Modules and PQ-trees in Robinson Spaces

M. CARMONA^{a,b}, V. CHEPOI^b, G. NAVES^b, AND P. PRÉA^{a,b}

^aLIS, École Centrale Marseille, Marseille, France

^bLIS, Aix-Marseille Université, CNRS, and Université de Toulon Marseille, France

{mikhael.carmona, victor.chepoi, guyslain.naves, pascal.prea}@lis-lab.fr

June 16, 2023

Abstract. A Robinson space is a dissimilarity space (X, d) on n points for which there exists a compatible order, *i.e.* a total order < on X such that x < y < z implies that $d(x, y) \leq d(x, z)$ and $d(y, z) \leq d(x, z)$. Recognizing if a dissimilarity space is Robinson has numerous applications in seriation and classification. A PQ-tree is a classical data structure introduced by Booth and Lueker to compactly represent a set of related permutations on a set X. In particular, the set of all compatible orders of a Robinson space are encoded by a PQ-tree. An mmodule is a subset M of X which is not distinguishable from the outside of M, *i.e.* the distances from any point of $X \setminus M$ to all points of M are the same. Mmodules define the mmodule-tree of a dissimilarity space (X, d). Given $p \in X$, a p-copoint is a maximal mmodule not containing p. The p-copoints form a partition of $X \setminus \{p\}$. There exist two algorithms recognizing Robinson spaces in optimal $O(n^2)$ time. One uses PQ-trees and one uses a copoint partition of (X, d).

In this paper, we establish correspondences between the PQ-trees and the mmodule-trees of Robinson spaces. More precisely, we show how to construct the mmodule-tree of a Robinson dissimilarity from its PQ-tree and how to construct the PQ-tree from the mmodule-tree. To establish this translation, additionally to the previous notions, we introduce the notions of δ -graph $G_{\overline{\delta}}$ of a Robinson space and of δ -mmodules, the connected components of $G_{\overline{\delta}}$. We also use the dendrogram of the subdominant ultrametric of d. All these results also lead to optimal $O(n^2)$ time algorithms for constructing the PQ-tree and the mmodule tree of Robinson spaces.

Keywords: Robinson dissimilarity; Classification, Seriation; Mmodule; PQ-Tree.

1. INTRODUCTION

The classical seriation problem asks to find a simultaneous ordering (or permutation) of the rows and the columns of the distance matrix D of a dissimilarity space (X, d) with the objective that small values should be concentrated around the main diagonal as closely as possible, whereas large values should fall as far from it as possible. This goal is best achieved by considering the so-called Robinson property [14]: a distance matrix D is said to have the Robinson property if the values of D increase monotonically in the rows and the columns when moving away from the main diagonal in both directions. In case of (0, 1)-matrices, the Robinson property is best known as the Consecutive One Property. A Robinson space is a dissimilarity space whose distance matrix can be transformed by permuting its rows and columns to a distance matrix having the Robinson property. The permutation which leads to a matrix with the Robinson property is called a compatible order.

A PQ-tree is a classical data structure introduced by Booth and Lueker [2] to efficiently encode a set of related permutations on a finite set X. All compatible orders of a Robinson space (X, d) can be encoded by a PQ-tree. This fact was used by several recognition algorithms for the Robinson spaces [1, 13, 17]; the algorithm of [13] was the first algorithm which recognizes Robinson spaces on n points in optimal $O(n^2)$ time. Even if optimal, the algorithm of [13] is far from being simple. Recently, in [3] we designed a simple and practical divide-and-conquer algorithm for recognition of Robinson spaces in optimal $O(n^2)$ time. This algorithm is based on the notions of mmodules and copoint partitions of dissimilarity spaces. An mmodule of a dissimilarity space (X, d) (generalizing the notion of a module in graph theory) is a subset M of X which is not distinguishable from the outside of M, i.e., the distances from any point of $X \setminus M$ to all points of M are the same. Mmodules define the mmodule-tree of a dissimilarity space (X, d). If p is any point of X, then p

In this paper, we establish correspondences between the PQ-trees and the mmodule-trees of Robinson spaces (X, d). Namely, we show how to derive the mmodule-tree from the PQ-tree of (X, d) and, vice-versa, how to construct the PQ-tree from the mmodule-tree of (X, d). We also show how to derive the branches of a PQ-tree from the copoint partitions of (X, d). We also describe optimal $O(n^2)$ algorithms for constructing the PQ-tree and the mmodule-tree of a Robinson space (X, d). To establish the cryptomorphism between PQ-trees and mmodules-trees, additionally to the previous notions, we introduce the notion of δ -graph $G_{\overline{\delta}}$ of a Robinson space (X, d). We prove that either $G_{\overline{\delta}}$ is connected for all $\delta > 0$ or there exists a unique value of δ for which $G_{\overline{\delta}}$ is not connected. In the later case, the connected components of $G_{\overline{\delta}}$ are called δ -mmodules. The dichotomy between the connectivity for all δ and the non-connectivity for some δ of $G_{\overline{\delta}}$ and the δ -modules in the second case are crucial in the construction of the PQ-tree and the translations between PQ-trees and mmodule trees. The dendrogram $\mathcal{T}_{\hat{d}}$ of the ultrametric subdominant \hat{d} of (X, d) is yet another important ingredient, used in the algorithm for the construction of the mmodule tree. Notice also that the algorithm for the construction of the PQ-tree from the mmodule tree uses the recognition of flat Robinson spaces from [3] as a subroutine. On the other hand, we present an optimal $O(n^2)$ algorithm for constructing the PQ-tree, using the p-copoints partition and the concept of p-proximity order, also introduced in [3]. Since this paper is a follow-up of [3], we refer to the paper [3] for a complete bibliography on Robinson spaces and on their recognition algorithms (in this paper, we cite only the recognition algorithms using PQ-trees).

The rest of the paper is organized as follows. In Section 2, we present classical notions that we use: Robinson dissimilarities, PQ-trees and mmodules. We end this section with an illustrative example. In Section 3 we characterize the sets of total orders on X that are representable by a PQ-tree and the subsets of X that correspond to nodes of the PQ-tree of a Robinson space (X, d). These results are used in the following two sections. In Section 4 we introduce the notion of a δ -graph $G_{\overline{\delta}}$ of a Robinson space and investigate the properties of its δ -mmodules. Using them, we show how to construct the PQ-tree of a Robinson space. In Section 5 we show how to construct for a Robinson space its mmodule tree from its PQ-tree and, vice versa, its PQ-tree from its mmodule tree. In Section 6 we show how to build the mmodule tree using partition refinement and the subdominant ultrametric. In Section 7 we show how to build the PQ-tree from any point p and the copoint partition of p and the p-proximity order introduced in [3].

2. Preliminaries

2.1. Robinson dissimilarities. Let $X = \{p_1, \ldots, p_n\}$ be a set of *n* elements, called *points*. A dissimilarity on X is a symmetric function *d* from X^2 to the nonnegative real numbers such that d(x,y) = 0 if x = y. Then d(x,y) is called the *distance* between x, y and (X, d) is called a *dissimilarity space*. A partial order on X is called *total* if any two elements of X are comparable. Since we will mainly deal with total orders, we abbreviately call them *orders*.

Definition 2.1 (Compatible order). Given a dissimilarity space (X, d), an order < on X is *compatible* if x < y < z implies that $d(x, z) \ge \max\{d(x, y), d(y, z)\}$. We denote by $\Pi(X, d)$ the set of compatible orders of (X, d). If < is a compatible order, then so is the order $<^{\text{op}}$ opposite to <.

Definition 2.2 (Robinson space). A dissimilarity space (X, d) is a *Robinson space* if it admits a compatible order, i.e., if $\Pi(X, d) \neq \emptyset$. Then (X, d) is said to be *Robinson*.

Equivalently, (X, d) is Robinson if its distance matrix $D = (d(p_i, p_j))$ can be symmetrically permuted so that its elements do not decrease when moving away from the main diagonal along any row or column. Such a dissimilarity matrix D is said to have the *Robinson property* [4, 5, 6, 14]. If $Y \subseteq X$, we denote by (Y,d) the dissimilarity space obtained by restricting d to Y; we call (Y,d) a subspace of (X,d). If (X,d) is a Robinson space, then any subspace (Y,d) of (X,d) is also Robinson and the restriction of any compatible order < of X to Y is compatible.

Definition 2.3 (Block). Let (X, d) be a Robinson space. A set $Y \subset X$ is called a *block* if Y is an interval in any compatible order of (X, d).

The ball of radius $r \ge 0$ centered at $x \in X$ is the set $B_r(x) = \{y \in X : d(x, y) \le r\}$. From the definition of compatible orders it follows all balls of a Robinson space are blocks. The diameter of a set $Y \subseteq X$ is diam $(Y) = \max\{d(x, y) : x, y \in Y\}$ and a pair $x, y \in Y$ such that $d(x, y) = \operatorname{diam}(Y)$ is called a diametral pair of Y.

Basic examples of Robinson dissimilarities are the ultrametrics and line-distances. A *line-distance* is provided by the standard distance $d(p_i, p_j) = |p_i - p_j|$ between n points $p_1 < \ldots < p_n$ of \mathbb{R} . Notice that any line-distance has exactly two compatible orders: the order $p_1 < \ldots < p_n$ defined by the coordinates of the points and its opposite. This leads to the following notion:

Definition 2.4 (Flat Robinson space). A Robinson space is *flat* is it has exactly two compatible orders, reverse of each other. All line-distances are flat but the converse is not true.

2.2. X-trees. Given a finite set X, an X-tree is an ordered rooted tree \mathcal{T} in which the exists a bijection between X and the set of leaves of \mathcal{T} and any inner node of \mathcal{T} has degree at least 2. We will use Greek letters as variables over nodes of trees but for convenience we will give the same name to the elements of X and the corresponding leaves of \mathcal{T} . As usually, we say that a node α is an ancestor of a node β if α belongs to a unique path of \mathcal{T} between β and the root. For two nodes α and β , we denote by $lca(\alpha, \beta)$ the *lowest common ancestor* of α and β . Given a node α of \mathcal{T} , we denote $X(\alpha) \subseteq X$ the set of leaves having α as an ancestor. We say that two X-trees \mathcal{T} and \mathcal{T}' are *isomorphic* if there exists an isomorphism f between the trees \mathcal{T} and \mathcal{T}' such that f(u) = u for any $u \in X$ and $X(f(\alpha)) = X(\alpha)$ for any inner node α of \mathcal{T} .

Definition 2.5 (Pertinent node). Given $S \subset X$ and an X-tree \mathcal{T} on X, we will say that a node α is S-pertinent or the pertinent node of S if α is the lowest node such that $S \subseteq X(\alpha)$.

In this paper we consider three types of X-trees: mmodule trees for arbitrary dissimilarity spaces (X, d), PQ-trees for Robinson spaces (X, d), and dendrograms for ultrametric spaces (X, d).

2.3. Ultrametrics. Recall, that a dissimilarity space (X, d) is an *ultrametric space* if it satisfies the three-point condition $d(x, y) \leq \max\{d(x, z), d(y, z)\}$ for all $x, y, z \in X$. Equivalently, the two largest distances among d(x, y), d(x, z), and d(y, z) are equal. The ultrametrics are thoroughly used in phylogeny and hierarchical clustering, because they can be represented by particular X-trees, called dendrograms. A *dendrogram* for an ultrametric space (X, d) is an X-tree \mathcal{T}_D with weighted edges such that each inner node α has the same distance to all leaves in the subtree rooted at α . The sets $X(\alpha)$ for nodes α of \mathcal{T}_D are called *clusters* and the set system \mathcal{H} consisting of all clusters is called a *hierarchy*. Any two clusters of \mathcal{H} are either disjoint or one is included in the another one. $\mathcal{H}(X)$ is unique, and $\mathcal{T}_D(X)$ is unique up to reordering children of each node. The dendrogram \mathcal{T}_D and the weights of its edges are constructed by the well-known *single-linkage clustering algorithm* [8, 10]. Then for any two points $x, y \in X$, d(x, y) equals the length of the unique path between x and y in \mathcal{T}_D or, equivalently, to twice the height of x and y in the subtree of \mathcal{T}_D rooted at the lowest common ancestor lca(x, y) of x and y.

We consider the dendrogram \mathcal{T}_D of an ultrametric space as unweighted, but we weight each inner node α of \mathcal{T}_D by the distance d(x, y) between any two leaves $x, y \in X(\alpha)$ such that $lca(x, y) = \alpha$; we denote the weight of α by $p(\alpha)$. Notice then when moving from any leaf to the root of \mathcal{T}_D , the weights of the nodes occurring on this path are strictly increasing. The representation of an ultrametric by a dendrogram in which the edges are weighted is called an *equidistant representation* and the representation in which the nodes are weighted is called a *vertex representation* [16]. The two representations are equivalent: node weights correspond to potential, and the weight of an edge is half the difference of potential between its two extremities. It is straightforward to compute the potentials from the differences of potential (setting the potential of any leaf to be 0), and vice versa. Notice that, in the vertex representation, the distance between two leaves x and y is equal to p(|ca(x,y)). In particular, for any inner node α and $x, y \in X(\alpha)$ such that x and y belong to different children of α , we have $d(x, y) = p(\alpha) = \text{diam}(X(\alpha))$.

One fundamental property of ultrametrics is the existence for each dissimilarity space (X, d) of the subdominant ultrametric \hat{d} on X: for any ultrametric d' on X such that $d' \leq d$ (i.e., $d'(x, y) \leq$ d(x, y) for all $x, y \in X$) we have $d' \leq \hat{d} \leq d$. The subdominant ultrametric \hat{d} can be defined as follows: for all $x, y \in X$, $\hat{d}(x, y)$ is the minimum over all paths P between x and y of the maximum weight of an edge on that path P:

$$\widehat{d}(x,y) = \min\{\max_{uv \in P} d(u,v) : P \text{ is a } (x,y)\text{-path}\}.$$

In combinatorial optimization, $\hat{d}(x, y)$ is called the *bottleneck distance* between x and y and a (x, y)path providing the minimum in the previous formula is called the *bottleneck shortest path* [15]. The subdominant ultrametric \hat{d} can be constructed in the following elegant way. Let T be a minimum spanning tree of the complete graph on X weighted by the values of the dissimilarity function d. Then for any $x, y \in X$, $\hat{d}(x, y)$ is the weight of the heaviest edge of the unique path of T between x and y [10]. We denote by $\mathcal{T}_{\hat{d}}$ the dendrogram of the ultrametric space (X, \hat{d}) ; sometimes we will say that $\mathcal{T}_{\hat{d}}$ is the dendrogram of the dissimilarity space (X, d). We can construct $\mathcal{T}_{\hat{d}}$ in the following iterative way (which seems us to be new): when using Prim's algorithm to compute the minimum spanning tree T of (X, d), one can build $\mathcal{T}_{\hat{d}}$ by inserting each vertex in $\mathcal{T}_{\hat{d}}$ at the moment when it is visited, leading to Algorithm 7 presented in the Appendix. This algorithm has complexity $O(n^2)$.

In this paper, we use ultrametrics as an illustrative example. In fact, for ultrametrics their dendrograms have the same shape as their PQ-trees and their mmodule trees. Additionally, we use the dendrogram $\mathcal{T}_{\hat{d}}$ of the ultrametric subdominant (X, \hat{d}) of a Robinson space (X, d) in our construction of the mmodule tree. The idea of constructing the subdominant ultrametric via the minimum spanning tree also occurs in our techniques.

2.4. **PQ-trees.** A PQ-tree is a tree-based data structure introduced by Booth and Lueker [2] in 1976 to efficiently encode a family of permutations on a set X in which various subsets of X occur consecutively.

Definition 2.6 (PQ-tree). A *PQ-tree* over a set X is an X-tree \mathcal{T} whose internal nodes are distinguished as either P-nodes or Q-nodes. Two PQ-trees are said to be *equivalent* if one can be transformed into the other by applying a sequence of the following two equivalence transformations.

- (1) Arbitrarily permute the children of a P-node.
- (2) Reverse the children of a Q-node.

The nodes of arity 2 can be equally viewed as P-nodes and as Q-nodes; in our notations, they will be considered as P-nodes.

We use the convention that P-nodes are represented by circles or ellipses and Q-nodes are represented by rectangles. For PQ-trees β_1, \ldots, β_k , we denote $P(\beta_1, \ldots, \beta_k)$ and $Q(\beta_1, \ldots, \beta_k)$ the PQ-trees whose root are a P-node, respectively a Q-node, with children β_1, \ldots, β_k in that order.

For convenience, we will abusively identify permutations and (total) orders. The *canonical order* of a PQ-tree \mathcal{T} over X is the permutation on X obtained by a left-to-right traversal of \mathcal{T} .

Definition 2.7 (Represented permutations of a PQ-tree). The set of represented permutations of a PQ-tree \mathcal{T} is the set of canonical orders of all PQ-trees equivalent to \mathcal{T} , and is denoted $\Pi(\mathcal{T})$. A set of orders/permutations Π is called *representable by a PQ-tree* if there exists a PQ-tree \mathcal{T} such that $\Pi(\mathcal{T}) = \Pi$.

Represented permutations may also be defined using composition of orders, as defined below.

Definition 2.8 (Composition of orders). Let X be a set, \mathcal{P} a partition of X, $<_{\mathcal{P}}$ an order on \mathcal{P} , and for each part $S \in \mathcal{P}$, $<_S$ an order on S. Then the *composition* of $<_{\mathcal{P}}$ and $(<_S)_{S \in \mathcal{P}}$ is the order < defined by x < y when

- (i) either there is $S \in \mathcal{P}$ with $x, y \in S$, and $x <_S y$,
- (ii) or there are $S, S' \in \mathcal{P}$ distinct, with $x \in S, y \in S'$ and $S <_{\mathcal{P}} S'$.

Then the permutations represented by a PQ-tree matches with orders obtained by composing an order on the children of the root with a choice of orders on each children of the root node, where the order on the children is

- in the case of a P-node: an arbitrary order,
- in the case of a Q-node: either the order of the children in the PQ-tree or its reverse.

Example 2.9. The PQ-tree \mathcal{T} of Figure 1 has one Q-node (the root) and one P-node α with $X(\alpha) = \{1, 2, 3\}$. The subtree rooted at α represents all the permutations of the elements 1, 2, 3. Consequently, the PQ-tree \mathcal{T} represents the 12 permutations of the form $(\pi, 4, 5, 6, 7)$ and $(7, 6, 5, 4, \pi)$, where π is any permutation on $\{1, 2, 3\}$.



FIGURE 1. A PQ-tree

Préa and Fortin [13] used PQ-trees to encode the compatible orderings of a Robinson dissimilarity space (X, d), because this set of orders is represented by a PQ-tree. We recall this correspondence. A (0, 1)-matrix A has the *Consecutive Ones Property* (C1P) if its columns can be permuted in such a way that in all rows the 1s appear consecutively. Such an order is called *compatible*. If Ais a C1P-matrix, then the sets of all its compatible permutations can be represented by a PQ-tree; Booth and Lueker designed an iterative algorithm, using PQ-trees, which determines if a matrix M has the C1P [2]. Let **B** denote the set of all distinct balls of a dissimilarity space (X, d). Let $M_{\mathbf{B}}$ be the $\{0, 1\}$ -matrix whose columns are indexed by the points of X and rows by the balls of **B**: for $x \in X$ and $B \in \mathbf{B}$ we define $M_{\mathbf{B}}(B, x) = 1$ if $x \in B$ and $M_{\mathbf{B}}(B, x) = 0$ otherwise. The following simple result of Mirkin and Rodin [12] links Robinson dissimilarities with C1P-matrices:

Proposition 2.10. [12] A dissimilarity space (X, d) is Robinson if and only if its matrix $M_{\mathbf{B}}$ satisfies the C1P. There exists a bijection between the set $\Pi(X, d)$ of orders compatible with d and the set of permutations compatible with $M_{\mathbf{B}}$.

Since the sets of all compatible permutations of a C1P-matrix can be represented by a PQ-tree [2], from Proposition 2.10 we obtain:

Corollary 2.11. The set $\Pi(X,d)$ of all compatible orders of a Robinson space (X,d) can be represented by a PQ-tree.

For a Robinson space (X, d), we denote by $\mathcal{T}_{PQ}(X, d)$, or \mathcal{T}_{PQ} for short, its PQ-tree (unique up to equivalence).

2.5. Mmodules and copoints. In this subsection, we recall the basic facts about the mmodules and copoints in dissimilarity spaces from our paper [3]. Let (X, d) be a dissimilarity space.

Definition 2.12 (Mmodule). A set $M \subseteq X$ is called an *mmodule* (a *metric module* or a *matrix module*) if M cannot be distinguished from outside, *i.e.*, for any $z \in X \setminus M$ and all $x, y \in M$ we have d(z, x) = d(z, y).

In graph theory, the subgraphs indistinguishable from the outside are called modules, explaining our choice of the term "mmodule". Denote by $\mathcal{M}(X,d)$ (or \mathcal{M} fo short) the set of all mmodules of (X,d). Trivially, \emptyset, X , and $\{p\}, p \in X$ are mmodules; we call them *trivial mmodules*. An mmodule M is called *maximal* if M is a maximal by inclusion mmodule different from X. Denote by $\mathcal{M}_{\max}(X,d)$ (or \mathcal{M}_{\max} for short) the set of all maximal mmodules of (X,d). We continue with the basic properties of mmodules.

