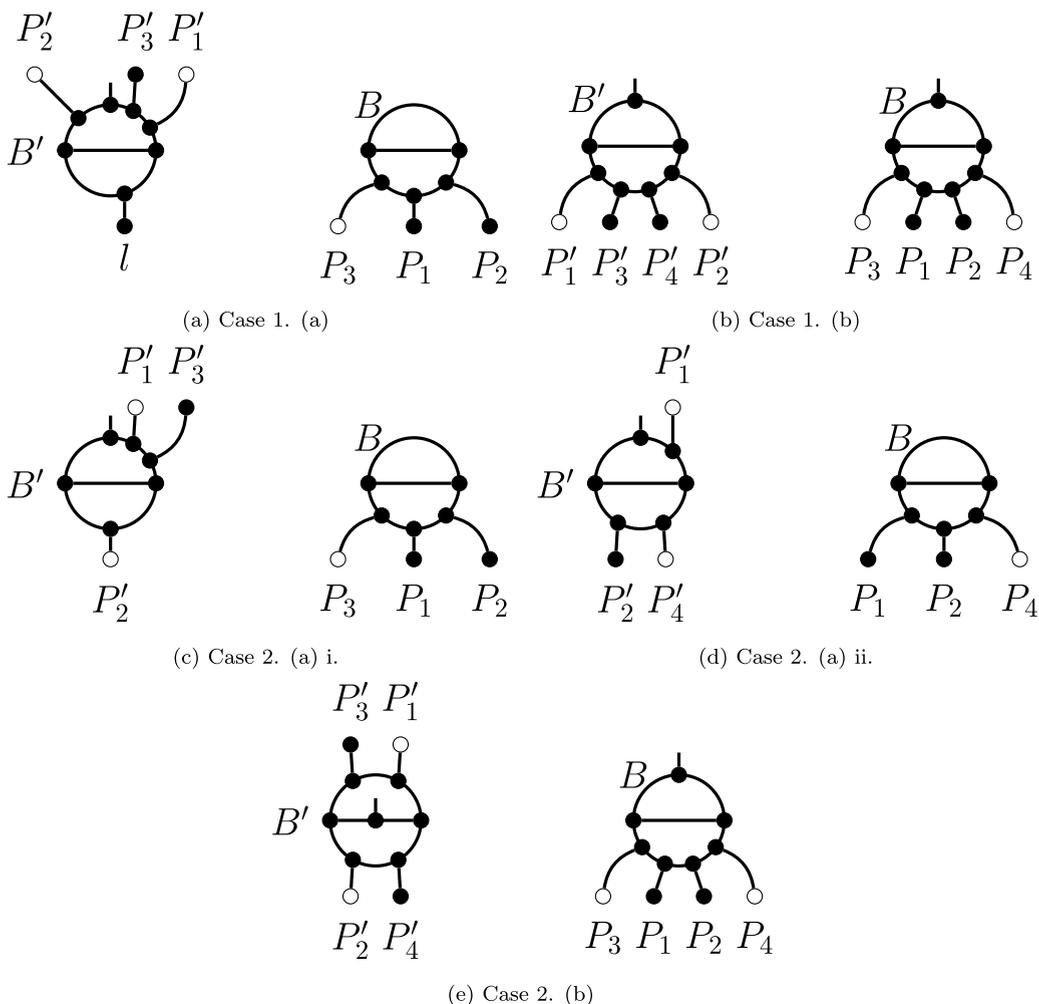
(b)  **$u'$  is in  $s'_3$** : Then to ensure that the leaves of  $P'_1$  and the leaves of  $P'_2$  are shortest distance-9 apart, we require  $P'_1$  and  $P'_2$  to be adjacent to level-2 blobs  $P'_3$  and  $P'_4$ , respectively. But then

$$d^{N'}(P'_3, P'_4) \geq 10.$$

In  $\bar{B}$ , the pendant blobs  $P_3, P_1; P_1, P_2$ ; and  $P_2, P_4$  are adjacent. So we have

$$d^N(P_3, P_4) = 9,$$

which contradicts **Claim 1**.



**Fig. 9.** The different cases from the proof of Claim 3. Pendant blobs are indicated by filled and unfilled leaves with the label  $P_i$  for some  $i$ . The filled vertices indicate a pendant level-2 blob of the form  $(2, 0, 0, 0)$ , whereas unfilled vertices indicate a pendant level-1 blob on two leaves.