Proposition 2.13. [3, Proposition 3.1] Let (X, d) be a dissimilarity space. The set $\mathcal{M} = \mathcal{M}(X, d)$ has the following properties:

- (i) $M_1, M_2 \in \mathcal{M}$ implies that $M_1 \cap M_2 \in \mathcal{M}$;
- (ii) if $M \in \mathcal{M}$ and $M' \subset M$, then $M' \in \mathcal{M}$ if and only if M' is an amodule of $(M, d|_M)$;
- (iii) if $M_1, M_2 \in \mathcal{M}, M_1 \cap M_2 \neq \emptyset$, then $M_1 \cup M_2 \in \mathcal{M}$, and if additionally $M_1 \setminus M_2 \neq \emptyset, M_2 \setminus M_1 \neq \emptyset$, then $M_1 \cup M_2, M_1 \setminus M_2, M_2 \setminus M_1$, and $M_1 \Delta M_2$ are mmodules;
- (iv) the union $M_1 \cup M_2$ of two intersecting maximal mmodules $M_1, M_2 \in \mathcal{M}$ is X;
- (v) if M_1 and M_2 are two disjoint maximal mmodules and M is a nontrivial mmodule contained in $M_1 \cup M_2$, then either $M \subset M_1$ or $M \subset M_2$;
- (vi) if $M_1, M_2 \in \mathcal{M}$ and $M_1 \cap M_2 = \emptyset$, then d(u, v) = d(u', v') for any (not necessarily distinct) points $u, u' \in M_1$ and $v, v' \in M_2$.

The next results show that the mmodules of a dissimilarity can be organized within a treestructure. We say that a family of subsets $\{M_1, \ldots, M_k\}$ of X is a *copartition* of X if $\{X \setminus M_1, \ldots, X \setminus M_k\}$ is a partition of X. For a set $M \subseteq X$, we denote its complement by $\overline{M} = X \setminus M$.

Lemma 2.14. [3, Lemma 3.7] Let (X, d) be a dissimilarity space. Then $\mathcal{M}_{\max}(X, d)$ is either a partition or a copartition of X.

Proposition 2.15. [3, Proposition 3.9] Let (X, d) be a dissimilarity space. There is a unique X-tree (up to children reorderings) with inner nodes labelled by \cup or \cap , such that:

- (i) if a node α is a \cup -node, then its arity is at least three and for any child β of α , $X(\beta)$ is an mmodule,
- (ii) if a node α is a \cap -node, then its arity is at least two, and for any proper subset $\{\beta_1, \ldots, \beta_i\}$ of children of α , $X(\beta_1) \cup \ldots X(\beta_i)$ is an mmodule.
- (iii) any proper mmodule appears exactly once as in (i) and (ii).

If \mathcal{M}_{\max} is a partition but not a bipartition, then the root is a \cup -node, while if \mathcal{M}_{\max} is a copartition (possibly a bipartition), it is a \cap -node. For a dissimilarity space (X,d), we call the X-tree defined in Proposition 2.15 the *mmodule-tree* of (X,d) and we denote it by $\mathcal{T}_M(X,d)$ (or \mathcal{T}_M for short). It would be tempting to believe that, for Robinson spaces, \cup -nodes correspond to Q-nodes of \mathcal{T}_{PQ} and \cap -nodes to P-nodes. We will see later that this is not always the case, and we will describe precisely the relationship between \mathcal{T}_{PQ} and \mathcal{T}_M .

Definition 2.16 (Copoint). A copoint at a point p (or a p-copoint) is any maximal by inclusion mmodule C not containing p; the point p is the attaching point of C.

The copoints of \mathcal{M} minimally generate \mathcal{M} , in the sense that each mmodule M is the intersection of all copoints containing M. Maximal by inclusion mmodules are copoints but the converse is not true. Denote by \mathcal{C}_p the set of all copoints at p plus the trivial mmodule $\{p\}$.

Lemma 2.17. [3, Lemma 3.4] For any point p of a dissimilarity space (X, d), the copoints of C_p are pairwise disjoint and define a partition of the set X.

We call $C_p = \{C_0 = \{p\}, C_1, \ldots, C_k\}$ a copoint partition of (X, d) with attaching point p. The copoint partition C_p is called *trivial* if C_p consists only of the points of X, i.e., $C_p = \{\{x\} : x \in X\}$, and *co-trivial* if $C_p = \{\{p\}, X \setminus \{p\}\}$, i.e., all points of $X \setminus \{p\}$ have the same distance to p.

We conclude this subsection with the definition of a quotient space of a dissimilarity space (X, d). In [3] we defined and used it in case of copoint partitions C_p . Now, we will define it for arbitrary partitions of X into mmodules.

Definition 2.18 (Quotient space). Let $\mathcal{M}' = \{M_1, \ldots, M_k\}$ be a partition of a dissimilarity space (X, d) into mmodules. The *quotient space* (\mathcal{M}', \hat{d}) of (X, d) has the mmodules of \mathcal{M}' as points and for $M_i, M_j, i \neq j$ of \mathcal{M}' we set $\hat{d}(M_i, M_j) := d(u, v)$ for an arbitrary pair $u \in M_i, v \in M_j$.

From the definition of mmodules and since \mathcal{M}' is a partition, the notion of a quotient space is well-defined because d(u, v) is the same for any choice of the points $u \in M_i$ and $v \in M_j$.

2.6. Examples. In order to illustrate the notions introduced in this section, we give the following example. In Figure 2 we present a Robinson space (X, d) on 12 points. In Figure 3 we provide its PQ-tree and its mmodule-tree. In Figure 4 we list all its non-trivial copoints, together with the point to which they are attached.

| D | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|----------|---|----------|----------|----------|---|---|---|---|---|----|----------|----------|
| 1 | 0 | 2 | 2 | 3 | 5 | 5 | 5 | 8 | 8 | 8 | 8 | 8 |
| 2 | | 0 | 1 | 2 | 5 | 5 | 5 | 8 | 8 | 8 | 8 | 8 |
| 3 | | | 0 | 2 | 5 | 5 | 5 | 8 | 8 | 8 | 8 | 8 |
| 4 | | | | 0 | 5 | 5 | 5 | 8 | 8 | 8 | 8 | 8 |
| 5 | | | | | 0 | 1 | 1 | 6 | 6 | 6 | 6 | 6 |
| 6 | | | | | | 0 | 1 | 6 | 6 | 6 | 6 | 6 |
| 7 | | | | | | | 0 | 6 | 6 | 6 | 6 | 6 |
| 8 | | | | | | | | 0 | 1 | 2 | 2 | 3 |
| 9 | | | | | | | | | 0 | 2 | 2 | 2 |
| 10 | | | | | | | | | | 0 | 2 | 2 |
| 11 | | | | | | | | | | | 0 | 2 |
| 12 | | | | | | | | | | | | 0 |

FIGURE 2. The distance matrix D of a Robinson space (X, d) with $X = \{1, \dots, 12\}$.



FIGURE 3. (A) The PQ-tree \mathcal{T}_{PQ} and (B) the mmodule-tree \mathcal{T}_M of the dissimilarity space from Figure 2.

3. Represented orders and nodes of a PQ-tree

In this section, first we characterize the set of orders that are representable by a PQ-tree and then we characterize the subsets of a Robinson space (X, d) that are the nodes of the PQ-tree of (X, d). These auxiliary results will be used in the next two sections.

| non-trivial mmodule | copoint for | non-trivial mmodule | copoint for |
|---------------------|-------------|------------------------|--------------------------|
| $\{2, 3\}$ | 1, 4 | $\{5, 6, 7\}$ | 1 to 4 and 8 to 12 |
| $\{1, 4\}$ | 2, 3 | $\{10, 11\}$ | 8, 9, 12 |
| $\{1, 2, 3, 4\}$ | 5 to 12 | $\{8, 9, 10, 12\}$ | 11 |
| $\{5, 6\}$ | 7 | $\{8, 9, 11, 12\}$ | 10 |
| $\{5, 7\}$ | 6 | $\{8, 9, 10, 11, 12\}$ | 1 to 7 |
| $\{6, 7\}$ | 5 | | |

FIGURE 4. The non-trivial mmodules of the dissimilarity space from Figure 2 that are copoints, together with the points to which they are attached.

3.1. Represented orders. In this subsection, we characterize the set Π of orders of X that are represented by PQ-trees.

Definition 3.1 (II-block). For a set Π of orders on X, a set $Y \subsetneq X$ is called a Π -block if Y is an interval in each order of Π . Then the blocks from Definition 2.3 are precisely the $\Pi(d)$ -blocks.

Lemma 3.2. Let \mathcal{T}_{PQ} be a PQ-tree over a set X and $\Pi(\mathcal{T}_{PQ})$ be the set of represented permutations of \mathcal{T}_{PQ} . Then a set $S \subseteq X$ is a $\Pi(\mathcal{T}_{PQ})$ -block if and only if

- (i) either there is a node α in \mathcal{T}_{PQ} with $X(\alpha) = S$,
- (ii) or there is a Q-node α in \mathcal{T}_{PQ} with children β_1, \ldots, β_k , and j, j' with $1 \le j < j' \le k$ such that $\{j, j'\} \ne \{1, k\}$ and $\bigcup_{i \in \{j, \ldots, j'\}} X(\beta_i) = S$.

Proof. Let $S \subseteq X$ be a $\Pi(\mathcal{T}_{PQ})$ -block, and α be the pertinent node of S. If $S = X(\alpha)$, case (i) holds. Otherwise, $S \subsetneq X(\alpha)$.

For the sake of contradiction, suppose that α is a P-node. If there is a child β of α and $x \in S \cap X(\beta)$, $y \in X(\beta) \setminus S$, then let $z \in S \cap (X(\alpha) \setminus X(\beta))$ be in another child. As S is a block, there is a compatible order < with x < z < y or y < x < z (say the former). By definition of the compatible orders of a PQ-tree, reversing the order on $X(\beta)$ provides another compatible order, with z < x < y, in contradiction with the fact that S is a block. Otherwise, S is the union of the sets induced by some children of α . Let $x, y, z \in X(\alpha)$ be in three distinct children of α , with $x, z \in S, y \notin S$. By property of P-nodes, there is a compatible order with x < y < z, contradicting the fact that S is a block.

Hence α is a Q-node. Let β_1, \ldots, β_k be its children. Then $\{i \in \{1, \ldots, k\} : \beta_i \cap S \neq \emptyset\}$ is an interval $\{j, \ldots, j'\}$ because S is a $\Pi(\mathcal{T}_{PQ})$ -block and by property of Q-nodes, with j < j' as α is S-pertinent. Finally, if there is $z \in \bigcup_{k \in \{j, \ldots, j'\}} \beta_k \setminus S$, let $x \in \beta_j \cap S$ and $y \in \beta_{j'} \cap S$, there is a compatible order with x < z < y, contradicting of the fact that S is a $\Pi(\mathcal{T}_{PQ})$ -block. Hence (ii) holds. The reverse direction is immediate.

Consider a set Π of orders on X, and say that two points $x, y \in X$ are *equivalent* if every maximal Π -block contains either none or both of them. This is clearly an equivalence relation denoted \approx_{Π} . We can use it to characterize when a set of orders is represented by a PQ-tree. To this end, let \mathcal{B}_{Π} denote the set of equivalence classes of \approx_{Π} .

Proposition 3.3. A set of orders Π on X is represented by a PQ-tree if and only if the restriction of Π on each $S \in \mathcal{B}_{\Pi}$ is represented by a PQ-tree \mathcal{T}_S , and

- (i) either Π is the set of orders obtained by composing any order on \mathcal{B}_{Π} with orders from each $\mathcal{T}_S, S \in \mathcal{B}_{\Pi}$,
- (ii) or there are at least three equivalence classes and there is an order $<_{\mathcal{B}}$ on \mathcal{B}_{Π} such that Π is the set of orders obtained by composing $<_{\mathcal{B}}$ or its reverse with orders from each $\mathcal{T}_S, S \in \mathcal{B}_{\Pi}$.

In that case, the root of the PQ-tree is a P-node in case (i) and a Q-node in case (ii), and its children are the PQ-trees \mathcal{T}_S of each equivalence class S of \approx_{Π} , in arbitrary order in case (i) and in order $<_{\mathcal{B}}$ (or its reverse) in case (ii).

Proof. Suppose first that Π is represented by a PQ-tree \mathcal{T} . Let β_1, \ldots, β_k be the children of the root. From Lemma 3.2, when the root is a P-node, the maximal blocks are the sets $X(\beta_i)$ and thus are also the equivalence classes of \approx_{Π} , whereas when the root is a Q-node, the maximal blocks are induced by intervals $\bigcup \{X(\beta_i) : i \in \{j, \ldots, j'\}\}$, implying that the equivalence classes of \approx_{Π} are also the set $X(\beta_i)$. The result then follows, with (i) corresponding to a P-node root, and (ii) corresponding to a Q-node root (< β being the order on the children of the root).

Conversely, suppose that each equivalence class of \approx_{Π} is represented, and either (i) or (ii) holds. Then it can be readily checked that the PQ-tree defined in the statement of the result does indeed represent Π .

3.2. Nodes of a PQ-tree. Sets that are simultaneously mmodules and blocks of a Robinson space (X, d) play a special role because in any compatible order their points can be ordered independently of the rest of the points. We prove that they correspond exactly with the nodes of the PQ-tree \mathcal{T}_{PQ} of (X, d).

Lemma 3.4. Let (X, d) be a Robinson space with a compatible order <'. Let S be an module that is an interval in <' and \leq_S be any compatible order on S. Let < be the total order on X defined by setting x < y when either $\{x, y\} \subset S$ and $x <_S y$, or $\{x, y\} \notin S$ and x <' y (equivalently, < is obtained from <' by reordering the elements of S according to \leq_S). Then < is a compatible order of (X, d).

Proof. Pick any x < y < z and we check that $d(x,z) \ge \max\{d(x,y), d(y,z)\}$. If $x, y, z \in S$, then $x <_S y <_S z$ and the result follows. If $|\{x, y, z\} \setminus S| \in \{2, 3\}$, then x <'y <'z and we are done again. If $x \notin S$, $y, z \in S$, then d(x, y) = d(x, z) because S is an mmodule, and $d(y, z) \le \max\{d(x, y), d(x, z)\}$ because either x <'y <'z or x <'z <'y' holds. Thus $d(x, z) \ge \max\{d(x, y), d(y, z)\}$. The case $x, y \in S$, $z \notin S$ is symmetric, while the case $x, z \in S$, $y \notin S$ cannot happen as S is an interval in <'.

Let < be a compatible order for (X, d) for which S is an interval. Let $<_{\overline{S}}$ be the order defined by setting $x <_{\overline{S}} y$ if either x < y and $\{x, y\} \notin S$, or y < x and $\{x, y\} \subseteq S$, that is $<_{\overline{S}}$ is the order obtained from < by reversing the interval S. We can easily generalize $<_{\overline{S}}$ to a subset S which is not an interval and we have the following elementary result:

Lemma 3.5. Let (X, d) be a Robinson space and $S \subseteq X$ an interval of a compatible order <. Then $<_{\overline{S}}$ is a compatible order if and only if S is an mmodule.

Proof. If S is an mmodule, then by Lemma 3.4 $\leq_{\overline{S}}$ is compatible. Conversely, let $\leq_{\overline{S}}$ be a compatible order. Let $y, z \in S$ with y < z, and let $x \notin S$, and say (by symmetry) that x < y < z. Then $d(x, y) \leq d(x, z)$. Since $x <_{\overline{S}} z <_{\overline{S}} y$ and $\leq_{\overline{S}}$ is compatible, we obtain $d(x, z) \leq d(x, y)$. Consequently, d(x, y) = d(x, z), yielding that S is an mmodule.

More generally, one can reorder the elements of a block as long as the order of the block itself remains compatible.

Lemma 3.6. For any node α of the PQ-tree \mathcal{T}_{PQ} of a Robinson space (X,d), the set $X(\alpha)$ is an *module of* (X,d).

Proof. By definition of PQ-trees, for any compatible order < of \mathcal{T}_{PQ} , $S := X(\alpha)$ is an interval and $<_{\overline{S}}$ is compatible. By Lemma 3.5, $X(\alpha)$ is an interval.

Using Proposition 2.13(vi), this justifies the notation $d(\alpha, \beta)$ for any two nodes α or β of \mathcal{T}_{PQ} or \mathcal{T}_M with $X(\alpha)$ and $X(\beta)$ disjoint, where $d(\alpha, \beta) = d(x, y)$ for any $x \in X(\alpha)$, $y \in X(\beta)$. Combining the last results, we get the following characterization of the subsets of X corresponding to the nodes of the PQ-tree of (X, d):

Theorem 3.7. Let (X, d) be a Robinson space and M be a subset of X. Then $X(\alpha) = M$ for some node α of \mathcal{T}_{PQ} if and only if M is a block and an mmodule of (X, d).

Proof. From Lemmas 3.2 and 3.6, for any node α of the PQ-tree, $X(\alpha)$ is an mmodule and a block. Conversely, consider a set $M \subseteq X$ that is both an mmodule and a block. By way of contradiction, suppose that there is no node α such that $M = X(\alpha)$. By Lemma 3.2, there is a Q-node α in \mathcal{T}_{PQ} with children β_1, \ldots, β_k , and j, j' with $1 \leq j < j' \leq k$ and $\{j, j'\} \neq \{1, k\}$ such that $M = X(\beta_j) \cup \ldots \cup X(\beta_{j'})$. Let < be a compatible order with $X(\beta_1) < \ldots < X(\beta_k)$. Then by Lemma 3.5, $\leq_{\overline{S}}$ is also a compatible order, with $X(\beta_1) <_{\overline{S}} X(\beta_j') <_{\overline{S}} X(\beta_j) <_{\overline{S}} X(\beta_k)$. But that order is not compatible with \mathcal{T}_{PQ} , a contradiction.

This leads to the following result, which involves flat Robinson spaces.

Corollary 3.8. Let (X, d) be a Robinson space in which all mmodules are trivial and $|X| \ge 3$. Then the following holds:

(i) (X, d) is flat,

(ii) \mathcal{T}_{PQ} has a single non-leaf node, that is a Q-node.

Proof. Since each mmodule is trivial, by Lemma 3.6, \mathcal{T}_{PQ} has a single non-leaf node α . Suppose for sake of contradiction that α is a P-node. Let $x, y, z \in X$ be distinct points, that are children of α . Then there exist compatible orders $<_1$, $<_2$, and $<_3$ with $x <_1 y <_1 z$, $y <_2 z <_2 x$, and $z <_3 x <_3 y$. Hence $d(x, z) \ge d(x, y) \ge d(y, z) \ge d(x, z)$, meaning that these three distances are equals. Consequently, all pairwise distances between the points of X are equal, thus any subset of points is an mmodule, a contraction. Thus α is a Q-node and (ii) is verified.

Clearly, (ii) implies (i).

Remark 3.9. It is worth observing that the converse of Corollary 3.8 does not hold, and dealing with this limitation is arguably one of the main technical difficulties that this paper addresses. This is illustrated by the simple example given in Figure 5. Later we will show that this happens when some maximal mmodule has larger diameter than its distance to other points; here $\{a, c\}$ has diameter 2, which is higher than the distance between the mmodules $\{a, c\}$ and $\{b\}$.



FIGURE 5. A flat Robinson space, together with its PQ-tree \mathcal{T}_{PQ} and its mmodule tree \mathcal{T}_M .

3.3. Distances and the PQ-tree. In this subsection, we present some results about the values of the dissimilarity relative to the nodes of the PQ-tree (and the mmodule tree). The next two lemmas motivate the notions and the results of the next section, and also relates to the properties of clusters and of the weights of nodes in dendrograms of ultrametrics.

Lemma 3.10. Let (X, d) be a Robinson space with PQ-tree \mathcal{T}_{PQ} and α a P-node in \mathcal{T}_{PQ} . Let β_1, \ldots, β_k be some of the children of α , then $S := X(\beta_1) \cup \ldots \cup X(\beta_k)$ is an mmodule.

Proof. If k = 1 or $S = X(\alpha)$, this follows from Theorem 3.7. Otherwise, let $x, y \in S$ be in two distinct children of α , and $z \in X(\alpha) \setminus S$. By property of the P-nodes, there are compatible orders < and <' with x < y < z and y <' x <' z. Thus $d(y, z) \leq d(x, z) \leq d(y, z)$, implying that d(x, z) = d(y, z); so S is an mmodule.

Lemma 3.11. Let (X, d) be a Robinson space with PQ-tree \mathcal{T}_{PQ} and mmodule tree \mathcal{T}_M . Let α be a P-node of \mathcal{T}_{PQ} or a \cap -node of \mathcal{T}_M . Then there exists $\delta > 0$ such that for any x, y appearing in two distinct children of α , we have $d(x, y) = \delta$.

Proof. Let β be a child of α . Then $X(\alpha) \setminus X(\beta)$ is an mmodule, by Proposition 2.15 when α is a \cap -node and by Lemma 3.10 when α is a P-node. Hence by Proposition 2.13(vi) the distances are uniform between $X(\beta)$ and $X(\alpha) \setminus X(\beta)$, and thus uniform between children of α .

As a consequence, for any α P-node of \mathcal{T}_{PQ} or \cap -node of \mathcal{T}_M , we denote $\rho(\alpha)$ the value δ from Lemma 3.11, that is the distance between children of α . Another observation is that, similarly to dendrograms, the diameters of nodes are almost strictly monotone in the PQ-tree.

Lemma 3.12. Let (X, d) be a Robinson space with PQ-tree \mathcal{T}_{PQ} . Let α be an internal node of \mathcal{T}_{PQ} and β a non-leaf child of α . Then

- (i) if α is a P-node, diam $(X(\beta)) \leq \rho(\alpha) = diam(X(\alpha));$
- (*ii*) if α is a Q-node, diam $(X(\beta)) \leq \min\{d(\beta, \beta') : \beta' \text{ child of } \alpha, \beta \neq \beta'\} \leq \operatorname{diam}(X(\alpha));$
- (iii) if diam $(X(\alpha)) =$ diam $(X(\beta))$, then α is a P-node, β is a Q-node, and for any non-leaf child γ of β , diam $(X(\gamma)) <$ diam $(X(\alpha))$.

Proof. Let $x, y \in X(\beta)$ and $z \in X(\alpha) \setminus X(\beta)$. By Theorem 3.7, $X(\beta)$ is a block and mmodule, hence for any compatible order < with x < y, either z < x or y < z. By symmetry we may assume x < y < z. Then $d(x, y) \le d(x, z) = d(y, z)$. If α is a P-node, then by Lemma 3.11 $d(x, z) = \rho(\alpha)$ and thus (i) holds. If α is a Q-node, by choosing $z \in \beta'$, we get (ii).

Suppose that $\delta := \operatorname{diam}(X(\alpha)) = \operatorname{diam}(X(\beta))$. We claim that α is a P-node. Assume that α has arity at least three (as otherwise it is a P-node by definition). Then for any β' child of α distinct from β , $d(\beta, \beta') = \delta$. Hence $S' := X(\alpha) \setminus X(\beta)$ is an mmodule. As α has at least three children, S' is not a set induced by a node of \mathcal{T}_{PQ} , thus by Theorem 3.7 is not a block. Because $X(\alpha)$ is a block, it means that there is a compatible order $\langle, x, z \in S' \text{ and } y \in X(\beta) \text{ with } x < y < z$. Let β_x and β_z be the children of α containing x and z respectively. Then, for each $x' \in S'$ with x' < y and each $z' \in S'$ with y < z', $\delta = d(x', y) \leq d(x', z') \leq \operatorname{diam}(X(\alpha)) = \delta$, proving that $S := X(\beta) \cup \{x \in S : x < y\}$ is an mmodule. Then, by Lemma 3.5, $\langle_{\overline{S}}$ is a compatible order. Hence β_x, β, β_z may be ordered in more than two ways, α is a P-node.

For the sake of contradiction, suppose furthermore that β is a P-node. Then $\rho(\alpha) = \rho(\beta) = \delta$. Let γ be a child of β . Then by Proposition 2.15, $X(\beta) \setminus X(\gamma)$ is an mmodule and $d(X(\gamma), X(\beta \setminus X(\gamma)) = \delta$. Thus $S := X(\alpha) \setminus X(\gamma)$ is also an mmodule. Let < be a compatible order with x < y < z for any $x \in X(\gamma), y \in X(\beta) \setminus X(\gamma)$ and $z \in X(\alpha) \setminus X(\beta)$ (such an order exists by the structure of \mathcal{T}_{PQ}). Then by Lemma 3.5, $<_{\overline{S}}$ is also a compatible order, contradiction because $X(\beta)$ is a block by Theorem 3.7. Thus β is a Q-node. Consequently, for any non-leaf child γ of β , diam $(X(\gamma)) < \text{diam}(X(\beta)) = \text{diam}(X(\alpha))$. Thus (iii) is proved.

3.4. Dendrograms and PQ-trees for ultrametrics. As an application of the results of this section, we prove that for ultrametrics, the X-trees \mathcal{T}_{PQ} and \mathcal{T}_D are isomorphic. Furthermore, we consider the following characterizations of ultrametric spaces by their PQ-trees (these results probably can be considered as half-folkloric, however we give their full proofs):

Proposition 3.13. A Robinson space (X, d) is ultrametric if and only all internal nodes of \mathcal{T}_{PQ} are *P*-nodes.

Proof. Suppose first that (X, d) is ultrametric and, by a way of contradiction, that its PQ-tree \mathcal{T}_{PQ} has a Q-node $\alpha = Q(\beta_1, \beta_2, \ldots, \beta_k)$ with $k \geq 3$. We set $\delta = \operatorname{diam}(X(\alpha)) = d(\beta_1, \beta_k)$. Let $i \in \{1, \ldots, k\}$ be minimum such that $d(\beta_1, \beta_i) = \delta$. If i = 2, then, for all $j \in \{2, \ldots, k\}$, $d(\beta_1, \beta_j) = \delta$, implying that $X(\beta_2) \cup \ldots \cup X(\beta_k)$ is an mmodule. By Lemma 3.2, it is also a block, and thus by Theorem 3.7 k = 2, contradiction. If i > 2, since $d(\beta_1, \beta_{i-1}) < \delta$ and $d(\beta_{i-1}, \beta_i) \leq d(\beta_1, \beta_i) = \delta$, by definition of ultrametric we have $d(\beta_{i-1}, \beta_i) = \delta$. Consequently, for all $1 \leq j < i \leq j' \leq k$, we have $d(\beta_j, \beta_{j'}) = \delta$. Thus $X(\beta_1) \cup \ldots \cup X(\beta_{i-1})$ and $X(\beta_i) \cup \ldots \cup X(\beta_k)$ are blocks and mmodules, by Theorem 3.7 i = k = 2, contradiction. Conversely, suppose that all internal nodes of \mathcal{T}_{PQ} of arity more than two are P-nodes and let $x, y, z \in X$. Let α be the lowest common ancestor of x, y, z. If two of them, say x and y, have a child of α as common ancestor, then we have $d(x, y) \leq d(x, z) = d(y, z)$. Otherwise, $|\mathsf{ca}(x, y)| = |\mathsf{ca}(x, z)| = \alpha$. Since α is a P-node of arity at least three, we have d(x, y) = d(y, z) = d(x, z).

Proposition 3.14. Let (X, d) be an ultrametric space. Then the X-trees \mathcal{T}_{PQ} and \mathcal{T}_{D} are isomorphic.

Proof. Let β be an internal node of \mathcal{T}_D . Then for any $x \notin X(\beta)$, let α be the least common ancestor of x and β in \mathcal{T}_D , we have $d(x,\beta) = \rho(\alpha)$. Thus $X(\beta)$ is an mmodule. Also, by definition of \mathcal{T}_D , $X(\beta)$ is a ball of radius $\rho(\beta)$ centered at any point in $X(\beta)$. From the definition of Robinson space, any ball is a block. By Theorem 3.7, as $X(\beta)$ is a block and an mmodule, there is a node β' in \mathcal{T}_{PQ} with $\beta = \beta'$.

Conversely, for any node β' in \mathcal{T}_{PQ} and any $x \notin X(\beta')$, let α' be the least common ancestor of β' and x. By Proposition 3.13, α' and β' are P-nodes, and thus $d(x,\beta') = \rho(\alpha')$. By Lemma 3.12, $\rho(\alpha') > \rho(\beta')$, hence $d(x, X(\beta')) > \operatorname{diam}(X(\beta'))$. Thus there is a node β in \mathcal{T}_D with $X(\beta) = X(\beta')$.

4. The graph $G_{\overline{\delta}}$ and the construction of the PQ-tree

In this section we introduce the graph $G_{\overline{\delta}}$ and the δ -mmodules, which are the most important notions defined in this paper. We use them together with the maximal mmodules to construct the PQ-tree of a Robinson space.

4.1. The graph $G_{\overline{\delta}}$ and δ -mmodules. In this subsection, we define and give properties of the graph $G_{\overline{\delta}}$ and δ -modules. Some of the properties are valid for any dissimilarity space (first part of Lemma 4.2, Lemmas 4.3 and 4.4), the others are only valid for Robinson spaces.

Definition 4.1 (Graphs $G_{\overline{\delta}}$, $G_{<\delta}, G_{\leq\delta}$, and δ -mmodules). Let (X, d) be a dissimilarity space and let $\delta > 0$. Then $G_{\overline{\delta}}$ is the graph with X as the set of vertices and edges $\{xy : x, y \in X, d(x, y) \neq \delta\}$. Let also $G_{<\delta} := (X, \{xy : x \neq y, d(x, y) < \delta\})$ and $G_{\leq\delta} := (X, \{xy : x \neq y, d(x, y) \leq \delta\})$. For $S \subseteq X$, we denote by $G_{\overline{\delta}}(S)$ the subgraph of $G_{\overline{\delta}}$ induced by S. The connected components of the graph $G_{\overline{\delta}}$ are called the δ -mmodules of (X, d), and their number is denoted c_{δ} .

Lemma 4.2. Let (X, d) be a dissimilarity space and $\delta > 0$ such that the graph $G_{\overline{\delta}}$ is not connected. Then each δ -mmodule is an mmodule. Moreover, if (X, d) is Robinson, then at most one δ -mmodule is not a block, and each δ -mmodule that is a block has diameter at most δ .

Proof. Let M be a δ -mmodule. Then for any $x, y \in M$, $z \notin M$, by definition of $G_{\overline{\delta}}$ we have $d(x, z) = \delta = d(z, y)$, hence M is an mmodule.

Suppose now that (X, d) is Robinson and let < be any compatible order, with minimum x_{\star} and maximum x^{\star} . Suppose that M does not contain x_{\star} (or symmetrically x^{\star}). Then for any $y, z \in M$ with y < z, we have $d(y, z) \leq d(x_{\star}, z) = \delta$, hence diam $(M) \leq \delta$. Since at most one connected component of $G_{\overline{\delta}}$ may contain both points x_{\star}, x^{\star} , we conclude that any other component has diameter at most δ .

Let M be a connected component of $G_{\overline{\delta}}$ with diam $(M) \leq \delta$. We assert that M is an interval of <. Let x < y < z with $x, z \in M, y \notin M$. Consider a path P from x to z in $G_{\overline{\delta}}$. Necessarily P contains an edge x'z' with $x', z' \in M$ and x' < y < z'. Then by definition of edges of $G_{\overline{\delta}}$ and since diam $(M) \leq \delta$, we have $d(x', z') < \delta$. Consequently, $d(x', y) \leq d(x', z') < \delta$, proving that $y \in M$, contrary to our choice of y. Thus M is an interval of <.

If there is a connected component M_0 of $G_{\overline{\delta}}$ with diam $(M_0) > \delta$, then all other connected components have diameter at most δ , and x_{\star}, x^{\star} is a diametral pair of M_0 . Hence for every compatible order, each other connected component M of $G_{\overline{\delta}}$ is an interval, hence M is a block.

Otherwise, if a connected component of $G_{\overline{\delta}}$ with diameter larger than δ does not exist, then we prove that there is no component M with $x_{\star}, x^{\star} \in M$ for any compatible order <. By way of contradiction assume there is one, and let $y \notin M$. For any $x, z \in M$ with x < y < z, we have $d(x, z) \ge \max\{d(x, y), d(y, z)\} = \delta$. Since diam $(M) \le \delta$, this yields $d(x, z) = \delta$. But then the points x such that x < y and z such that y < z cannot belong to the same connected component of $G_{\overline{\delta}}$. This contradicts the fact that x_{\star} and x^{\star} belong to M. Consequently, in this case each connected component is an interval in any compatible order, hence is a block.

The following result shows that either the graph $G_{\overline{\delta}}$ is connected for all values of $\delta > 0$ or there exists a unique positive value of δ such that $G_{\overline{\delta}}$ is not connected. Furthermore, we characterize the dissimilarity spaces for which the second option occurs.

Lemma 4.3. Let (X, d) be a dissimilarity space such that \mathcal{M}_{\max} is a copartition of X. Then there exists a unique $\delta > 0$ such that for any maximal mmodule M, for any $x \in M$ and $y \in X \setminus M$, we have $d(x, y) = \delta$. Consequently, the graph $G_{\overline{\delta}}$ is not connected and each connected component of $G_{\overline{\delta}}$ is the complement of a maximal mmodule. Conversely, if there exists $\delta > 0$ such that $G_{\overline{\delta}}$ is not connected, then \mathcal{M}_{\max} is the copartition of X consisting of the complements of the δ -mmodules.

Proof. First, let \mathcal{M}_{\max} be a copartition. Let M, M' be two maximal mmodules, and let $x \in M$, $x' \in X \setminus M, y' \in M'$ and $y \in X \setminus M'$. We assert that d(x, x') = d(y, y'), allowing us to set $\delta = d(x, x')$. As \mathcal{M}_{\max} is a copartition, $X \setminus M' \subset M$ and $X \setminus M \subset M'$, hence $x' \in M'$ and $y \in M$. Since $x, y \in M, x' \in X \setminus M$ and M is an mmodule, we deduce that d(x, x') = d(y, x'). Analogously, since $x', y' \in M', y \in X \setminus M'$ and M' is an mmodule, we get d(x', y) = d(y', y), and thus d(x, x') = d(y, y'). Then $G_{\overline{\delta}}$ is not connected as each maximal mmodule and its complement define a cut of $G_{\overline{\delta}}$. The connected components of $G_{\overline{\delta}}$ are the subsets of the partition defined by the complements of maximal mmodules.

Conversely, let $\delta > 0$ be such that the graph $G_{\overline{\delta}}$ is not connected. Then any arbitrary union of connected components of $G_{\overline{\delta}}$ is an mmodule. Thus, for each component C of $G_{\overline{\delta}}$, its complement $M = X \setminus C$ is an mmodule. We assert that M belongs to \mathcal{M}_{\max} . Let M' be an mmodule containing M. Then $C' := X \setminus M'$ is a subset of C. Since M' is an mmodule, for any $x \in C', y \in M', d(x, y) = \delta$ holds. This implies that M' and C' define a cut of $G_{\overline{\delta}}$, thus C' is a union of connected components of $G_{\overline{\delta}}$. Since $C' \subseteq C$ and C is a connected component of $G_{\overline{\delta}}$, we conclude that C' = C and M' = M, establishing the maximality of M.

We can actually give a simple characterization of the unique value of δ such that the graph $G_{\overline{\delta}}$ is not connected.

Lemma 4.4. Let (X, d) be a dissimilarity space such that \mathcal{M}_{\max} is a copartition of X, and $\delta > 0$ be the unique value such that $G_{\overline{\delta}}$ is not connected. Let T be a minimum spanning tree on the complete graph on vertex set X, with weights given by d. Then

 $\delta = \max\{d(x,y) : xy \in T\} = \min\{\delta' > 0 : the graph (X, \{xy : x \neq y, d(x,y) \le \delta'\}) is connected\}.$

Proof. Let $T \subseteq \binom{X}{2}$ be a minimum-weight spanning tree on X. Since $G_{\overline{\delta}}$ is not connected, T must contain an edge with weight δ , hence $\max\{d(x,y) : xy \in T\} \ge \delta$.

Let e = xy be any edge of T. If e joins two components of $G_{\overline{\delta}}$, then its weight is δ . Else, let M be the connected component of $G_{\overline{\delta}}$ containing x and y. Pick any $z \notin M$ (such z exists since $G_{\overline{\delta}}$ is not connected). We may assume that y lies between x and z in the tree T. Then $T \setminus \{e\} \cup \{xz\}$ is a spanning tree. By minimality of T, $d(x, y) \leq d(x, z)$. Since $x \in M, z \notin M$, we also have $d(x, z) = \delta$. Consequently, $d(x, y) \leq \delta$ for any edge of T. This proves the first inequality.

As $G_{\overline{\delta}}$ is not connected, the graph $G_{<\delta} := (X, \{xy : d(x, y) < \delta\})$ is not connected. Moreover $G_{\leq \delta} := (X, \{xy : d(x, y) \leq \delta\})$ is a supergraph of the complement of $G_{\overline{\delta}}$. As the complement of a not-connected graph is connected, $G_{\leq \delta}$ is connected, proving the last inequality. \Box

Definition 4.5 (Connected and non-connected dissimilarity spaces, large ρ -mmodules). Let ρ be the minimum value such that the graph $G_{\leq \rho} = (X, \{xy : x \neq y, d(x, y) \leq \rho\})$ is connected. If the graph $G_{\overline{\rho}}$ is not connected, then we say that the dissimilarity space (X, d) is non-connected. Otherwise, all graphs $G_{\overline{\delta}}$ are connected for $\delta > 0$, and we say that the dissimilarity space (X, d) is connected. If (X, d) is a non-connected Robinson space and $G_{\overline{\rho}}$ contains a connected component with diameter larger that ρ (see Lemma 4.2), then we call this component a large ρ -mmodule.

Using the relationship between the minimum spanning tree and the dendrogram $\mathcal{T}_{\hat{d}}$ of the subdominant ultrametric \hat{d} of d, we get that ρ is the weight of the root in the vertex representation of $\mathcal{T}_{\hat{d}}$. Observe also that ρ coincides with $\rho(\alpha)$ when α is a P-node root of \mathcal{T}_{PQ} or a \cap -node root of \mathcal{T}_M . The next result establishes some properties of large ρ -mmodules.

Lemma 4.6. Let (X, d) be a non-connected Robinson space containing a large ρ -mmodule S_0 . Then S_0 has the following properties:

- (i) there is a unique bipartition $S_0 = S_{\star} \cup S^{\star}$ of S_0 into two blocks,
- (*ii*) diam $(S_{\star}) \leq \rho$ and diam $(S^{\star}) \leq \rho$,
- (*iii*) $d(x,y) \ge \rho$ for any $x \in S_{\star}, y \in S^{\star}$,
- (iv) if there exists $\delta > 0$ such that $G_{\overline{\delta}}(S_0)$ is not connected, then $\delta > \rho$ and the connected components of $G_{\overline{\delta}}(S_0)$ are S_{\star} and S^{\star} .

Proof. Let $y \in X \setminus S_0$, and < be any compatible order for (X, d). Since diam $(S_0) > \rho$, S_0 contains at least two points. Let xz be any edge of $G_{\overline{\rho}}(S_0)$ and suppose that x < z. If $d(x, z) < \rho$, then, as $d(x, y) = d(y, z) = \rho$, either x < z < y or y < x < z holds. Otherwise, by definition of the edges of $G_{\overline{\rho}}$ we have $d(x, z) > \rho$, and thus x < y < z holds. Setting $E_{>\rho} := \{x'z' \in E(G_{\overline{\rho}}) : d(x', z') > \rho\}$, it implies that for any $xz \in E(G_{\overline{\rho}})$ and $y \in X \setminus S_0$, y is between x and z in any compatible order if and only if $xz \in E_{>\rho}$.

We can extend the previous argument to any pair of vertices x, z of S_0 . Since S_0 is connected in $G_{\overline{\rho}}$, there exists at least one (x, z)-path and let $P = (x = x_0x_1, x_1x_2, \dots, x_{\ell-1}x_{\ell} = z)$ be an arbitrary (x, z)-path. Then the parity of the number of edges x_ix_{i+1} of P such that y is between x_i and x_{i+1} is odd if and only if y is between $x = x_0$ and $z = x_{\ell}$. In particular, this parity is the same for all paths with extremities x and z. Fixing $x \in S_0$, we can thus define the following bipartition of S_0 :

$$S^{\star} := \{z \in S_0 : \text{for each } (x, z) \text{-path } P \text{ of } G_{\delta^*}, |P \cap E_{>\rho}| \text{ is even}\},\$$

$$S_{\star} := \{z \in S_0 : \text{for each } (x, z) \text{-path } P \text{ of } G_{\delta^*}, |P \cap E_{>\rho}| \text{ is odd} \}.$$

Then for any $y \in X \setminus S_0$, y is between any pair $x \in S_{\star}$, $z \in S^{\star}$, hence $X \setminus S_0$, S_{\star} and S^{\star} are blocks, and this bipartition is unique, establishing (i).

By construction, the bipartition (S_{\star}, S^{\star}) has the properties (ii) and (iii). For (iv), suppose there exists $\delta > 0$ such that $G_{\overline{\delta}}(S_0)$ is not connected. Then $\delta \neq \rho$, as S_0 is a connected component of $G_{\overline{\rho}}$. The inequality $\delta < \rho$ is also impossible, since the complete bipartite graph on (S_{\star}, S^{\star}) would be a subgraph of $G_{\overline{\delta}}(S_0)$. Hence $\delta > \rho$. By (ii), each of the sets S_{\star} and S^{\star} induces a connected subgraph in $G_{\overline{\delta}}(S_0)$, hence S_{\star} and S^{\star} are the connected components of $G_{\overline{\delta}}(S_0)$.

The existence of large ρ -mmodules will induce some irregularities in both tree representations of Robinson dissimilarities. The next definitions capture those irregularities, and will be useful when comparing PQ-trees and mmodule trees.

Definition 4.7 (δ -special, large, δ -conical, apex, split and standard nodes). Let (X, d) be a Robinson space with mmodule tree \mathcal{T}_M and PQ-tree \mathcal{T}_{PQ} . Let $\delta > 0$.

A \cap -node $\alpha = \cap(\beta_1, \ldots, \beta_k)$ of \mathcal{T}_M is called δ -special if for all distinct $j, j' \in \{1, \ldots, k\}$, we have $d(X(\beta_j), X(\beta_{j'})) = \delta$ and there is $i \in \{1, \ldots, k\}$ such that $\operatorname{diam}(X(\beta_i)) > \delta$ holds. Then β_i is unique and called the *large* child of α . A \cap -node is *special* if it is δ -special for some $\delta > 0$.

A Q-node $\alpha = Q(\beta_1, \dots, \beta_k)$ of \mathcal{T}_{PQ} is called δ -conical if there is a child β_i such that for all $j \in \{1, \dots, k\} \setminus \{i\}$, we have $d(X(\beta_i), X(\beta_j)) = \delta$. Then β_i is unique and called the *apex* child of α . A Q-node is *conical* if it is δ -conical for some $\delta > 0$.

If α is the apex child of a δ -conical Q-node and $G_{\overline{\delta}}(X(\alpha))$ is not connected, then α is called a *split node*. If a node α of \mathcal{T}_{PQ} is not split, then it is *standard*.

The uniqueness of β_i in both definitions can be readily checked:

- The uniqueness of the large child of a special \cap -node derives from Lemma 4.2.
- Suppose that a conical node $\alpha = Q(\beta_1, \dots, \beta_k)$ has two apex children β_i and β_j . First notice that the distance between β_i and the other children is the same that the distance between β_j and the other children (its value is $d(X(\beta_i), X(\beta_j))$). It would be possible to exchange the nodes β_i and β_j in the list of the children of α , a contradiction.