This covers all cases for whenever two level-2 blobs are adjacent. In all cases, we were able to find a contradiction with regard to the inter-taxa distances or to Claim 1.  $\square$

**Claim 4.** A pendant level-2 blob may not be adjacent to both a pendant level-1 blob and a leaf simultaneously in  $\bar{B}$  (and in  $\bar{B}'$ ).

**Proof.** Suppose that a pendant level-1 blob  $P_1$  is adjacent to a pendant level-2 blob  $P_2$ , and some leaf  $l$  is adjacent to  $P_2$  in  $\bar{B}$ . To realize these distances in  $\bar{B}'$ , we must have that  $P_1'$  and  $P_2'$ , the pendant level-2 and the level-1 blobs that correspond to  $P_1$  and  $P_2$  must be adjacent, and that  $l$  must be adjacent to  $P_1'$ . Since level-1 blobs may be adjacent to at most one level-2 blob, in both  $B$  and  $B'$ ,  $P_1$  and  $P_2'$  must be adjacent to a pole or  $u$  or  $u'$ . We now split into cases depending on the position of  $u$  in  $\bar{B}$ .

1.  **$u$  is adjacent to  $p_1$ :** We have

$$d^N(P_1, u) - d^N(P_2, u) = 4 - 6 = -2.$$

In  $\bar{B}'$ , we have  $d^{N'}(P_1', p_1') = d^{N'}(P_2', p_1') = 4$ . It follows that

$$d^{N'}(P_1', u') - d^{N'}(P_2', u') \geq 0,$$

which contradicts Claim 1.

2.  **$u$  is not adjacent to  $p_1$ :** Let  $v$  be a vertex in  $\bar{B}$  such that  $d^N(p_1, v) = 2$  and  $v$  is not the neighbor of  $l$ . We claim that  $v$  is either a pole or equal to  $u$ .

Note that  $p_1$  must be adjacent to a pole since  $P_1$  can be adjacent to at most one pendant level-2 blob, and  $P_1$  cannot be adjacent to leaves or other pendant level-1 blobs by Claim 2. The shortest path from  $p_1$  to  $v$  must contain this pole. Suppose for a contradiction that  $v$  is either a neighbor of a leaf or that  $v$  is a connection of some pendant blob. If  $v$  is a neighbor of a leaf  $l'$ , then

$$d^N(P_1, l) = 6,$$

meaning that  $P'_1$  must be adjacent to  $l'$  in  $\bar{B}'$ . But this is impossible since  $P'_1$  is adjacent to  $P'_2$  and  $l$ . Secondly, if  $v$  is a connection of a pendant level-1 blob  $P_3$ , then

$$d^N(P_1, P_3) = 8,$$

but this is impossible since two pendant level-1 blobs must have shortest distance at least 10 by Claim 3. Finally, if  $v$  is a connection of a pendant level-2 blob  $P_4$ , then

$$d^N(P_1, P_4) = 9,$$

which means that the corresponding pendant level-1 blob must be adjacent either to  $P'_2$  or  $l$  in  $\bar{B}'$ . But both of these are forbidden by Claim 2. Therefore  $v$  must be a pole or  $u$ .

But this means that if  $u$  was not placed in the main path of  $\bar{B}$  that did not contain  $p_1$ , then  $\bar{B}$  would have parallel edges. So  $u$  must be contained in one of these two main sides. This means that

$$d^N(P_1, u) - d^N(P_2, u) = 5 - 7 = -2.$$

In  $B'$ , as in the previous case, we have that

$$d^{N'}(P'_1, u') - d^{N'}(P'_2, u') \geq 0,$$

which clearly contradicts Claim 1

These cover all possibilities for a pendant level-2 blob to be adjacent to a pendant level-1 blob and to a leaf. In all cases, we reach a contradiction.  $\square$

**Claim 5.**  $\bar{B}$  (and  $\bar{B}'$ ) contain at most one pendant level-1 blob.

**Proof.** Suppose for a contradiction that  $\bar{B}$  contained two pendant level-1 blobs  $P_1$  and  $P_2$ . We know that they must be shortest distance at least 10 apart. Since  $d^N(P_1, p_1) = d^N(P_2, p_2) = 3$ , we require that  $d^N(p_1, p_2) \geq 4$ .