4.2. Construction of the PQ-tree. The three next propositions describe how to build the nodes of the PQ-tree of a Robinson dissimilarity through the analysis of its ρ -mmodules.

Proposition 4.8. Let (X, d) be a connected Robinson space. Then the following assertions hold:

- (i) \mathcal{M}_{\max} is a partition of X with $|\mathcal{M}_{\max}| \geq 3$,
- (ii) each maximal mmodule is a block,
- (iii) the quotient space $(X/\mathcal{M}_{\max}, d)$ is flat,
- (iv) the compatible orders on X are exactly the composition of each of the two compatible orders of $(X/\mathcal{M}_{\max}, \hat{d})$ with the compatible orders of each maximal mmodule,
- (v) the root of \mathcal{T}_{PQ} is a Q-node, whose children are the PQ-trees of the maximal mmodules, sorted by the compatible orders of $(X/\mathcal{M}_{\max}, \hat{d})$.

Proof. If $\mathcal{M}_{\max} = \{M_1, \ldots, M_k\}$ is a copartition of X, then by Lemma 4.3, $G_{\overline{\rho}}$ is not connected, contradicting the hypothesis. Hence (i) holds.

Consider the quotient space $(X/\mathcal{M}_{\max}, \hat{d})$. By construction, its mmodules are all trivial. Hence by Corollary 3.8, $(X/\mathcal{M}_{\max}, \hat{d})$ is flat and has a unique compatible order $<_{\mathcal{M}_{\max}}$ up to reversal, that is, (iii) holds. We may assume that $M_1 <_{\mathcal{M}_{\max}} \ldots <_{\mathcal{M}_{\max}} M_k$. Then for each compatible order < on X, for each choice of $x_i \in M_i$ for $i \in \{1, \ldots, k\}$ the restriction of < to $\{x_1, \ldots, x_k\}$ coincides with $<_{\mathcal{M}_{\max}}$ or its reversal, that is either $x_1 < \ldots < x_k$ or $x_k < \ldots < x_1$. This implies that each M_i is an interval for <, hence (ii) holds.

By Theorem 3.7, each M_i is a node β_i in \mathcal{T}_{PQ} . By Lemma 3.4, the relative order of elements in M_i can be chosen independently from the order of the blocks. Thus (iv) holds. Finally by Proposition 3.3, it implies (v).

Proposition 4.9. Let (X, d) be a non-connected Robinson space and suppose that the diameter of each ρ -mmodule is at most ρ . Then the root of \mathcal{T}_{PQ} is a P-node whose children are the PQ-trees of each ρ -mmodule.

Proof. Let M be a ρ -mmodule. By Lemma 4.2, M is an mmodule and a block. By Theorem 3.7, there exists a node β_M in \mathcal{T}_{PQ} such that $X(\beta_M) = M$. Moreover, by Lemma 3.4, in any compatible order <, reordering the elements of M into an order compatible with β_M gives a compatible order

on X. Furthermore, since for any $x, y \in X$ that are not in the same mmodule, $d(x, y) = \rho$ holds, any order between the blocks corresponding to each ρ -mmodule is compatible. Hence each ρ -mmodule is a maximal block, and the result follows by Proposition 3.3.

Proposition 4.10. Let (X, d) be a non-connected Robinson containing a large ρ -mmodule S_0 . Let S_1, \ldots, S_k be the other ρ -mmodules. Then the root of $\mathcal{T}_{PQ}(S_0)$ is a Q-node $Q(\beta_1, \ldots, \beta_\ell)$ or a P-node $P(\beta_1, \beta_2)$ (and $\ell = 2$), and the root of the PQ-tree $\mathcal{T}_{PQ}(X)$ is a special Q-node $Q(\beta_1, \ldots, \beta_{i-1}, \beta, \beta_i, \ldots, \beta_\ell)$, obtained by adding an apex child β to the root of $\mathcal{T}_{PQ}(S_0)$, where

$$\beta = \begin{cases} \mathcal{T}_{PQ}(S_1) & \text{if } k = 1, \\ P(\mathcal{T}_{PQ}(S_1), \dots, \mathcal{T}_{PQ}(S_k)) & \text{if } k \ge 2. \end{cases}$$

Proof. By Lemma 4.6, there is a bipartition $S_0 = S_{\star} \cup S^{\star}$ of S_0 into two blocks, with diam $(S_{\star}) \leq \rho$, diam $(S^{\star}) \leq \rho$, and $d(x, y) \geq \rho$ for each $x \in S_{\star}, y \in S^{\star}$.

We claim that the root of $\mathcal{T}_{PQ}(S_0)$ is a Q-node or has arity two. If $G_{\overline{\delta}}[S_0]$ is connected for every $\delta > 0$, then by Proposition 4.8, the root of $\mathcal{T}_{PQ}(S_0)$ is a Q-node. Otherwise, let $\delta > 0$ be such that $G_{\overline{\delta}}(S_0)$ is not connected. By Lemma 4.6(iv), $\delta > \rho$ and $G_{\overline{\delta}}(S_0)$ has two connected components S_{\star} and S^{\star} , each of diameter less than δ . By Proposition 4.9, the root of $\mathcal{T}_{PQ}(S_0)$ is a P-node $P(\mathcal{T}_{PQ}(S_{\star}), \mathcal{T}_{PQ}(S^{\star}))$.

Let β_1, \ldots, β_l be the children of the root α of $\mathcal{T}_{PQ}(S_0)$, with $k \geq 2$. By Lemma 3.2, S_{\star} and S^{\star} are induced by consecutive children of α , that is, up to symmetry, there is $i \in \{2, \ldots, \ell\}$ such that $S_{\star} = \bigcup_{i=1}^{l-1} X(\beta_i)$ and $S^{\star} = \bigcup_{i=1}^{\ell} X(\beta_i)$. Let β be defined as in the statement of the result.

We claim that $\beta = \mathcal{T}_{PQ}(X \setminus S_0)$. If k = 1 this is immediate from the definition of β . If $k \ge 2$, then $G_{\overline{\rho}}(X \setminus S_0)$ is not connected and its components are precisely S_1, \ldots, S_k . Thus the claim follow by Proposition 4.9.

Then we show that $\mathcal{T}_{PQ}(X) = Q(\beta_1, \ldots, \beta_{i-1}, \beta, \beta_i, \ldots, \beta_\ell)$. Let < be a compatible order of (X, d). By Lemma 4.6, S_{\star} and S^{\star} are blocks. Notice that the restriction of < to S_0 is represented by $\mathcal{T}_{PQ}(S_0)$. By Lemma 4.2, S_1, \ldots, S_k are blocks, implying that the restriction of < to $X \setminus S_0$ is represented by β . Moreover as $d(S_{\star}, S_j) = d(S_j, S^{\star}) = \rho < \max\{d(x, y) : x \in S_{\star}, y \in S^{\star}\} = \operatorname{diam}(S_0)$, we have that S_j is between S_{\star} and S^{\star} in any compatible order. Thus < is represented by $Q(\beta_1, \ldots, \beta_{i-1}, \beta, \beta_i, \ldots, \beta_\ell)$.

Conversely, let < be an order represented by $Q(\beta_1, \ldots, \beta_{i-1}, \beta, \beta_i, \ldots, \beta_\ell)$ with $S_{\star} < S^{\star}$. We show that < is a compatible order of (X, d). Let x < y < z be a triplet of points in X. As the restriction of < is represented by $\mathcal{T}_{PQ}(S_0)$, if $x, y, z \in S_0$, then $\max\{d(x, y), d(y, z)\} \leq d(x, z)$. If $x, y \in S_0$, $z \in X \setminus S_0$, then as $x, y \in S_{\star}$, $d(x, y) \leq \rho = d(y, z) = d(x, z)$. The case $y, z \in S_0$, $x \in X \setminus S_0$ is similar. If $x, z \in S_0$ and $y \in X \setminus S_0$, then $x \in S_{\star}$, $z \in S^{\star}$, hence $d(x, z) \geq \rho = d(x, y) = d(y, z)$. If $x, y \in X \setminus S_0$ and $z \in S_0$, then $d(x, y) \leq \rho = d(y, z) = d(x, z)$. The case $x \in S_0$, $y, z \in X \setminus S_0$ is similar. Finally, if $x, y, z \in X \setminus S_0$, as the restriction of < to $X \setminus S_0$ is represented by β , again $\max\{d(x, y), d(y, z)\} \leq d(x, z)$. Hence < is compatible. \Box

Propositions 4.8 to 4.10 lead to Algorithm 1 that builds the PQ-tree of (X, d) using $G_{\overline{\rho}}$. It requires an algorithm able to compute a compatible order of a flat Robinson space on Line 4, otherwise it can only compute the structure of the PQ-tree, without the ordering of children of Q-nodes. We gave such an algorithm in our paper [3, Proposition 6.16], that runs in time $O(|X|^2)$. The value of ρ can be efficiently computed by Lemma 4.4, as fast as the computation of a minimum spanning tree of a complete graph. Determining the maximal mmodules on Line 3 will be possible using an algorithm presented in Section 6.

On line 12, the value of *i* in Proposition 4.10 is computed as the minimal value i^* such that (*) $d(\beta_{i^*}, \beta_{\ell}) \leq \rho$ and $d(\beta_{i^*-1}, \beta_{i^*}) \geq \rho$; we now prove that this computation is correct. We use the notations of Proposition 4.10; the root of $\mathcal{T}_{PQ}(X)$ is $Q(\beta_1, \ldots, \beta_{i-1}, \beta, \beta_i, \ldots, \beta_{\ell})$ and $d(\beta, \beta_j) = \rho$ for each $j \in \{1, \ldots, l\}$. First observe that $d(\beta_i, \beta_\ell) \leq d(\beta, \beta_\ell) = \rho$ and $d(\beta_{i-1}, \beta_i) \geq d(\beta, \beta_i) = \rho$, ALGORITHM 1. Computes the PQ-tree of (X, d) using the ρ -mmodules.

deltaPqTree(S)

Input: a Robinson space (X, d) (implicit), a set $S \subseteq X$. **Output:** the PQ-tree $\mathcal{T}_{PQ}(S)$. 1: if (S, d) is connected then \triangleright Proposition 4.8 2: let M_1, \ldots, M_l be the maximum mmodules of (S, d)let $x_1 \in M_1, \ldots, x_\ell \in M_\ell$ 3: let $x_{\sigma(1)} < \ldots < x_{\sigma(\ell)}$ be a compatible order of the flat Robinson space $\{x_1, \ldots, x_\ell\}$ 4: return $Q(\text{deltaPqTree}(M_{\sigma(1)}), \dots \text{deltaPqTree}(M_{\sigma(\ell)}))$ 5: \triangleright Lemma 4.4 6: Compute ρ for (S, d)7: let S_0, S_1, \ldots, S_k be the connected components of the graph $G_{\overline{\rho}}$ on vertex set S 8: let $\mathcal{T}_0, \ldots, \mathcal{T}_k$ = deltaPqTree $(S_0), \ldots$, deltaPqTree (S_k) \triangleright Proposition 4.10 if there is $j \in \{0, \ldots, k\}$ with diam $(S_j) > \rho$ then 9: $S_i \leftrightarrow S_0, \mathcal{T}_0 \leftrightarrow \mathcal{T}_i$ \triangleright ensures S_0 is the large ρ -mmodule 10: let $Q(\beta_1, \ldots, \beta_\ell) := \mathcal{T}_0$, or $P(\beta_1, \beta_\ell) := \mathcal{T}_0$ and $\ell = 2$ 11: let $i \in \{2, \ldots, \ell\}$ be minimal such that $d(\beta_i, \beta_\ell) \leq \rho$ and $d(\beta_{i-1}, \beta_i) \geq \rho$, 12:let $\beta := \mathcal{T}_1$ if $k = 1, \beta := P(\mathcal{T}_1, \dots, \mathcal{T}_k)$ if $k \ge 2$ 13:return $Q(\beta_1, \ldots, \beta_{i-1}, \beta, \beta_i, \ldots, \beta_\ell)$ \triangleright conical node with apex child β 14:15: return $P(\mathcal{T}_0,\ldots,\mathcal{T}_k)$ \triangleright Proposition 4.9

hence (*) holds for *i*. Now suppose for the sake of contradiction that there exists $i' \in \{1, \ldots, i-1\}$ for which (*) holds. Then for all $j \in \{i', \ldots, i-1\}$ and $j' \in \{i, \ldots, \ell\}$,

$$\rho = d(\beta, \beta_i) \le d(\beta_{i-1}, \beta_i) \le d(\beta_i, \beta_{j'}) \le d(\beta_{i'}, \beta_{\ell}) \le \rho,$$

and for all $j \in \{i', ..., i-1\}$ and $j' \in \{1, ..., i'-1\}$

 $\rho \leq d(\beta_{i'-1}, \beta_{i'}) \leq d(\beta_{j'}, \beta_j) \leq d(\beta_1, \beta_{i-1}) \leq d(\beta_1, \beta) = \rho,$

proving that all those quantities equal ρ . In particular, for all $x \in X(\beta_{i'}) \cup \ldots \cup X(\beta_{i-1})$ and $y \in X(\beta_1) \cup \ldots \cup X(\beta_{i'-1}) \cup X(\beta_i) \cup \ldots \cup X(\beta_{\ell}), d(x,y) = \rho$, contradicting the fact that S_0 is connected in $G_{\overline{\rho}}$.

5. Translation between PQ-trees and mmodule trees

In this section, we show how to build the mmodule tree of a Robinson space (X, d) from its PQ-tree, and *vice-versa*, how to build the PQ-tree from the mmodule tree. This cryptomorphism is illustrated by Figure 6.

5.1. The translation between \mathcal{T}_{PQ} and \mathcal{T}_M . The cryptomorphism between the two trees relies on the following remark: since Propositions 4.8 to 4.10 cover all possible cases, we can "invert" their statements depending on the root of \mathcal{T}_{PQ} and of whether (X, d) is connected or not. More precisely we have the following result:

Proposition 5.1. Let (X, d) be a Robinson space with PQ-tree \mathcal{T}_{PQ} , then the set of maximum mmodules \mathcal{M}_{max} is described as follows:

- (1) If $\mathcal{T}_{PQ} = P(\beta_1, \dots, \beta_k)$, then (X, d) is non-connected and $X(\beta_1), \dots, X(\beta_k)$ are the ρ -mmodules, all of diameter at most ρ , and $\mathcal{M}_{max} = \{X \setminus X(\beta_1), \dots, X \setminus X(\beta_k)\}.$
- (2) If $\mathcal{T}_{PQ} = Q(\beta_1, \ldots, \beta_k)$ and (X, d) is connected, then $\mathcal{M}_{\max} = \{X(\beta_1), \ldots, X(\beta_k)\}.$
- (3) If $\mathcal{T}_{PQ} = Q(\beta_1, \dots, \beta_k)$ and (X, d) is non-connected, then there is a large ρ -mmodule S_0 , and there exists $i \in \{2, \dots, k-1\}$ such that $S_0 = X \setminus X(\beta_i)$. The root of \mathcal{T}_{PQ} is conical with apex child β_i . Moreover,



FIGURE 6. The translations between mmodule trees and PQ-trees, as provided by Algorithms 2 and 3; here ϕ denotes the bijection from mmodule trees to PQ-trees. In cases (b), (c), none of the nodes is special or conical. In case (d), $\phi(b_k)$ can also be $P(\gamma_1, \gamma_2)$ (then $\ell = 2$), and if k = 2 the apex node is simply $\phi(\beta_1)$. In case (f): the large node is a \cap -node when l = 2, and it may happen that the apex node is reduced to a leaf (in which case γ_i is standard).

 $\begin{array}{l} (3.1) \ if \ c_{\rho} = 2, \ then \ \mathcal{M}_{\max} = \{X(\beta_i), X \setminus X(\beta_i)\}, \\ (3.2) \ if \ c_{\rho} \ge 3, \ then \ \beta_i = P(\gamma_1, \dots, \gamma_{c_{\rho}-1}) \ is \ a \ split \ node \ and \ \mathcal{M}_{\max} = \{X \setminus X(\gamma_i) : i \in \{1, \dots, c_{\rho}-1\}\} \cup \{X(\beta_i)\}. \end{array}$

Proof. For (1), as the root of \mathcal{T}_{PQ} is a P-node, Proposition 4.9 is the sole proposition allowing this conclusion, hence there is $\rho > 0$ with $c_{\rho} \geq 3$. Then by Lemma 4.3, $\mathcal{M}_{\text{max}} = \{X \setminus X(\beta_1), \ldots, X \setminus X(\beta_k)\}$.

Otherwise the root of \mathcal{T}_{PQ} is a Q-node. For (2), the only proposition where $G_{\overline{\delta}}$ is always connected is Proposition 4.8, from which we get that case.

For (3), Proposition 4.10 is the only applicable proposition, hence there is $\rho > 0$ such that $G_{\overline{\rho}}$ is not connected, and has a large ρ -mmodule S_0 . It remains to prove what is \mathcal{M}_{max} in that case, but it actually easily follows from Lemma 4.3.

5.2. From \mathcal{T}_{PQ} to \mathcal{T}_M . This leads to Algorithm 2 to compute the mmodule tree from the PQ-tree of a Robinson space. Given the PQ-tree \mathcal{T}_{PQ} of a Robinson space (X, d), we denote by $\rho(\mathcal{T}_{PQ})$ the unique value δ for which $G_{\overline{\delta}}$ is not connected, if it exists, otherwise $\rho(\mathcal{T}_{PQ})$ is undefined. We can compute $\rho = \rho(\mathcal{T}_{PQ})$ efficiently in the following way:

- if the root of \mathcal{T}_{PQ} is a P-node, then $\rho := d(\alpha, \beta)$, where α and β are two distinct children of the root. This follows from Proposition 5.1 (1),
- otherwise, the root of \mathcal{T}_{PQ} is a Q-node with children β_1, \ldots, β_k , with $k \geq 3$. Then there is at most one $i \in \{2, \ldots, k-1\}$ such that for all $j \in \{1, \ldots, k\} \setminus \{i\}$, and $\rho = d(\beta_i, \beta_j)$. This follows from Proposition 5.1 (3). Checking all possibilities for i allows to find ρ (and i) in time O(k), as it is sufficient to check that $d(\beta_1, \beta_i)$, $d(\beta_{i-1}, \beta_i)$, $d(\beta_i, \beta_{i+1})$ and $d(\beta_i, \beta_k)$ are all equal (then that value is ρ). Then the root of \mathcal{T}_{PQ} is a conical node with apex child β_i . If no such i exists, then the situation is that of Proposition 5.1 (2), the root of \mathcal{T}_{PQ} is not conical and ρ is undefined.

ALGORITHM 2. Computes the mmodule tree of a Robinson space (X, d) from its PQ-tree.

mmodTree($\mathcal{T}_{PQ}(S)$)

Input: a Robinson space (X, d) (implicit), a PQ-tree $\mathcal{T}_{PQ}(S)$ for a subspace S of (X, d). **Output:** the module tree $\mathcal{T}_M(S)$ of S. 1: match $\mathcal{T}_{PQ}(S)$ with 2: case Leaf x: return Leaf x3: 4: case $P(\beta_1, ..., \beta_k)$: **return** \cap (mmodTree(β_1),..., mmodTree(β_k)) \triangleright Proposition 5.1(1) 5:case $Q(\beta_1,\ldots,\beta_k)$: 6: if $\mathcal{T}_{PQ}(S)$ is not conical then 7: **return** \cup (mmodTree(β_1),..., mmodTree(β_k)) \triangleright Proposition 5.1(2) 8: 9: let $\rho := \rho(\mathcal{T}_{PQ}(S))$ and β_i the apex child of $\mathcal{T}_{PQ}(S)$ let $\mathcal{T}_0 := \cup (\mathsf{mmodTree}(\beta_1), \dots, \mathsf{mmodTree}(\beta_{i-1}), \mathsf{mmodTree}(\beta_{i+1}), \dots, \mathsf{mmodTree}(\beta_k))$ 10: if $\rho(\beta_i)$ is undefined or $\rho(\beta_i) < \rho$ then 11: \triangleright Proposition 5.1(3.1) **return** \cap (\mathcal{T}_0 , mmodTree(β_i)) special 12:13:let $\gamma_1, \ldots, \gamma_\ell$ be the children of β_i **return** \cap (\mathcal{T}_0 , mmodTree(γ_1), ..., mmodTree(γ_ℓ)) special \triangleright Proposition 5.1(3.2) 14:

Theorem 5.2. Let (X,d) be a Robinson space and \mathcal{T}_{PQ} be its PQ-tree. Then $\mathsf{mmodTree}(\mathcal{T}_{PQ})$ correctly computes the mmodule tree of (X,d) in time O(|X|).

Proof. The correctness mostly follows by induction from Proposition 5.1, we only explain the differences between the conditions in Proposition 5.1 and Algorithm 2.

On line 7, testing whether $\mathcal{T}_{PQ}(S)$ is conical is equivalent to checking whether there is apex child, in which case (S, d) is not connected and Proposition 5.1(3) applies. Otherwise (S, d) is connected and Proposition 5.1(2) applies.

Consider the case when the execution runs through line 9. The conical child β_i is $X \setminus S_0$. We must determine c_{ρ} to decide between Proposition 5.1(3.1) and (3.2). As $X(\beta_i)$ is the union of the ρ -mmodules other than S_0 we may use $\rho(\beta_i)$. Indeed, $c_{\rho} > 2$ if and only if $G_{\overline{\rho}}(X(\beta_i))$ is not connected. Hence if $c_{\rho} = 2$, then $S_0, X(\beta_i)$ are the ρ -mmodules of S and the return at line 12 is correct. Otherwise, by Proposition 4.9, the ρ -mmodules other than S_0 are the sets induced by the children of β_i , proving that the return at line 14 is also correct.

The complexity follows from the previous remark that $\rho(\alpha)$ can be computed in time O(k) where k is the number of children of the node α . Then we use the fact he the sum of arities of the nodes in \mathcal{T}_{PQ} is no more than 2|X| because each inner node has arity at least 2 and the number of leaves is |X|, thus the total cost for computing all the $\rho(\alpha)$ is O(|X|). The rest of the algorithm can be computed in time proportional to the size of the PQ-tree, that is in $\Theta(|X|)$.

5.3. From \mathcal{T}_M to \mathcal{T}_{PQ} . Propositions 4.8 to 4.10 also allow to derive the PQ-tree of a Robinson space from its mmodule tree, except for the ordering of children of Q-nodes. This is done in Algorithm 3. We analyse this algorithm.

ALGORITHM 3. Computes the PQ-tree of a Robinson space (X, d) from its mmodule tree.

$pqTree(\mathcal{T}_M(S))$

Input: a Robinson space (X, d) (implicit), an module tree $\mathcal{T}_M(S)$ for a subspace S of (X, d). **Output:** the PQ-tree $\mathcal{T}_{PQ}(S)$ of S.

1: match $\mathcal{T}_M(S)$ with 2: case Leaf x: return Leaf x3: 4: case $\cup (\beta_1, \ldots, \beta_k)$: let $\beta_{\sigma(1)} < \ldots < \beta_{\sigma(k)}$ be a compatible order of the flat Robinson space X/\mathcal{M}_{\max} 5:return $Q(pqTree(\beta_{\sigma(1)}), \dots, pqTree(\beta_{\sigma(k)}))$ \triangleright Proposition 4.8 6: 7: case $\cap (\beta_1, \ldots, \beta_k)$: let $\rho = d(\beta_1, \beta_k)$ 8: if $\mathcal{T}_M(S)$ is special with large child β_i then 9: 10: $\beta_i \leftrightarrow \beta_k$ \triangleright ensures i = klet $Q(\gamma_1, \ldots, \gamma_\ell) := pqTree(\beta_k)$ \triangleright Proposition 4.10 11: let $j := findBipartition(\rho, \gamma_1, \ldots, \gamma_\ell)$ 12:let $\beta := pqTree(\beta_1)$ if $k = 2, \beta := P(pqTree(\beta_1), \dots, pqTree(\beta_{k-1}))$ if $k \ge 3$ 13:return $Q(\gamma_1, \ldots, \gamma_j, \beta, \gamma_{j+1}, \ldots, \gamma_\ell)$ conical with apex β \triangleright Proposition 4.10 14:**return** $P(pqTree(\beta_1), \ldots, pqTree(\beta_k))$ \triangleright Proposition 4.9 15:

findBipartition($\rho, \gamma_1, \ldots, \gamma_k$)

Input: a non-connected Robinson space (X, d) (implicit) with a large ρ -module S_0 of G_{δ^*} and bipartition (S_{\star}, S^{\star}) , and the children $\gamma_1, \ldots, \gamma_{\ell}$ of the Q-node root of $\mathcal{T}_{PQ}(S_0)$ (by Proposition 4.10).

Output: The unique $j \in \{1, \ldots, l-1\}$ such that for $S_{\star} := X(\gamma_1) \cup \ldots \cup X(\gamma_i)$ and $S^{\star} :=$ $X(\gamma_{i+1}) \cup \ldots \cup X(\gamma_{\ell}).$ 1: let $i_0 := \max\{i \in \{1, \dots, \ell - 1\} : d(\gamma_i, \gamma_\ell) > \rho\}$ 2: return $\min\{i \in \{i_0, \dots, \ell - 1\} : d(\gamma_i, \gamma_{i+1}) \ge \rho\}$ \triangleright exists as diam $(S_0) > \rho$

Lemma 5.3. Under the hypothesis of Proposition 4.10, findBipartition $(\rho, \gamma_1, \ldots, \gamma_k)$ from Algorithm 3 correctly computes the bipartition (S_{\star}, S^{\star}) of S_0 in time O(l).

Proof. We know that j exists by Proposition 4.10. Let j' be the value returned by findBipartition from Algorithm 3, and let $S := X \setminus S_0$. Denote $S_i = X(\gamma_i)$ for any $i \in \{1, \ldots, \ell\}$. Let < be a compatible order with $S_1 < \ldots < S_j < S < S_{j+1} < \ldots < S_\ell$. As $d(S_{i_0}, S_\ell) > \rho = d(S, S_\ell) \ge 0$ $d(S_{j+1}, S_{\ell})$, we have that $i_0 < j+1$. This implies that j' is well defined as $d(S_j, S_{j+1}) \ge d(S_j, S) = \rho$, and $j' \leq j$.

By way of contradiction suppose that j' < j. We prove that $T := S_{j'+1} \cup \ldots \cup S_j \cup S$ is a union of ρ mmodules, a contradiction to the fact that S_0 is a maximal mmodule. Notice that $S_{j'+1} < \ldots < S_j <$ S, hence it is sufficient to show that $d(S_1, S_{j'+1}) = d(S_{j'+1}, S_l) = \rho$ and $d(S_1, S) = d(S, S_{j+1}) = \rho$. The latter inequalities follow from the definition of S, we prove the former. By definition of j', $d(S_{j'}, S_{j'+1}) \ge \rho$, but $S_1 < S_{j'} < S_{j'+1} \le S_j < S$ implies that $d(S_{j'}, S_{j'+1}) \le d(S_1, S) = \rho$, hence $d(S_{j'}, S_{j'+1}) = \rho$. By the maximality of i_0 and since $j' \ge i_0$, $d(S_{j'+1}, S_\ell) \le \rho$. Then because $S_{j'+1} \leq S_j < S < S_l$, we get $d(S_{j'+1}, S_l) \geq d(S, S_l) = \rho$, hence the last equality follows. **Theorem 5.4.** Let (X, d) be a Robinson space and \mathcal{T}_M be its mmodule tree. Then $pqTree(\mathcal{T}_M)$ correctly computes the PQ-tree \mathcal{T}_{PQ} of (X, d) in time O(|X|) without counting the cost of ordering the children of each Q-node.

Proof. If $\mathcal{T}_M = \bigcup(\beta_1, \ldots, \beta_k)$, then by Proposition 2.15, \mathcal{M}_{\max} is a partition with maximal mmodules $X(\beta_1), \ldots, X(\beta_k)$. By Lemma 4.3, $G_{\overline{\delta}}$ is connected for any $\delta > 0$. By Proposition 4.8, $\mathcal{T}_{PQ} = Q(T_1, \ldots, T_k)$ where T_1, \ldots, T_k are the PQ-tree of $X(\beta_1), \ldots, X(\beta_k)$ given in a compatible order. This proves that the return at line 6 is correct.

If $\mathcal{T}_M = \cap(\beta_1, \ldots, \beta_k)$, then by Proposition 2.15, \mathcal{M}_{\max} is a copartition, the ρ -mmodules are $X(\beta_1), \ldots, X(\beta_k)$ and their complements are the maximal mmodules of (X, d). By Lemma 4.3, $d(X(\beta_i), X(\beta_j)) = \rho$. If (X, d) does not contain large ρ -mmodules, then by Proposition 4.9, the returns at line 15 is correct.

If some ρ -mmodule has diameter greater than ρ , say diam $(X(\beta_k)) > \rho$, then by Proposition 4.10, the root of the PQ-tree of $S_0 := X(\beta_k)$ is a Q-node. By Lemma 4.6, S_0 has a bipartition into two blocks S_{\star}, S^{\star} , which must match with consecutive children of the root of $\mathcal{T}_{PQ}(S_0)$. By Lemma 5.3, findBipartition correctly computes that bipartition, and then by Proposition 4.10, the return at line 14 is correct.

The diameter of the sets induced by nodes of the PQ-tree can be computed simultaneaously: for a P-node the diameter is the distance between any two children, while for a Q-node, the diameter is the distance between the two extremal children. To compute the diameter of a set induced by an mmodule tree, we first compute its PQ-tree (as the algorithm will compute it eventually, this does not add any cost), then compute its diameter in constant time.

Then the complexity of the algorithm, without counting the ordering at line 5 and the recursive calls, is proportional to the arity k of the root node of \mathcal{T}_M , and ℓ in case it returns at line 14. Notice that the last case happens when transforming a Q-node whose subset induces a connected Robinson subspace into a Q-node whose subset induces a non-connected Robinson subspace. Hence it happens at most once for any Q-node in the final PQ-tree $\mathcal{T}_{PQ}(X)$. Thus, counting the recursive calls (but still not line 5), the complexity of the algorithm is proportional to the sum of arities in \mathcal{T}_M and \mathcal{T}_{PQ} , which is O(|X|) as each inner node has arity at least 2.

Another consequence of these translations between PQ-tree and mmodule tree is that a nodeto-node correspondence for most of the nodes of those trees:

Proposition 5.5. Let (X, d) be a Robinson space, with PQ-tree \mathcal{T}_{PQ} and mmodule tree \mathcal{T}_M . For any node α in \mathcal{T}_M , either there exists a node α' in \mathcal{T}_{PQ} with $X(\alpha) = X(\alpha')$ or α is the large child of a special node. For any node β' in \mathcal{T}_{PQ} , either there exists a node β in \mathcal{T}_M with $X(\beta) = X(\beta')$, or β' is the split child of a conical node α' . Moreover, if α is a node of \mathcal{T}_M and α' a node of \mathcal{T}_{PQ} with $X(\alpha) = X(\alpha')$, then:

- (i) α is a non-special \cap -node if and only if α' is a P-node,
- (ii) α is a \cup -node if and only if α' is a non-conical Q-node,
- (iii) α is a special \cap -node if and only if α' is a conical Q-node.

5.4. **Mmodules trees of ultrametrics.** As an application of the results of this section, we show that for ultrametrics \mathcal{T}_M is isomorphic to \mathcal{T}_D and \mathcal{T}_{PQ} . We characterize the ultrametric spaces via their mmodule trees in the following way:

Proposition 5.6. If (X,d) is an ultrametric space, then the X-trees \mathcal{T}_D , \mathcal{T}_{PQ} , and \mathcal{T}_M are isomorphic. Furthermore, a dissimilarity space (X,d) is ultrametric if and only if its mmodule-tree \mathcal{T}_M satisfies the following conditions:

- (i) the internal nodes of \mathcal{T}_M are all \cap -nodes,
- (ii) for every node α of \mathcal{T}_M and child β of α , we have diam $(X(\beta)) < \text{diam}(X(\alpha))$.

Proof. Suppose first that (X, d) is an ultrametric space. Then, by Proposition 3.13, \mathcal{T}_{PQ} contains only P-nodes. By Proposition 5.1(1), all internal nodes of \mathcal{T}_M are non-special \cap -nodes with no large component and are in one-to-one correspondence to those of \mathcal{T}_{PQ} , proving (i) and (ii), and that \mathcal{T}_{PQ} and \mathcal{T}_M are isomorphic. By Proposition 3.14, they are also isomorphic to \mathcal{T}_D .

Conversely, suppose that \mathcal{T}_M satisfies (i) and (ii). Let $x, y, z \in X$ and α be the common least ancestor of x, y, z in \mathcal{T}_M . If x, y, z are in distinct children, then $d(x, y) = d(y, z) = d(x, z) = \rho(\alpha)$ by (i). Otherwise, two of them are in a common child, say x and y. Then $d(x, y) < \rho(\alpha)$ by (ii), and $d(x, z) = d(y, z) = \rho(\alpha)$ by (i). Thus (X, d) is an ultrametric.

6. Construction of the mmodule tree using partition refinement

In Section 5 we established a correspondence between the PQ-tree \mathcal{T}_{PQ} and the mmodule tree \mathcal{T}_M of a Robinson space (X, d), allowing to derive one such tree from another. In Section 4 we showed how to construct \mathcal{T}_{PQ} from the maximal mmodules \mathcal{M}_{max} of (X, d). In this section, we show how to build the mmodule tree \mathcal{T}_M recursively from top-to-bottom, using a partition refinement algorithm and the dendrogram $\mathcal{T}_{\hat{d}}$ of the ultrametric subdominant (X, \hat{d}) . This also allows to construct \mathcal{M}_{max} and thus to get full algorithmic translations between the trees \mathcal{T}_{PQ} and \mathcal{T}_M .

6.1. Stable partitions and partition refinement. A partition of a set X is a family of sets $\mathcal{P} = \{B_1, \ldots, B_m\}$ such that $B_i \cap B_j = \emptyset$ for any $i \neq j$ and $\bigcup_{i=1}^k B_i = X$. The sets B_1, \ldots, B_m are called the *classes* of \mathcal{P} .

Definition 6.1 (Stable partition). A partition $\mathcal{P} = \{B_1, \ldots, B_m\}$ of a dissimilarity space (X, d) is a *stable partition* if for any $i \in \{1, \ldots, m\}$, B_i is an mmodule.

A non-stable partition \mathcal{P} can be transformed into a stable partition by applying the classical operation of *partition refinement*, which proceeds as follows. Algorithm 8 (see the Appendix) maintains the current partition \mathcal{P} and for each class B of \mathcal{P} maintains the set Z(B) of all points outside B which still have to be processed to refine B. While \mathcal{P} contains a class B with nonempty Z(B), the algorithm pick any point z of Z(B) and partition B into maximal classes that are not distinguishable from z, *i.e.* for any such new class $B' \subseteq B$ and any $x, x' \in B'$ we have d(x,z) = d(x',z). Finally, the algorithm removes B from \mathcal{P} and insert each new class B' in \mathcal{P} and sets $Z(B') := (B \setminus B') \cup (Z(B) \setminus \{z\})$. Notice that each class B is partitioned into subclasses by comparing the distances of points of B to the point $z \notin B$ and such distance items never occur in later comparisons. Also, if the final stable partition has classes B'_1, \ldots, B'_t , then the distances between points in the same class B'_i are never compared to other distances. This algorithm is formalized in Algorithm 8, where one would call stablePartition(\mathcal{P}) to get a stable partition from \mathcal{P} . The complexity of refinePart in Algorithm 8 is $O(\sum_{i=1}^k |B_i| \times |B \setminus B_i|)$, the complexity of refining \mathcal{P} into \mathcal{P}' with Algorithm 8 is $O(\sum_{P \in \mathcal{P}'} |P| \times |X \setminus P|)$. The copoint partition \mathcal{C}_p of (X,d) can be constructed by applying Algorithm 8 to the partition $\{p\}$.

The effect of Algorithm 8 applied to a partition of a subset $S \subseteq X$ of a dissimilarity space (X, d) is described in Lemma 9.7, which asserts that stablePartition(\mathcal{P}) is the less refined refinement of \mathcal{P} into mmodules of (S, d).

We now present Algorithm 4, a variant of the stable partition algorithm, that uses S-trees to represent sets. This will allow us to use the dendrogram $\mathcal{T}_{\hat{d}}$ of the ultrametric subdominant to represent X, providing us with extra information that will be needed to obtain an efficient algorithm to build the mmodule tree.

Lemma 6.2. Let (X, d) be a dissimilarity space and let $\mathcal{T}(S)$ be an S-tree for some subset $S \subseteq X$. Let $q \in X \setminus S$ and $\mathcal{T}(S_1), \ldots, \mathcal{T}(S_n) := \mathsf{pivotTree}(q, \mathcal{T}(S))$. Then for all $i \in \{1, \ldots, n\}, \mathcal{T}(S_i)$ is either a subtree of $\mathcal{T}(S)$ or the join of some children of a node in $\mathcal{T}(S)$. ALGORITHM 4. A refinement algorithm where sets are represented by X-trees

stableTrees($\mathcal{T}(S_1), \ldots, \mathcal{T}(S_k)$)

- **Input:** a dissimilarity space (X, d) (implicit), $\mathcal{T}(S_i)$ an S_i -tree for $i \in \{1, \ldots, k\}$, where $\{S_1, \ldots, S_k\}$ is a partition of a subset $S \subseteq X$.
- **Output:** $\mathcal{T}(M_i)$ an M_i -tree for $i \in \{1, \dots, \ell\}$, where $\{M_1, \dots, M_\ell\}$ is a partition of S into mmodules of (S, d).
- 1: for $i \in \{1, ..., k\}$ do
- 2: yield from refineTree($\mathcal{T}(S_i), S_1 \cup \ldots \cup S_{i-1} \cup S_{i+1} \cup \ldots \cup S_k)$

 $refineTree(\mathcal{T}(S), Z(S))$

2: if $Z(S) = \emptyset$ then

- 3: return $\mathcal{T}(S)$
- 4: let $q \in Z(S)$
- 5: let $\mathcal{T}(S_1), \ldots, \mathcal{T}(S_k) := \mathsf{pivotTree}(q, \mathcal{T}(S))$
- 6: for $i \in \{1, ..., k\}$ do

7: **yield from** refineTree($\mathcal{T}(S_i), S_1 \cup \ldots \cup S_{i-1} \cup S_{i+1} \cup \ldots \cup S_k \cup Z(S) \setminus \{q\}$)

pivotTree $(q, \mathcal{T}(S))$

Input: a dissimilarity space (X, d) (implicit), an *S*-tree $\mathcal{T}(S)$ for some subset $S \subseteq X$, and $q \in X \setminus S$. Output: $\mathcal{T}(S_i)$ an S_i -tree for $i \in \{1, ..., n\}$, where $S_1, ..., S_n$ is a partition of *S*. 9: if d(q, x) is constant for $x \in \mathcal{T}(S)$ then 10: $\[return \mathcal{T}(S) \]$ 11: let Node $(\beta_1, ..., \beta_k) := \mathcal{T}(S)$ 12: let $I := \{i \in \{1, ..., k\} : d(q, x) \text{ is constant for } x \in X(\beta_i)\}$ and $J := \{1, ..., k\} \setminus I$ 13: for $j \in J$ do 14: $\[yield from pivotTree}(q, \beta_j) \]$ 15: let $\{d_1, ..., d_\ell\} := \{d(q, \beta_i) : i \in I\}$ 16: for $j \in \{1, ..., \ell\}$ do 17: $\[yield join(\{\beta_i : i \in I, d(q, \beta_i) = d_j\}) \]$ join $(\{\alpha_1, ..., \alpha_k\})$ 20: return $\left\{ \begin{array}{c} \alpha_1 & \text{if } k = 1, \\ \text{Node}(\alpha_1, ..., \alpha_k) & \text{otherwise.} \end{array} \right.$

Proof. We proceed by induction on the size of $\mathcal{T}(S)$. If d(q, x) is constant for $x \in S$, then n = 1 and $\mathcal{T}(S_1) = \mathcal{T}(S)$ (line 9). Let $i \in \{1, \ldots, n\}$. If $\mathcal{T}(S_i)$ is yielded at line 14, then the result holds by induction. Otherwise, it is yielded at line 17, hence $\mathcal{T}(S_i)$ is the join of some children of the root.

Lemma 6.3. Let (X, d) be a dissimilarity space and let $\mathcal{T}(S)$ be an S-tree for some subset $S \subseteq X$. Let $q \in X \setminus S$ and $\mathcal{T}(S_1), \ldots, \mathcal{T}(S_n) := \mathsf{pivotTree}(q, \mathcal{T}(S))$. Then for all $i \in \{1, \ldots, n\}$, d(q, x) is constant for $x \in \mathcal{T}(S_i)$.

Proof. This easily follows by induction on the size of $\mathcal{T}(S)$.

The fundamental property of the stable partition algorithm is that it outputs the maximal mmodules included in some parts of the initial partition. This property will only be preserved when working with S-trees whose structure respects the mmodules of the dissimilarity space.

Definition 6.4. Let (X, d) be a dissimilarity space and $S \subseteq X$. An *S*-tree \mathcal{T} is *coherent* if for each mmodule M of X with $M \subseteq S$, for each child β of the M-pertinent node in \mathcal{T} , either $X(\beta) \subset M$ or $X(\beta) \cap M = \emptyset$.

Notice that any subtree of a coherent tree is itself coherent.

Lemma 6.5. Let (X, d) be a dissimilarity space and let $\mathcal{T}(S)$ be a coherent S-tree for some $S \subseteq X$. Let $q \in X \setminus S$ and $\mathcal{T}(S_1), \ldots, \mathcal{T}(S_n) := \mathsf{pivotTree}(q, \mathcal{T}(S))$. Then $\mathcal{T}(S_1), \ldots, \mathcal{T}(S_n)$ are coherent. Moreover, let $M \subsetneq S$ be an amodule of S, then there is $i \in \{1, \ldots, n\}$ such that $M \subseteq S_i$.

Proof. Let M be a proper mmodule of S. By induction on the size of $\mathcal{T}(S)$, first we prove the claim that there exist $i \in \{1, \ldots, n\}$ and a node α of $\mathcal{T}(S_i)$ such that $M = X(\alpha)$ or $M = X(\beta_1) \cup \ldots X(\beta_k)$ for some children β_1, \ldots, β_k of α . Then we obtain the assertion of the lemma by applying this claim to all proper mmodules of S.

If d(q, x) is constant for $x \in S$, then n = 1, $\mathcal{T}(S_1) = \mathcal{T}(S)$ and the claim follows from the coherence of $\mathcal{T}(S)$. If the root of $\mathcal{T}(S)$ is not *M*-pertinent, then as $\mathcal{T}(S)$ is coherent, $M \subseteq X(\beta_i)$ for some child β_i of the root. If $i \in I$, β_i is in the join of some $\mathcal{T}(S_j)$ yielded at line 17 and the claim holds as β_i is coherent, else the claim holds by induction, from line 14 because β_i is coherent.

Otherwise the root is *M*-pertinent. Since *M* is an mmodule and $\mathcal{T}(S)$ is coherent, there is a subset $I' \subseteq I$ such that $M = \bigcup_{i \in I'} X(\beta_i)$, and there is $j \in \{1, \ldots, \ell\}$ such that $d_j = d(q, M)$. Then *M* is a subset of leaves of the join yielded on line 17 at iteration *j*, establishing the claim. \Box

The next proposition establishes that stableTrees is semantically equivalent to stablePartition.