- $p_1$  and  $p_2$  are contained in the same main path  $s$  of  $\bar{B}$ :** Consider the path from  $p_1$  to  $p_2$  that contains only the vertices of the main path  $s$ . Since we require  $d^N(p_1, p_2) \geq 4$ , we need at least three vertices in this path excluding  $p_1$  and  $p_2$ . By Claims 2 and 4, these three vertices must be two connections  $p_3, p_4$  of pendant level-2 blobs and the vertex  $u$ . In particular,  $p_1$  and  $p_2$  must be adjacent to  $p_3$  and  $p_4$ , and  $p_3$  and  $p_4$  must be adjacent to  $u$ . It follows from Claim 2 that  $s$  contains only these five vertices.

Now consider the two main paths  $s_1$  and  $s_2$  of  $B$  that is not  $s$ . If these main paths are both empty, then  $d^N(P_1, P_2) = 9$ , which contradicts the fact that  $d^N(P_1, P_2) \geq 10$ . So they must both contain vertices. Let  $v_i$  denote the vertex in  $s_i$  such that  $d^N(v_i, p_1) = 2$ , for  $i = 1, 2$ . Firstly, if  $v_1$  is a neighbor of some leaf  $l$ , then  $d^N(P_1, l) = 6$ , meaning that  $l$  must be adjacent to  $P'_1$  in  $N'$ . But this would imply that  $P'_1$  is adjacent to a leaf  $l$  and a pendant level-2 blob  $P'_3$  in  $\bar{B}'$ , which contradicts Claim 4. Secondly, if  $v_1$  is a connection of a pendant level-1 blob  $P_5$ , then  $d^N(P_1, P_5) = 8$ . But two pendant level-1 blobs must be shortest distance at least 10 apart. So  $v_1$  must be a connection of a pendant level-2 blob. Similarly,  $v_2$  must be a connection of a pendant level-2 blob. But this implies that  $\bar{B}'$  contains four pendant level-1 blobs.

The main path of  $\bar{B}'$  with  $u'$  contains exactly two pendant level-1 blobs; the other two main paths of  $\bar{B}'$  contain exactly one pendant level-1 blob each. Consider these two latter main paths. By Claims 2, 3, and 4 these two main paths may contain an additional pendant level-2 blob each, but no other leaves. This means that the pendant level-1 blobs in these two main paths are shortest distance at most 9 to one another, which is a contradiction. Therefore, the vertices  $v_i$  for  $i = 1, 2$  cannot be neighbors of leaves/connections of pendant blobs, meaning that  $\bar{B}$  contains parallel edges, which is a contradiction.

- $p_1$  and  $p_2$  are not contained in the same main path of  $\bar{B}$ :** Let  $s_1$  and  $s_2$  denote the main paths of  $\bar{B}$  that contain  $p_1$  and  $p_2$ , respectively. If  $s_1$  and  $s_2$  do not contain the vertex  $u$ , then  $d^N(P_1, P_2) \leq 9$  and we are done.

So suppose without loss of generality that  $s_1$  contains the vertex  $u$ . Since we require  $d^N(p_1, p_2) \geq 4$ , considering the path between  $P_1$  and  $P_2$  that uses only the edges from  $s_1$  and  $s_2$ , without using the vertex  $u$ , we see that  $P_1$  and  $P_2$  must be adjacent to pendant level-2 blobs  $P_3, P_4$ , respectively. In particular, this path contains the subpath  $p_1 p_3 v p_4 p_2$  for some pole  $v$  of  $\bar{B}$ . Therefore  $p_1$  must be adjacent to  $u$  in  $\bar{B}$ . Then,

$$d^N(P_1, u) - d^N(P_3, u) = 4 - 6 = -2.$$

In  $\bar{B}'$ , we have  $d^{N'}(P'_1, p'_1) = d^{N'}(P'_3, p'_1) = 4$ . It follows that

$$d^{N'}(P'_1, u') - d^{N'}(P'_3, u') \geq 0,$$

which is a contradiction.

This covers all cases for when  $\bar{B}$  contains more than one pendant level-1 blob, which all result in a contradiction. Therefore the claim follows.  $\square$

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