Proposition 6.6. Let (X,d) be a dissimilarity space and $\mathcal{T}(S_1), \ldots, \mathcal{T}(S_k)$ be coherent trees, where S_1, \ldots, S_k is a partition of X. Let $\mathcal{T}(R_1), \ldots, \mathcal{T}(R_\ell) := \text{stableTrees}(\mathcal{T}(S_1), \ldots, \mathcal{T}(S_k))$. Then R_1, \ldots, R_ℓ are the maximal by inclusion mmodules of X contained in S_1, \ldots, S_k .

Proof. By Lemma 6.5, for each such maximal mmodule M, there is $i \in \{1, \ldots, \ell\}$ such that $M \subseteq R_i$. It remains to prove that, for $i \in \{1, \ldots, \ell\}$, R_i is an mmodule.

We check the following invariant: for each call refineTree(T(S), Z(S)), for each $u \notin S \cup Z(S)$, d(x, u) is constant for $x \in S$. This is trivial in line 2. Then consider a call refineTree(T(S), Z(S))for which the invariant holds, and let us prove it for the recursive calls happening at line 7. For iteration *i*, let $u \in X \setminus (Z(S_i) \cup S_i) = \{q\} \cup (X \setminus Z(S) \setminus S)$. If $u \in X \setminus Z(S) \setminus S$, then d(x, u) is constant for $x \in S$ hence for $x \in S_i$. Otherwise for u = q, S_i is a set yielded by pivotTree $(q, \mathcal{T}(S))$, and the invariant follows by Lemma 6.3.

Consequently, for any $i \in \{1, \ldots, \ell\}$, $\mathcal{T}(R_i)$ is returned at line 3, for some call refine $\mathsf{Tree}(\mathcal{T}(R_i), \emptyset)$. Thus by the invariant, $\mathcal{T}(R_i)$ is an mmodule.

The complexity of Algorithms 4 and 8 are asymptotically equivalent:

Lemma 6.7. Let (X,d) be a dissimilarity space and $\mathcal{T}(S_1), \ldots, \mathcal{T}(S_k)$ be coherent trees, where S_1, \ldots, S_k is a partition of X. Then $\mathcal{T}(R_1), \ldots, \mathcal{T}(R_\ell) := \text{stableTrees}(\mathcal{T}(S_1), \ldots, \mathcal{T}(S_k))$ takes $O(\sum_{i=1}^{\ell} |R_i| |X \setminus R_i|)$ time.

Proof. Notice that refineTree($\mathcal{T}_{\hat{d}}(S), Z(S)$) is called at most $|X \setminus S|$ times, because at each call, some element q is chosen and removed from Z(S). For a given $q \in X \setminus S$, we must evaluate whether d(q, x) is constant for $x \in S'$. In time O(|S|), we can decide that property for each node in $\mathcal{T}_{\hat{d}}(S)$. We charge a cost of O(1) on each pair (q, x) with $x \in S$. This allows to solve lines 9 and 12 in all calls to pivotTree $(q, \mathcal{T}_{\hat{d}}(S))$ for all S with $q \notin S$ in total time $O(|X \setminus R_i|)$, where $q \in R_i$. Summing over all $q \in X$, we get $O(\sum_{i=1}^{n} |R_i||X \setminus R_i|)$.

It remains to evaluate the cost of line 15. Using a binary search tree, associating to each distance the children at that distance, this has cost $O(|I| \log \ell)$, which we can amortized by charging a cost of log ℓ to an element of each child β_i , for $i \in I$. Notice that this element is, from this step, split from each of the other $\ell - 1$ parts, hence from at least $\log \ell$ elements. This implies that the total charge accumulated by an element during the main call to stableTrees is less than the number of trees returned. Thus the total cost of line 15 is at most $O(\sum_{i=1}^{n} |R_i| |X \setminus R_i|)$.

6.2. ρ -Components and the maximal mmodules. In this subsection, we study the relationships between the maximal mmodules and the ρ -components. They will lead us to an efficient algorithm to find the maximal mmodules of a Robinson dissimilarity and to build its mmodule tree. First, we define the ρ -components of a dissimilarity space (recall that ρ is the minimum value for which the graph $G_{\leq \rho}$ is connected):

Definition 6.8 (ρ -components). The ρ -components of a dissimilarity space (X, d) are the connected components of the graph $G_{<\rho}$.

Lemma 6.9. Let (X, d) be a connected Robinson space with $\mathcal{T}_M(X) = \cup(\beta_1, \ldots, \beta_k)$. Let C be a ρ -component of (X, d). Then

- (i) either there exists $I \subseteq \{1, \ldots, k\}$ such that $C = \bigcup_{i \in I} X(\beta_i)$,
- (ii) or there exists $i \in \{1, \ldots, k\}$ such that $\operatorname{diam}(X(\beta_i)) = \rho, \ \beta_i = \cap(\gamma_1, \ldots, \gamma_\ell)$, and there is $j \in \{1, \ldots, \ell\}$ such that $C = X(\gamma_i)$.

Proof. Suppose that (i) does not happen, i.e., there is some $i \in \{1, \ldots, k\}$ such that $C \cap X(\beta_i) \neq \emptyset$ and $X(\beta_i) \setminus C \neq \emptyset$. By Lemma 3.12 and Proposition 5.5, diam $(X(\beta_i)) \leq \min\{d(\beta_i, \beta_j) : j \in \{1, \ldots, k\} \setminus \{i\}\} \leq \rho$, and thus for all $x \in C \cap X(\beta_i)$ and $y \in X(\beta_i) \setminus C$, we have $d(x, y) = \rho$. This implies that the Robinson space $(X(\beta_i), d)$ is non-connected, with $\rho(X(\beta_i)) = \rho = \operatorname{diam}(X(\beta_i))$, hence $\beta_i = \cap(\gamma_1, \ldots, \gamma_\ell)$ is non-special. Then for all $x \in X(\beta_i)$ and $z \in X \setminus X(\beta_i)$, we have $d(x, z) \geq \rho$. Thus each $X(\gamma_i)$ is a ρ -component, establishing (ii).

In case (i), the ρ -component C is said to be *giant*, while in case (ii), it is said to be *dwarf*. Making that distinction, the next theorem gives a way to find most of maximal mmodules of a connected Robinson space using the stable partition algorithm.

Proposition 6.10. Let (X, d) be a connected Robinson space with $\mathcal{T}_M = \cup(\beta_1, \ldots, \beta_k)$. Let $i \in \{1, \ldots, k\}$ and Y be a ρ -component intersecting $X(\beta_i)$. Let \mathcal{P} be the stable partition obtained by calling stablePartition($\{Y, X \setminus Y\}$).

- (1) If Y is a giant ρ -component, then $\mathcal{P} = \mathcal{M}_{\max}$.
- (2) If Y is a dwarf ρ -component with $Y = X(\gamma)$ for some child γ of β_i , then $\mathcal{P} = \mathcal{M}_{\max} \setminus \{X(\beta_i)\} \cup \{Y, X(\beta_i) \setminus Y\}.$

Proof. By Proposition 2.15, the maximal mmodules \mathcal{M}_{max} of (X, d) are $\{X(\beta_1), \ldots, X(\beta_k)\}$.

In case (1), by Lemma 6.9, $Y = \bigcup_{i \in I} X(\beta_i)$ for some $I \subset \{1, \ldots, k\}$, hence Y and $X \setminus Y$ are unions of maximal mmodules. Therefore the maximal mmodules contained in Y and $X \setminus Y$ are exactly the maximal mmodules of X, thus by Lemma 9.7, $\mathcal{P} = \mathcal{M}_{\text{max}}$ holds.

In case (2), for each β_j with $j \in \{1, \ldots, k\} \setminus \{i\}, X(\beta_j) \subseteq X \setminus Y$ holds, hence $X(\beta_j) \in \mathcal{P}$. Moreover, since $(X(\beta_i), d)$ is not connected, the children of β_i are its ρ -mmodules, thus Y and $X(\beta_i) \setminus Y$ are mmodules in $X(\beta_i)$. By Proposition 2.13(ii), Y and $X(\beta_i) \setminus Y$ are also mmodules in (X, d). Hence by Lemma 9.7, $\mathcal{P} := \mathcal{M}_{\max} \setminus \{X(\beta_i)\} \cup \{Y, X(\beta_j) \setminus Y\}$.

In the case of dwarf ρ -components, we still need to retrieve the maximal mmodule $X(\beta_i)$:

Lemma 6.11. Let (X,d) be a connected Robinson space and $\{X_1, \ldots, X_k\}$:= stablePartition($\{Y, X \setminus Y\}$). Then a ρ -component Y of (X,d) is dwarf if and only if there are distinct and uniquely defined indices $i, j \in \{1, \ldots, k\}$ such that $Y = X_i$, $d(Y, X_j) = \rho$ and for all $h \in \{1, \ldots, k\} \setminus \{j\}$, we have $d(Y, X_h) = d(X_j, X_h)$. In that case, $Y \cup X_j$ is a maximal mmodule of (X, d).

Proof. Let Y be a dwarf ρ -component. From Proposition 6.10, and using the same notations, $Y = X(\gamma)$ and $X_j = X(\gamma) \setminus Y$ for some j. Then j has the required properties, since $X(\gamma)$ is an mmodule. Conversely, for any index j with those properties, $Y \cup X_j$ is an mmodule. As $X(\gamma)$ is the maximum mmodule containing Y, for any $j' \neq j$, $Y \cup X_{j'}$ is not an mmodule, proving that j is unique. If Y is a giant ρ -component, then either Y is the union of at least 2 maximal mmodules, in which case i does not exist, or Y is a maximal mmodule, and if j exists, then $Y \cup X_j$ is an mmodule, a contradiction.

Now, we consider the case of non-connected spaces.

Lemma 6.12. Let (X, d) be a non-connected Robinson space. Then any ρ -mmodule S of diameter at most ρ is also a ρ -component.

Proof. Clearly S is the union of ρ -components, because for any $x \in S$ and $y \in X \setminus S$, $d(x, y) = \rho$ by definition of ρ -mmodules. Suppose there is a ρ -component C with $C \subsetneq S$. By definition of ρ -components, for each $x \in C$, $y \in S \setminus C$, we have $d(x, y) \ge \rho$. Since diam $(S) \le \rho$, we get $d(x, y) = \rho$, whence C is a ρ -component, a contradiction.

Proposition 6.13. Let (X,d) be a non-connected Robinson space and let C_1, \ldots, C_k be its ρ components. Let $I := \{i \in \{1, \ldots, k\} : C_i \text{ is not a } \rho\text{-mmodule}\}$. Then exactly one of the following
assertions holds:

- (1) |I| = 0; in this case, $\mathcal{M}_{\max} = \{\overline{C_1}, \ldots, \overline{C_k}\}$ and there are no large ρ -mmodules.
- (2) $|I| \ge 2$; in this case, $S_0 := \bigcup_{i \in I} C_i$ is a large ρ -mmodule, and $\mathcal{M}_{\max} = \{\overline{C_j} : j \in \{1, \dots, k\} \setminus I\} \cup \{\overline{S_0}\}$. Moreover, the graph $H := (I, \{ii': \text{ there are } x \in C_i, y \in C_{i'} \text{ such that } d(x, y) > \rho\})$ is connected and bipartite, with bipartition $I = I_{\star} \cup I^{\star}$, and the maximal mmodules of S_0 are given by stablePartition($\{S_{\star}, S^{\star}\}$), where $S_{\star} := \bigcup_{i \in I_{\star}} C_i$ and $S^{\star} := \bigcup_{i \in I^{\star}} C_i$.

Proof. Since (X, d) is non-connected, by Lemma 4.2, each ρ -mmodule is an mmodule, and at most one ρ -mmodule S_0 has diameter greater than ρ . All the ρ -mmodules except S_0 are ρ -components by Lemma 6.12. If there is no such S_0 , then this immediately leads to case (1).

We may now assume that S_0 exists. Then by Lemma 4.6, there is a bipartition $S_0 = S_{\star} \cup S^{\star}$. By Lemma 4.6(iii), S_{\star} and S^{\star} are unions of ρ -components, and $S_0 = \bigcup_{i \in I} C_i$. By Lemma 4.3, $\mathcal{M}_{\max} = \{\overline{C_j} : j \in \{1, \dots, k\} \setminus I\} \cup \{\overline{S_0}\}$. Furthermore, the graph H is connected, because any connected component is an ρ -mmodule by definition and S_0 does not contain a proper ρ -mmodule. By Lemma 4.6(ii), $I_{\star} \cup I^{\star}$ with $I_{\star} := \{i \in I : C_i \subseteq S_{\star}\}$ and $I^{\star} := \{i \in I : C_i \subseteq S^{\star}\}$ is the (unique) bipartition of H.

Suppose that there is a non-trivial mmodule M of S_0 with $x \in M \cap S_{\star} \neq \emptyset$ and $y \in M \cap S^{\star} \neq \emptyset$. Let $z \in S_0 \setminus M$, say $z \in S_{\star} \setminus M$. Then $\rho \leq d(z, y) = d(z, x) \leq \rho$ by Lemma 4.6(ii) and (iii) and the fact that M is an mmodule. Also for $w \in X \setminus S_0$, we have $d(w, x) = d(w, y) = \rho$. Hence M is a ρ -mmodule of X, a contradiction. Thus, for any maximal mmodule M of S_0 , either $M \subseteq S_{\star}$ or $M \subseteq S^{\star}$, hence by Lemma 9.7, the maximum mmodules of S_0 are provided by stablePartition($\{S_{\star}, S^{\star}\}$)).

Propositions 6.10 and 6.13 can be used to compute the mmodule tree of a Robinson dissimilarity in optimal $O(|X|^2)$ time in a top-down way, that is root first then recursively on each child. The alternative way to compute the mmodule tree of an arbitrary dissimilarity space is to compute the copoints of a point and to sort them, leading to a root-to-leaf path. Then recurse on all subtrees attached to that path. This gives an optimal $O(|X|^2)$ -time algorithm [7]. Our Algorithm 5 is more complicated, nevertheless, we think that it shed complimentary light on the links between mmodule trees and the dendrogram of the ultrametric subdominant.

Proposition 6.14. Let (X, d) be a Robinson space, mmoduleTree(X) correctly computes the mmodule tree of X.

ALGORITHM 5. Computes the mmodule tree of (X, d)

$\mathsf{mmoduleTree}(S)$

Input: a Robinson space (X, d), an mmodule $S \subseteq X$. **Output:** The mmodule tree of S1: if |S| = 1 then 2: return Leaf x, where $\{x\} = S$ 3: let C_1, \ldots, C_k be the ρ -component of S \triangleright assume $|C_1| \leq |C_i|$ for any $i \in \{1, \ldots, k\}$ 4: let $J := \{i \in \{1, \dots, k\} : C_i \text{ is a } \rho \text{-mmodule}\} \text{ and } I := \{1, \dots, k\} \setminus I$ \triangleright Proposition 6.13(1) 5: if $I = \emptyset$ then **return** \cap (mmoduleTree(C_1),..., mmoduleTree(C_k)) 6: 7: if $J = \emptyset$ then let S_1, \ldots, S_ℓ := stablePartition({ $C_1, S \setminus C_1$ }) with $S_1 \subseteq C_1$ 8: for $i \in \{1, \ldots, \ell\}$ do 9: if for all $j \in \{2, \dots, \ell\} \setminus \{i\}, d(S_1, S_j) = d(S_i, S_j)$ then 10:let $\{M_1, ..., M_{\ell-2}\} = \{ \mathsf{mmoduleTree}(S_i) : j \in \{2, ..., \ell\} \setminus \{i\} \}$ 11: **return** \cup (mmoduleTree($S_1 \cup S_i$), $M_1, \ldots, M_{\ell-2}$) 12: \triangleright Proposition 6.10(2) **return** \cup (mmoduleTree $(S_1), \ldots,$ mmoduleTree (S_ℓ)) \triangleright Proposition 6.10(1) 13:14: let $\{\beta_1, \ldots, \beta_{k'}\}$:= {mmoduleTree (C_j) : $j \in J$ } 15: let $H = (I, \{ij: \text{ there is } x \in C_i, y \in C_j, \text{ with } d(x, y) > \rho\})$ 16: let $I = I_{\star} \cup I^{\star}$ be the unique bipartition of $H, S_{\star} := \bigcup_{i \in I} C_i$ and $S^{\star} := \bigcup_{i \in I^{\star}} C_i$ 17: let S_1, \ldots, S_ℓ := stablePartition({ S_\star, S^\star }) 18: **if** ℓ = 2 **then** \triangleright Proposition 6.13(2), with |I| = 2 and d(x, y) constant for $x \in S_*$, $y \in S^*$ 19: **return** \cap ($\beta_1, \ldots, \beta_{k'}, \cap$ (mmoduleTree(S_{\star}), mmoduleTree(S^{\star})) 20: **return** \cap ($\beta_1, \ldots, \beta_{k'}, \cup$ (mmoduleTree(S_1), ..., mmoduleTree(S_ℓ))) \triangleright Proposition 6.13(2)

Proof. Obviously the return at line 2 is correct. The space (S, d) is not connected precisely when there is no ρ -mmodule, that is when $J = \emptyset$. Thus, the return at line 6 is a direct consequence of Proposition 6.13(1) as J is non-empty.

If $J = \emptyset$, then (S, d) is connected and Proposition 6.10 applies. Deciding whether the ρ component C_1 is dwarf or giant is done in lines 9 to 12, following Lemma 6.11. Consequently,
the returns at line 12 and 13 are correct by Proposition 6.10.

Otherwise, $J \neq \emptyset$ implies that (S, d) is not connected and Proposition 6.13 applies. As $I \neq \emptyset$ we are in case (1) of Proposition 6.13. If $\ell = 2$, notice that we must have $\{S_1, S_2\} = \{S_{\star}, S^{\star}\}$: $S_0 = S_{\star} \cup S^{\star}$ has only two maximal mmodules and thus the root of its mmodule tree is a \cap -node. This justifies the return at line 19. If $\ell > 2$, we follow Proposition 6.13(2), proving that line 20 is also correct.

6.3. From the dendrogram $\mathcal{T}_{\hat{d}}$ to the mmodule tree \mathcal{T}_M . To make Algorithm 5 efficient, one need to efficiently compute the ρ -components at each recursive step. To this end, we use the dendrogram $\mathcal{T}_{\hat{d}}$ of the ultrametric subdominant (X, \hat{d}) . This is possible since the maximal clusters of $\mathcal{T}_{\hat{d}}$ correspond to ρ -components.

Lemma 6.15. Let (X, d) be a dissimilarity space, α be an internal node in the dendrogram $\mathcal{T}_{\hat{d}}$, and β be a child of α . Then $X(\beta)$ is a $p(\alpha)$ -component of $X(\alpha)$.

Proof. By the definition and construction of $\mathcal{T}_{\hat{d}}$, for any $x \in X(\beta)$ and $y \in X(\alpha) \setminus X(\beta)$ we have $d(x,y) \geq \hat{d}(x,y) = p(\alpha)$. Hence $X(\beta)$ is an union of components C_1, \ldots, C_ℓ of $G_{< p(\alpha)}(X(\alpha))$. If $X(\beta)$ is not a $p(\alpha)$ -component, then $\ell > 1$. Let $x \in C_1$ and $y \in X(\beta) \setminus C_1$. Then there is a path from x to y in $X(\beta)$ with maximum weight at most $p(\beta) < p(\alpha)$. This path contains an edge x'y'

with $x \in C_1$, $y \in X(\beta) \setminus C_1$. But then $d(x', y') < p(\alpha)$, which is impossible. Hence $X(\beta)$ is a $p(\alpha)$ -component.

In order to apply stableTrees (Algorithm 4) to the dendrogram $\mathcal{T}_{\hat{d}}$, we need:

Lemma 6.16. For any dissimilarity space (X, d), the dendrogram $\mathcal{T}_{\hat{d}}$ is coherent.

Proof. Let M be an mmodule, and α be the M-pertinent node in $\mathcal{T}_{\hat{d}}$, and suppose $X(\alpha) \neq M$. Let β_1, \ldots, β_k be the children of α intersecting M $(k \geq 2)$. By way of contradiction, suppose that there is $i \in \{1, \ldots, k\}$ with $X(\beta_i) \cap M \neq \emptyset$ and $X(\beta_i) \setminus M \neq \emptyset$. Since $X(\beta_i)$ is a $p(\alpha)$ -component, there exists $x, y \in X(\beta_i)$ with $x \in M$, $y \notin M$ and $d(x, y) < p(\alpha)$. Let $z \in X(\beta_j)$ for some $j \neq i$. Then $d(y, z) \geq p(\alpha) > d(y, x)$, hence $z \notin M$ and $M \subseteq X(\beta_i)$. This contradicts the fact that α is M-pertinent.

Theorem 6.17. Using stableTrees as a stable partition algorithm, one can implement mmoduleTree to run in time $O(|X|^2)$.

Proof. To prove the theorem, we need to establish that (1) at each recursive call, we can build the dendrogram of the ultrametric subdominant for that subset; (2) all these computations can be performed efficiently. Consider a call to mmoduleTree($\mathcal{T}_{\hat{d}}(S)$). Suppose that $\mathcal{T}_{\hat{d}}(S) = \text{Node}(\beta_1, \ldots, \beta_k)$, and notice that $C_i = X(\beta_i)$ and $\mathcal{T}_{\hat{d}}(C_i) = \beta_i$ for all $i \in \{1, \ldots, k\}$ by Lemma 6.15.

We start by proving (1). First, we justify the call stablePartition($\{C_1, S \setminus C_1\}$) in line 8. $\mathcal{T}_{\hat{d}}(C_1)$ is available as a child in $\mathcal{T}_{\hat{d}}(S)$. Then removing that child, we get a coherent tree $\mathcal{T}(S \setminus C_1)$ (notice that it may not be a dendrogram). Next we prove, through several claims, that all calls to stablePartition return dendrograms of the ultrametric subdominants of their respective subsets.

Claim 6.18. Let $\mathcal{T}(S_i)$ be an S_i -tree obtained at lines 8 or 17. If diam $(S_i) \leq \rho$, then $\mathcal{T}_{\hat{d}}(S_i) = \mathcal{T}(S_i)$.

Proof. If $\mathcal{T}(S_i)$ is a subtree of $\mathcal{T}_{\hat{d}}(S)$, then $\mathcal{T}_{\hat{d}}(S_i) = \mathcal{T}(S_i)$. Otherwise let $\mathcal{T}(S_i) = \text{Node}(\beta_1, \ldots, \beta_n)$ where β_1, \ldots, β_n define a proper subset of children of a node α in $\mathcal{T}_{\hat{d}}(S)$. By the properties of dendrograms, there exist $x \in S_i$ and $y \in X(\alpha) \setminus S_i$ with $d(x, y) = p(\alpha)$. As S_i is a ρ -component, we deduce $p(\alpha) \geq \rho$. Thus α is the root of $\mathcal{T}_{\hat{d}}(S)$. Now let $x, y \in S_i$ be in distinct children of α . Then $d(x, y) \geq \rho$, but also $d(x, y) \leq \rho$ since diam $(S_i) \leq \rho$. Consequently, $d(x, y) = \rho$. Hence any two children of $\mathcal{T}(S_i)$ are at the same distance ρ , proving that $\mathcal{T}_{\hat{d}}(S_i) = \mathcal{T}(S_i)$.

Claim 6.19. For $j \in \{1, \ldots, \ell\}$, let $\mathcal{T}(S_j)$ be an S_j -tree obtained at line 8. Then $\mathcal{T}_{\hat{d}}(S_j) = \mathcal{T}(S_j)$.

Proof. If there is a child γ of the root of $\mathcal{T}_M(S)$ with $X(\gamma) = S_j$, then $\operatorname{diam}(S_j) \leq \min_{\gamma'} d(S_j, \gamma')$ where γ' ranges over the other children of the root of \mathcal{T}_M . Hence $\operatorname{diam}(S_j) \leq \rho$ and the claim follows by Claim 6.18.

Otherwise, S_1 is a dwarf component and S_j is either S_1 or S_i in line 12. In either case, diam $(S_j) \leq \rho$ and again Claim 6.18 applies.

Claim 6.20. For $j \in \{1, \ldots, \ell\}$, let $\mathcal{T}(S_j)$ be an S_j -tree obtained at line 17. Then $\mathcal{T}_{\hat{d}}(S_j) = \mathcal{T}(S_j)$.

Proof. By Lemma 4.6, diam $(S_{\star}) \leq \rho$ and diam $(S^{\star}) \leq \rho$. Hence diam $(S_j) \leq \rho$ and the claim follows by Claim 6.18.

Claims 6.19 and 6.20 imply that almost all recursive calls to mmoduleTree are valid since we know the dendrogram for each set. It remains to consider the case of $S_1 \cup S_i$ in line 12, which happens when C_1 is a dwarf component. Then $S_1 = C_1$. If S_i is a single ρ -component, then $\mathcal{T}(S_i)$ is a single child of the root of $\mathcal{T}_{\hat{d}}(S)$ and $\mathcal{T}_{\hat{d}}(S_1 \cup S_i) = \text{Node}(\mathcal{T}(S_1), \mathcal{T}(S_i))$. Otherwise, S_i is a union of ρ -components and $\mathcal{T}(S_i)$ is a join of several children of the root of $\mathcal{T}_{\hat{d}}(S)$, and $\mathcal{T}_{\hat{d}}(S_1 \cup S_i)$ is obtained by adding $\mathcal{T}(S_1)$ as a child to $\mathcal{T}(S_i)$. Thus, the recursive call mmoduleTree $(S_1 \cup S_i)$ is also valid. We also have to justify the call stablePartition($\{S_{\star}, S^{\star}\}$) in line 17. Consider S_{\star} . If $|I_{\star}| = 1$, then S_{\star} is a ρ -component and thus $\mathcal{T}_{\hat{d}}(S_{\star}) = \mathcal{T}(C_i)$ for $i \in I_{\star}$. Otherwise, by definition of H, for each $i, i' \in I_{\star}$, $x \in C_i$ and $y \in C_{i'}$, we have $d(x, y) \ge \rho$ (since C_i and $C_{i'}$ are ρ -components) and $d(x, y) \le \rho$ (as, in H, I_{\star} is an independent set of vertices). This implies that $\mathcal{T}_{\hat{d}}(S_{\star})$ is the join of the $\mathcal{T}(C_i)$ for $i \in I_{\star}$. Similarly, $\mathcal{T}_{\hat{d}}(S^{\star})$ is the join of $\mathcal{T}(C_i)$ for $i \in I^{\star}$. This concludes the proof of assertion (1).

We now prove the assertion (2) that $\mathsf{mmoduleTree}(X)$ can be implemented in $O(|X|^2)$. First by Proposition 9.6 the dendrogram $\mathcal{T}_{\hat{d}}(X)$ can be computed in $O(|X|^2)$. Then we analyse the cost of $\mathsf{mmoduleTree}(\mathcal{T}_{\hat{d}}(S))$ without counting the recursive calls, depending on the line of return. Observe that the cost of lines 3 and 4 is $O(\sum_{i=1}^{k} |C_i||S \setminus C_i|)$. We will relate in each case the cost to the number N of pairs of elements in distinct children of the root of $\mathcal{T}_M(S)$.

If mmoduleTree($\mathcal{T}_{\hat{d}}(S)$) returns on line 6 (the case of a non-special \cap -node), then the total cost is $O(\sum_{i=1}^{k} |C_i| | S \setminus C_i|)$, which is proportional to N. As we will see in the next two cases, this case can be charged with an additional cost, still proportional to N.

If mmoduleTree($\mathcal{T}_{\hat{d}}(S)$) returns on line 13 (the case of a \cup -node discovered through a giant component C_1), then the total cost is

$$O\left(\sum_{i=1}^{k} |C_i| |S \setminus C_i| + \sum_{i=1}^{\ell} |S_i| |S \setminus S_i|\right)$$

(counting line 8). The left-hand term is the number of pairs of elements in distinct children of the root of $\mathcal{T}_M(S)$. By Lemma 6.9, each component C_i is either dwarf or giant. If C_i is giant, $x \in C_i$ and $y \in S \setminus C_i$, then x and y are not in the same ρ -component, hence those pairs x, y are counted in $\sum_{i=1}^{\ell} |S_i| |S \setminus S_i|$. Thus, without counting the additional contribution from dwarf components, we get a cost proportional to N. It remains to count the pairs x, y where x and y are in two distinct dwarf components that are part of the same S_i . In that case $\mathcal{T}_M(S_i) = \cup(\gamma_1, \ldots, \gamma_m)$ where $X(\gamma_1), \ldots, X(\gamma_m)$ are the dwarf components from that S_i . We thus charge the uncounted cost induced by those dwarf components to the call $\mathsf{mmoduleTree}(\mathcal{T}_{\hat{d}}(S_i))$ (the charged cost is proportional to its N value).

If mmoduleTree($\mathcal{T}_{\hat{d}}(S)$) returns on line 12 (the case of a \cup -node discovered from a dwarf component), the analysis is similar to the previous case. Notice that there is an additional cost of $O(|S_1||S_i|)$ induced in line 8 by the fact that S_1 and S_i are not mmodules. We charge it to mmoduleTree($S_1 \cup S_i$) as S_1 is a dwarf component of the mmodule $S_1 \cup S_i$.

If mmoduleTree($\mathcal{T}_{\hat{d}}(S)$) returns on lines 19 or 20 (the case of a special \cap -node), then the total cost is

$$O\left(\sum_{i=1}^{k} |C_i| |S \setminus C_i| + \sum_{i \in I} |C_i| |(S_{\star} \cup S^{\star}) \setminus C_i| + \sum_{i=1}^{l} |S_i| |(S_{\star} \cup S^{\star}) \setminus S_i|\right).$$

Let $i \in \{1, \ldots, k\}$. If $i \in J$, then $C_i = X(\beta_j)$ for some $j \in \{1, \ldots, k'\}$, that is C_i is the set induced by some child of $\mathcal{T}_M(S)$. Otherwise, $i \in I$. If $C_i = \bigcup_{i \in L} S_i$ for some $L \subset \{1, \ldots, \ell\}$, then $|C_i||(S_{\star} \cup S^{\star}) \setminus C_i| \leq \sum_{j \in L} |S_j||(S_{\star} \cup S^{\star}) \setminus S_j|$. Otherwise there is some $j \in \{1, \ldots, \ell\}$ such that $C_i \cap S_j \neq \emptyset$ and $S_j \setminus C_i \neq \emptyset$. We may assume that $S_j \subseteq S_{\star}$ (the case $S_j \subseteq S^{\star}$ is similar). Since diam $(S_{\star}) \leq \rho$, we obtain diam $(S_j) \leq \rho$. Thus for any $x \in S_j \cap C_i$ and $y \in S_j \setminus C_i$, $d(x,y) = \rho$. Thus $\mathcal{T}_M(S_j) = \cap(\gamma_1, \ldots, \gamma_m)$ with $\rho(S_j) = \rho$ and $X(\gamma_1), \ldots, X(\gamma_m)$ are ρ -components of S, one of them being C_i . That is, C_i is a dwarf component of $S_{\star} \cup S^{\star}$. Similarly to the two previous case, we may charge the cost related to the dwarf components to the corresponding recursive call mmoduleTree (S_j) . To conclude that case, we get that the total cost is composed of one term that is proportional to the number of pairs of elements separated by the current call:

$$\sum_{j \in J} |C_j| |S \setminus C_j| + \sum_{i=1}^l |S_i| |S \setminus S_i|,$$

and another term corresponding to dwarfs components in $S_{\star} \cup S^{\star}$, that is charged one their respective recursive calls.

Finally, each call incurs a cost proportional to the number of pairs of distinct elements of S that are not together in a deeper recursive call. Hence each pair of $\binom{X}{2}$ is counted exactly once, thus the total complexity is $O(|X^2|)$.

6.4. Nodes of $\mathcal{T}_{\hat{d}}$ and nodes of \mathcal{T}_M and \mathcal{T}_{PQ} . We conclude this section with a characterization of nodes of \mathcal{T}_M and \mathcal{T}_{PQ} that correspond to nodes of $\mathcal{T}_{\hat{d}}$.

Lemma 6.21. Let (X, d) be a Robinson space with PQ-tree \mathcal{T}_{PQ} and let β be an internal node of \mathcal{T}_{PQ} . Then one of the following assertions holds:

- (i) $X(\beta)$ is a cluster of $\mathcal{T}_{\hat{d}}$,
- (ii) β is P-node, β is the child of a Q-node α , and for each child γ of β , $X(\gamma)$ is a cluster of $\mathcal{T}_{\hat{d}}$.

Proof. Suppose that $X(\beta)$ is not a cluster, in particular β is not the root of \mathcal{T}_{PQ} , and let α be its parent node. Let $\rho := \rho(X(\beta))$ be the minimum value such that the graph $G_{\leq \rho}(X(\beta))$ is connected. Let also C be the minimal cluster containing $X(\beta)$, and let ρ' be the weight of the node corresponding to C in the vertex representation of $\mathcal{T}_{\hat{d}}$. In particular, $\min\{d(x, z) : x \in X(\beta), z \in C \setminus X(\beta)\} \leq \rho'$. By Lemma 3.12 this implies $\rho \leq \operatorname{diam}(X(\beta)) \leq \rho'$.

If $\rho < \rho'$, then there would be a cluster with value at most ρ containing $X(\beta)$, contradicting the minimality of C. Thus $\rho = \text{diam}(X(\beta)) = \rho'$, which implies that $G_{\overline{\rho}}(X(\beta))$ is not connected, and each of its ρ -components has diameter at most ρ . By Proposition 4.9, β is a P-node, and any children γ is a ρ -component of $X(\beta)$.

By way of contradiction, suppose that α is a P-node. By Lemma 3.12(iii), $\rho(\alpha) > \rho$. As $X(\alpha)$ is a block, for all $x \in X(\alpha)$ and $y \in X \setminus X(\alpha)$, $d(x, y) \ge \rho(\alpha) > \rho$. Also, as α is a P-node, for each $x \in X(\beta)$ and $y \in X(\alpha) \setminus X(\beta)$, $d(x, y) = \rho(\alpha) > \rho$. But then, $X(\beta)$ is a cluster of value ρ , contradiction. Thus α is a Q-node.

Since we proved that any node of the PQ-tree \mathcal{T}_{PQ} that does not induce a cluster of $\mathcal{T}_{\hat{d}}$ has a Q-node parent, we deduce that each child of the P-node β induces a cluster. Thus (ii) is proved. \Box

Leveraging the translation between PQ-trees and mmodule trees, we get:

Lemma 6.22. Let (X, d) be a Robinson space with mmodule tree \mathcal{T}_M and β be an internal node of \mathcal{T}_M . Then one of the following assertions holds:

- (i) $X(\beta)$ is a cluster of $\mathcal{T}_{\hat{d}}$,
- (ii) β is the large child of a \cap -node,
- (iii) β is a \cap -node and is the child of a \cup -node, and for each child γ of β , $X(\gamma)$ is a cluster of $\mathcal{T}_{\hat{d}}$.

Proof. By Proposition 5.5, either β is the large child of a special node α (that is (ii) holds), or there is a node β' in the PQ-tree \mathcal{T}_{PQ} with $X(\beta') = X(\beta)$. In the later case, by Lemma 6.21, either $X(\beta')$ is a cluster (and so is $X(\beta)$, thus (i) holds), or β' is a P-node child of a Q-node α' . Again, we assume the later. Then there is a node α in \mathcal{T}_M with $X(\alpha) = X(\alpha')$ by Proposition 5.5.

Since $X(\alpha) = X(\alpha'), X(\beta) = X(\beta'), \beta'$ is a P-node and α' a Q-node, by applying Proposition 5.1 to α' , we conclude that β is a \cap -node and one of three possibilities happens:

Case 1: α' is non-conical, then α is a U-node, β is a child of α . Then, as $X(\beta)$ is not a cluster, there is another child β' of α with $d(\beta, \beta') = \rho(\beta)$, hence by Lemma 3.12, diam $(X(\beta)) = \rho(\beta)$. This implies that β has no large child, and each of its child is a cluster, thus (iii) holds.

Case 2: α' is conical, but its apex is not β' , then α has a large child γ , γ is a \cup -node or have arity two, and β is a child of γ . As in the previous case, as $X(\beta)$ is not a cluster, its diameter is $\rho(\beta)$ and each of its child is a cluster, whence (iii) holds.

Case 3: α' is conical with apex β' , then α is a special \cap -node. Also β' cannot be split (otherwise there would not be a node with leaf set $X(\beta')$ in \mathcal{T}_M), hence β is a child of α . Then for each $x \in X(\beta), y \notin X(\beta), d(x, y) \ge \rho(\alpha) > \rho(\beta)$ by Lemma 3.12. Thus $X(\beta)$ is a cluster, whence (i) holds.

7. Translation between copoint partitions and PQ-trees and mmodule trees

In our previous paper [3], the copoints of a point p were at the heart of our divide-and-conquer recognition algorithm. This is due to the fact that the copoints of p together with $\{p\}$ define a partition C_p of $X \setminus \{p\}$. In this section, we provide a correspondence between the copoint partition C_p and the trees \mathcal{T}_M and \mathcal{T}_{PQ} of a Robinson space (X, d). First, for any dissimilarity space (X, d)we characterize the copoints of C_p in terms of subtrees of the mmodule tree \mathcal{T}_M rooted at the nodes of the unique path $\Psi(p)$ between $\{p\}$ and the root of \mathcal{T}_M . This allows us to establish that the total number of copoints of (X, d) is at most 2|X| - 1. Second, we characterize the nodes on the unique path $\Upsilon(p)$ of the PQ-tree \mathcal{T}_{PQ} of a Robinson space (X, d) between the leaf $\{p\}$ and the root of \mathcal{T}_{PQ} . We also locate the copoints of C_p with respect to the nodes of this path $\Upsilon(p)$ and the p-proximity order, introduced in [3].

7.1. Translation between C_p and $\Psi(p)$. The next result characterizes the copoints attached at p in terms of subtrees of \mathcal{T}_M .

Proposition 7.1. Let (X,d) be a dissimilarity space with mmodule tree \mathcal{T}_M . For any $p \in X$, the *p*-copoints of X are:

- (i) $X(\alpha) \setminus X(\beta)$ for each \cap -node $\alpha \in \Psi(p)$ with β be the child of α in $\Psi(p)$,
- (ii) $X(\beta)$ for each \cup -node $\alpha \in \Psi(p)$ and each child β of α such that $\beta \notin \Psi(p)$).

Proof. Pick any $\alpha \in \Psi(p)$. Let $S := X(\alpha) \setminus X(\beta)$ if α is a \cap -node with child $\beta \in \Psi(p)$ or $S := X(\beta)$ for a child $\beta \notin \Psi(p)$ of α if α is a \cup -node. By Proposition 2.15, S is an amodule. Moreover, also by Proposition 2.15, any mmodule properly containing S contains $X(\alpha)$ and p, hence S is a p-copoint.

Conversely, let S be a p-copoint, in particular S is an mmodule. By Proposition 2.15, the following holds:

- either S is the leaf-set of the union of some children of a \cap -node α . Then by maximality of S, as $X(\alpha)$ is an mmodule, $p \in X(\alpha)$. Let S' be $\bigcup \{X(\beta) : \beta \text{ child of } \alpha, p \notin X(\beta)\}$. Again by Proposition 2.15, S' is an mmodule, and $S \subseteq S', p \notin S'$. By maximality of S, S = S'.
- or S is the leaf-set of a child β of a \cup -node α . Then by maximality of S, as $X(\alpha)$ is an mmodule, $p \in X(\alpha)$.

This concludes the proof.

From Lemma 2.17 it follows that any dissimilarity space (X, d) contains at most |X|(|X| - 1) copoints. In fact, by Proposition 7.1 the number of copoints is always linear in the size of X:

Corollary 7.2. The number of copoints of a dissimilarity space (X, d) is at most 2|X| - 1.

Proof. By Proposition 7.1, each node of the mmodule tree induces at most as many copoints as its arity. As the sum of arities equals the number of nodes minus one, and each inner node as arity at least 2, we get the result. \Box

Since by Proposition 5.6 all inner nodes of the mmodule tree of an ultrametric space are \cap -nodes, from Proposition 7.1 we obtain the following observation:

Corollary 7.3. The p-copoints of an ultrametric space (X, d) are the sets of the form $X(\alpha) \setminus X(\beta)$, where $\alpha \in \Psi(p)$ and β is the child of α in $\Psi(p)$.

7.2. Translation between C_p and $\Upsilon(p)$. We already know by Theorem 3.7 that for each node α of the PQ-tree, $X(\alpha)$ is an mmodule. Next we determine which mmodules do not correspond to nodes of \mathcal{T}_{PQ} .

Lemma 7.4. Let (X,d) be a Robinson space and \mathcal{T}_{PQ} its PQ-tree. Let $M \subseteq X$. Then M is an module of (X,d) if and only if

- (i) either there is a node $\alpha \in \mathcal{T}_{PQ}$ such that $M = X(\alpha)$,
- (ii) or there is a P-node $P(\beta_1, \ldots, \beta_k) \in \mathcal{T}_{PQ}$ and $I \subset \{1, \ldots, k\}$ non-empty such that $M = \bigcup_{i \in I} X(\beta_i)$,
- (iii) or there is a δ -conical Q-node $\alpha = Q(\gamma_1, \dots, \gamma_l) \in \mathcal{T}_{PQ}$, with apex child γ_j , and $M = X(\alpha) \setminus X(\gamma_j)$,
- (iv) or there is a δ -conical Q-node $\alpha = Q(\gamma_1, \dots, \gamma_l) \in \mathcal{T}_{PQ}$, with split child γ_j , and a subset B of children of γ_j , such that $M = X(\alpha) \setminus \bigcup_{\beta \in B} X(\beta)$.

Proof. By Proposition 2.15, either (a) there is a node β in \mathcal{T}_M with $M = X(\beta)$, or (b) there is a \cap -node $\alpha = \cap(\beta_1, \ldots, \beta_k)$ and $I \subsetneq \{1, \ldots, k\}, |I| \ge 2$ such that $M = \bigcup_{i \in I} X(\beta_i)$.

In case (a), suppose (i) does not hold, then by Proposition 5.5 β is a large child of a special Q-node α . By Lemma 3.12, α is not a large child itself, hence there is a P-node α' in \mathcal{T}_{PQ} with $X(\alpha) = X(\alpha')$. By Proposition 4.10, $\alpha' = Q(\gamma_1, \ldots, \gamma_{i-1}, \beta', \gamma_i, \ldots, \gamma_\ell)$, with $X(\alpha) \setminus X(\beta') = X(\beta)$, hence (iii) holds.

In case (b), α is not a large child because k = 2, hence by Proposition 5.5 there is a P-node α' in \mathcal{T}_{PQ} with $X(\alpha) = X(\alpha')$. If α has no split child, then by Proposition 4.9, for each β_i , there is a child β'_i of α with $X(\beta_i) = X(\beta'_i)$, and (ii) follows. Thus we may assume that there is a split child, say β_k . By Proposition 4.10, $\alpha' = Q(\gamma_1, \ldots, \gamma_{j-1}, \beta', \gamma_j, \ldots, \gamma_\ell)$ with $X(\alpha') \setminus X(\beta') = X(\beta_k)$ and $\beta' = P(\gamma_1, \ldots, \gamma_{k-1})$ such that for each $i \in \{1, \ldots, k-1\}, X(\gamma_i) = X(\beta_i)$. If $k \in I$, (iv) holds, while if $k \notin I$, (iii) holds on β' .

Our next result establishes a correspondence between the copoints of \mathcal{C}_p and the nodes of $\Upsilon(p)$.

Theorem 7.5. Let (X, d) be a Robinson space. For any $p \in X$, the copoints of \mathcal{C}_p are:

- (1) $X(\alpha) \setminus X(\beta)$ for each P-node $\alpha \in \Upsilon(p)$ with child $\beta \in \Upsilon(p)$,
- (2) $X(\beta)$ for each Q-node $\alpha \in \Upsilon(P)$ and each child $\beta \notin \Upsilon(p)$, when, if α is conical, p is not in the apex child of α ,
- (3) $X(\alpha) \setminus X(\beta)$ for each δ -conical Q-node $\alpha \in \Upsilon(p)$ with standard apex child $\beta \in \Upsilon(p)$, and $G_{\overline{\delta}}(X(\beta))$ is connected,
- (4) $X(\alpha) \setminus X(\gamma)$ for each δ -conical Q-node $\alpha \in \Upsilon(p)$ with split child $\beta \in \Upsilon(p)$, and $\gamma \in \Upsilon(p)$ child of β .

Proof. Let M be a p-copoint. Then M is an mmodule and by Lemma 7.4 one of the four following cases occurs.

- (i) There is a node α in *T_{PQ}* such that *M* = *X*(α). As *p* ∉ *X*(α), α is not the root of *T_{PQ}*, and let γ be its parent. By maximality of *M*, *p* ∈ *X*(γ). By Lemma 7.4(ii) γ is not a P-node, hence is a Q-node. Suppose that it is conical and *p* is in an apex child α' of γ. Then *X*(γ) \ *X*(α') is an mmodule containing *X*(α) and not *p*, contradicting the maximality of *M*. Thus case (2) applies.
- (ii) There is a node $\alpha = P(\beta_1, \dots, \beta_k)$ in \mathcal{T}_{PQ} and $I \subsetneq \{1, \dots, k\}$ such that $M = \bigcup_{i \in I} X(\beta_i)$. By maximality of $M, p \in X(\alpha)$ and |I| = k - 1, hence $M = X(\alpha) \setminus X(\beta_i)$ for the unique $i \in \{1, \dots, k\} \setminus I, p \in X(\beta_i)$ and case (1) applies.
- (iii) There is a δ -conical Q-node $\alpha = Q(\beta_1, \dots, \beta_k)$, with β_i apex, and $M = X(\alpha) \setminus X(\beta)$. Then as $X(\alpha)$ is an mmodule, by maximality of $M, p \in X(\alpha)$ and thus $p \in X(\beta_i)$. Suppose that

 $G_{\overline{\delta}}(X(\beta_i))$ is not connected, let S be one of its δ -mmodule not containing p. Then $M \cup S$ is an mmodule not containing p, contradicting the maximality of p. Thus case (3) applies.

(iv) There is a δ -conical Q-node $\alpha = Q(\beta_1, \ldots, \beta_k)$ with an apex child β_i such that the graph $G_{\overline{\delta}}(X(\beta_i))$ is not connected, and there is a subset Γ of children of β_i such that $M = X(\alpha) \setminus \bigcup_{\gamma \in \Gamma} X(\gamma)$. As $X(\alpha)$ is an mmodule, by maximality of $M, p \in X(\alpha)$ hence $p \in X(\gamma^*)$ for some $\gamma^* \in \Gamma$. Then by maximality of $M, \Gamma = \{\gamma^*\}$, and case (4) applies.

Conversely, let M be a set as in one of the cases (1) to (4). Then by Lemma 7.4, M is an mmodule. Moreover, any mmodule properly containing M must contain $X(\alpha)$, hence contains p, proving that M is a p-copoint.

7.3. $\Upsilon(p)$ and the *p*-proximity order. We recall the definition of *p*-proximity orders of Robinson spaces, which was one of the ingredients of our recognition algorithm in [3]:

Definition 7.6 (p-Proximity order [3]). Let (X, d) be a Robinson space with a compatible order < and let p be a point of X. A *p*-proximity order (relatively to <) is a total order \prec on C_p such that if $C, C' \in C_p$ and $C \prec C'$, then:

(PO1) $d(C, p) \le d(C', p);$

(PO2) if X is sorted according to <, then no point of C' is located between p and a point of C.

A *p*-proximity order exists for every compatible order and can be efficiently computed, even without the knowledge of the compatible order < [3]. Actually, in [3, Algorithm 6.1] we constructed a *universal* compatible order: an order < on C_p which is a *p*-proximity order relatively to any compatible order $< \in \Pi(X, d)$; in what follows we will consider only universal *p*-proximity orders. Given a universal *p*-proximity order <, suppose that the copoints of C_p are ordered in the following way:

$$\{p\} := C_0 \prec C_1 \prec \ldots \prec C_k.$$

For any C_i we denote by $[C_0, C_i]$ the points in the copoints between C_0 and C_i in the ordered set $(\mathcal{C}_p, \prec): [C_0, C_i] := C_0 \cup \ldots \cup C_i$. We call $[C_0, C_i]$ an *initial interval* of \prec . Since \prec is a *p*-proximity order for all compatible orders, any initial interval $[C_0, C_i]$ is a block.

Next, we will characterize the copoints $C \in C_p$ for which the initial interval $[C_0, C]$ is also an mmodule. Since the nodes of $\Upsilon(p)$ are exactly the subsets of X which are simultaneously mmodules and blocks and also contain p, these intervals will correspond to nodes of $\Upsilon(p)$. Let $\Upsilon(p) = (\alpha_0, \alpha_1, \ldots, \alpha_m)$, where α_0 correspond to p and α_m corresponds to the root of \mathcal{T}_{PQ} . Then $\{p\} = X(\alpha_0) \subsetneq X(\alpha_1) \subsetneq \ldots \subsetneq X(\alpha_m) = X$ is a chain of subsets of X which are mmodules and blocks containing p. However, in view of Theorem 7.5, only those $X(\alpha_i)$ where α_i is standard correspond to initial intervals of \prec . We now formalize these ideas, starting with a definition motivated by the previous discussion.

Definition 7.7 (frontier). A copoint C is a *frontier* if $[C_0, C]$ is an mmodule.

We establish the correspondence between frontiers and standard nodes of $\Upsilon(p)$.

Theorem 7.8. Let (X, d) be a Robinson space, p a point of X, and $S \subseteq X$ with $p \in S$. Let \prec be a universal p-proximity order. Then there is a standard node $\alpha \in \Upsilon(p)$ with $X(\alpha) = S$ if and only if there exists a frontier $C \in \mathcal{C}_p$ with $[C_0, C] = S$.

Proof. Let $\alpha \in \Upsilon(p)$ be a standard node. By Theorem 7.5, each copoint intersecting $X(\alpha)$ is contained in $X(\alpha)$. Let $\mathcal{C}_p(\alpha)$ be the set of copoints contained in $X(\alpha)$. Let $C' \in \mathcal{C}_p(\alpha)$ and $C'' \in C_p \setminus C_p(\alpha)$, and suppose by way of contradiction that $C'' \prec C'$. Consider a compatible order \prec . Let $x' \in C'$ and $x'' \in C''$. We may assume (up to reversal of \prec) that $p \prec x''$.

As $X(\alpha)$ is a block by Theorem 3.7, x'' is not between p and x' in <, hence x' < x''. Moreover, < being a p-proximity order, by (PO2) and C'' < C', x' is not between p and x'' in <, hence

 $x' . Then because <math>X(\alpha)$ is a block, by Lemma 3.5, $<_{X(\alpha)}$ is a compatible order, with $p <_{X(\alpha)} x' <_{X(\alpha)} x''$, in contradiction with the fact that < is a universal *p*-proximity order. Thus, if *C* is the maximum element in $\mathcal{C}_p(\alpha)$ for <, then $X(\alpha) = [C_0, C]$ holds.

if C is the maximum element in $C_p(\alpha)$ for \prec , then $X(\alpha) = [C_0, C]$ holds. Conversely, let $C \in C_p$ be a frontier, meaning by definition that $[C, C_p]$ is an mmodule and a block. By Theorem 3.7, there is a node α in \mathcal{T}_{PQ} with $X(\alpha) = [C_0, C]$. Clearly $\alpha \in \Upsilon(p)$. Suppose by contradiction that α is not standard, *i.e.* α is a split node, child of a δ -conical node β . Let γ be the child of α with $p \in X(\gamma)$. Then by Theorem 7.5, $X(\beta) \setminus X(\gamma)$ is a p-copoint intersecting C, but the p-copoints are disjoint, hence this is a contradiction.

The algorithm from [7] can be rephrased and applied to build the mmodule tree over a dissimilarity space. Recall that it is based on the partition into p-copoints and then building the path of the mmodule tree from p to the root. Our understanding of mmodules and of PQ-trees together with the algorithm from [3] lead to an alternative approach to the construction of the PQ-tree, which also provides the orders of the children of Q-nodes. Toward this goal, we first characterize the frontiers corresponding to each kind of nodes of the PQ-tree: P-node, non-conical Q-node, or conical Q-node with or without a split child.

Let (X, d) be a Robinson space, $p \in X$, and C_1, \ldots, C_k be the *p*-copoints, and let \prec be a *p*-proximity order on \mathcal{C}_p . We assume that $\{p\} = C_0 \prec C_1 \prec \ldots \prec C_k$. Let $i \in \{1, \ldots, k\}$. By definition, C_i is a frontier if and only if for each $j \in \{1, \ldots, i\}$ and each $j' \in \{i + 1, \ldots, n\}$, we have $d(p, C_{j'}) = d(C_j, C_{j'})$. This allows to determine all the frontiers in time $O(k^2)$: for each $j' \in \{1, \ldots, k\}$, let $j \in \{0, \ldots, j'\}$ be maximum such that $d(p, C_{j'}) = d(C_j, C_{j'})$ and mark $C_{j+1}, \ldots, C_{j'-1}$ as non-frontier. Then all non-marked copoints are frontiers.

Once we know that C_i is a frontier, let $\alpha_i \in \Upsilon(p)$ be the node with $X(\alpha_i) = [C_0, C_i]$, and we can determine the root of α_i , using Theorem 7.5.

(1) If i > 2 and C_{i-1} is not a frontier, then α_i is a Q-node. Let $j \in \{1, \ldots, i-1\}$ be maximum with C_j a frontier (or j = 0 if C_i is the first frontier). Then $\alpha_j, \mathcal{T}_{PQ}(C_{j+1}), \ldots, \mathcal{T}_{PQ}(C_i)$ are the children of α_i . Indeed those non-frontier copoints correspond to the case (2) in Theorem 7.5. If α_i is conical, then p is not in its apex child.

(2) Else, α_i is either a P-node, a conical Q-node with α_{i-1} apex and not split, or a conical Q-node with split child β and α_{i-1} a child of β . Let $\delta = d(p, C_i)$, in any of these cases $G_{\overline{\delta}}([C_0, C_i])$ is not connected, let K_1, \ldots, K_m be its connected component, with K_1 having the largest diameter.

- (2.1) If diam $(K_1) \leq \delta$, there is no large component, hence α_i is a P-node $P(\beta_1, \ldots, \beta_l)$, and each component corresponds to a child of α_i by Proposition 4.9. In that case, α_{i-1} is the child β_j of α_i containing p, hence exactly one of the following cases hold:
 - (2.1.1) either l > 2 and $\mathcal{T}_{PQ}(C_k) = P(\beta_1, \dots, \beta_{j-1}, \beta_{j+1}, \dots, \beta_l);$
 - (2.1.2) or l = 2 and $\mathcal{T}_{PQ}(C_k) = \beta_{3-j}$.
 - In both cases, diam $(C_k) \leq \delta$.
- (2.2) Else if m = 2, then, α_i is a δ -conical Q-node whose apex child α_{i-1} is not split by Proposition 4.10. In this case, $C_k = X(\alpha_i) \setminus X(\alpha_{i-1})$, and one of the following cases occurs:
 - (2.2.1) either $\mathcal{T}_{PQ}(C_k) = P(\beta_1, \beta_2)$ and then $\alpha_i = Q(\beta_1, \alpha_{i-1}, \beta_2)$;
 - (2.2.2) or $\mathcal{T}_{PQ}(C_k) = Q(\beta_1, \dots, \beta_l)$, and there is $j \in \{2, \dots, l\}$ with
 - $\alpha_i = Q(\beta_1, \ldots, \beta_{j-1}, \alpha_{i-1}, \beta_j, \ldots, \beta_k);$
 - In both cases, diam $(C_k) > \delta$.
- (2.3) Else, also by Proposition 4.10, m > 2 and α_i is a δ -conical Q-node with a split child β . The children of β are in one-to-one correspondence with the components K_2, \ldots, K_m , one of them being α_{i-1} . In that case, $\mathcal{T}_{PQ}(C_k) = Q(\beta_1, \ldots, \beta_l)$ with apex child β_j , diam $(C_k) > \delta$, and one of the following cases hold:
 - (2.3.1) either β_j is a split child, that is $\beta_j = P(\gamma_1, \dots, \gamma_n)$ with $d(X(\gamma_1), X(\gamma_n)) = \delta$, then $\alpha_i = Q(\beta_1, \dots, \beta_{j-1}, Q(\gamma_1, \dots, \gamma_n, \alpha_{i-1}), \beta_{j+1}, \dots, \beta_k);$

ALGORITHM 6. Computes the PQ-tree of a Robinson space (X, d) using the copoints attached at some point p.

pqTree2(S)

Input: A Robinson space (X, d) (implicit), a set $S \subseteq X$. **Output:** $\mathcal{T}_{PQ}(S)$ the PQ-tree of (S, d). 1: let $p \in S$ 2: if |S| = 1 then 3: return Leaf p4: let $C_0 = \{p\}, C_1, \ldots, C_k = \text{stablePartition}(\{p\}, S \setminus \{p\})$ \triangleright with $C_0 \prec C_1 \prec \ldots \prec C_k$ 5: return copointsToPqTree (p, C_1, \ldots, C_k) copointsToPqTree (p, C_1, \ldots, C_k) 6: let (L, i, R) := nextFrontier (p, C_1, \ldots, C_k) 7: let $T_p := \text{copointsToPqTree}(p, C_1, \dots, C_i)$ if $i > 0, T_p = \text{Leaf } p$ if i = 08: if i < k - 1 then let $[\beta_1, \ldots, \beta_l]$ = map(pqTree2, L) ++ $[T_p]$ ++ map(pqTree2, R) 9: return $Q(\beta_1, \ldots, \beta_l)$ \triangleright Case (1) 10:11: let $\alpha := pqTree2(C_k), \delta := d(p, C_k)$, and $D = diam(C_k)$ $\triangleright C_{k-1}$ is a frontier 12: match α with 13: case $P(\beta_1, \ldots, \beta_l)$ with $D = \delta$: \triangleright Case (2.1.1) return $P(\beta_1,\ldots,\beta_l,T_p)$ 14:15: case $P(\beta_1, \ldots, \beta_l)$ with $D < \delta$ or $Q(\beta_1, \ldots, \beta_l)$ with $D \leq \delta$: \triangleright Case (2.1.2) return $P(\alpha, T_p)$ 16:17: case $P(\beta_1, \beta_2)$ with $D > \delta$: \triangleright Case (2.2.1) return $Q(\beta_1, T_p, \beta_2)$ 18:19: case $Q(\beta_1, \ldots, \beta_l)$ with $D > \delta$: if α is δ -conical with split child $\beta_j = P(\gamma_1, \ldots, \gamma_n)$ then \triangleright Case (2.3.1) 20:return $Q(\beta_1,\ldots,\beta_{j-1},P(\gamma_1,\ldots,\gamma_n,T_p),\beta_{j+1},\ldots,\beta_l)$ 21:else if α is δ -conical with standard apex child β_i then \triangleright Case (2.3.2) 22:return $Q(\beta_1,\ldots,\beta_{j-1},P(\beta_j,T_p),\beta_{j+1},\ldots,\beta_l)$ \triangleright New split child 23:else \triangleright Case (2.2.2) 24:let (j, j + 1) be an admissible hole in α 25:26:return $Q(\beta_1,\ldots,\beta_j,T_p,\beta_{j+1},\ldots,\beta_l)$ \triangleright New apex child

nextFrontier (p, C_1, \ldots, C_k)

Input: A Robinson space (X, d) (implicit), $p \in X$ and $C_1 \prec C_2 \prec \ldots \prec C_k$ the *p*-copoints with \prec a universal *p*-proximity order.

Output: (L, i, R) where i < k is maximum such that C_i is a frontier (or i = 0 if there is no such frontier), L + R contains C_{i+1}, \ldots, C_k and there is a compatible order such that $L + \lfloor p \rfloor + R$ is increasing.

27: let $L := [], R := [C_k], i := k \text{ and } l := k$ 28: while $l \ge i$ do 29: for j := i - 1 to 1 do 30: if $(d(C_j, C_l) < d(p, C_l) \text{ and } C_l \in L)$ or $(d(C_j, C_l) > d(p, C_l) \text{ and } C_l \in R)$ then 31: $\bot \leftarrow C_j \cdot L, R \leftarrow [C_{j+1}, \dots, C_{i-1}] + R, \text{ and } i \leftarrow j$ 32: if $(d(C_j, C_l) < d(p, C_l) \text{ and } C_l \in R)$ or $(d(C_j, C_l) > d(p, C_l) \text{ and } C_l \in L)$ then 33: $\bot \leftarrow R \leftarrow C_j \cdot R, L \leftarrow [C_{j+1}, \dots, C_{i-1}] + L, \text{ and } i \leftarrow j$ 34: $\bot l \leftarrow l - 1$ 35: return (reverse(L), i - 1, R) (2.3.2) or β_j is standard, then $\alpha_i = Q(\beta_1, \dots, \beta_{j-1}, P(\beta_j, \alpha_{i-1}), \beta_{j+1}, \dots, \beta_l)$.

This leads to Algorithm 6, that builds the PQ-tree from the *p*-copoints. We use the notation $[e_1, \ldots, e_n]$ for a list or sequence of *n* elements; [] denotes the empty list. The *append* operation on list is denoted ++, while \cdot is the *insert first* operation; thus $[e_1, \ldots, e_n] + [f_1, \ldots, f_p] = e_1 \cdot ([e_2, \ldots, e_n] + [f_1, \ldots, f_p])$. We also use the map operation, defined by $map(f, [e_1, \ldots, e_n]) = [f(e_1), \ldots, f(e_n)]$. Applying the operation \cdot takes constant-time on single-linked list, and we assume that ++ and map are implemented as linear-time operations.

Algorithm 6 builds the *p*-copoints using the stable partition algorithm from [3, Algorithm 6.1], which returns the copoints in a universal *p*-proximity order. Then it builds recursively the PQtree $\mathcal{T}_{PQ}(C_k)$, and deduce $\mathcal{T}_{PQ}(X)$ from the previous analysis. The case analysis presented above justifies procedure copointsToPqTree. Algorithm 6 also relies on the procedure nextFrontier which finds the last frontier C_i before C_k and sorts the children of the root when this root is a Qnode. Those children are given by a permutation of the sequence provided by the *p*-proximity order $[C_0, C_i], C_{i+1}, \ldots, C_k$. The procedure nextFrontier builds a compatible pre-order from this *p*proximity order, by using the inner instructions of the main loop of [3, Algorithm 6.2]. Consequently the correctness of nextFrontier can be derived from the correctness of the construction in [3] of the compatible order from the *p*-proximity order.

Algorithm 6 can be implemented in $O(|X|^2)$ using [3, Algorithm 6.1] to compute the stable partition, and [3, Algorithm 4.1] to find the admissible hole at line 25. The analysis follows the same arguments as in [3, Theorem 7.2]. Therefore we can state:

Theorem 7.9. Given a Robinson space (X, d), Algorithm 6 computes $\mathcal{T}_{PO}(X)$ in time $O(|X|^2)$.

7.4. Copoints and frontiers in ultrametrics. We end this section with a characterization of ultrametric spaces in terms of copoints and frontiers:

Proposition 7.10. A dissimilarity space (X,d) is ultrametric if and only if for any $p \in X$ and any p-copoint C, C is a frontier and diam $(C) \leq d(p, C)$.

Proof. Let $p \in X$ and $C_o := \{p\} \prec C_1 \prec \ldots \prec C_k$ be the *p*-copoints in increasing universal *p*-proximity order. Let $\Upsilon(p) = \{\alpha_0, \alpha_1, \ldots, \alpha_{k'}\}$, sorted by decreasing depth; α_0 = Leaf *p* and $\alpha_{k'} = \mathcal{T}_{PQ}(X)$.

Suppose that (X, d) is ultrametric. By Proposition 3.13, $\mathcal{T}_{PQ}(X)$ contains only P-nodes; thus by Theorem 7.5, k = k' and $C_i = X(\alpha_i) \setminus X(\alpha_{i-1})$ for all $i \in \{1, \ldots, k\}$. As $[C_0, C_i] = X(\alpha_i)$, by Theorem 3.7 it is an mmodule, hence C_i is a frontier. Moreover, for each child β of α_i distinct from α_{i-1} , $X(\beta)$ is a block and $d(p, \beta) = d(p, C_i) = \rho(\alpha_i)$, hence diam $(\beta) \leq \rho(\alpha_i)$ and thus diam $(C_i) \leq d(p, C_i)$.

Conversely, suppose that for each $i \in \{1, ..., k\}$, C_i is a frontier with diam $(C_i) \leq d(p, C_i)$. By Theorem 7.8, k = k' and $X(\alpha_i) = [C_0, C_i]$ for each $i \in \{1, ..., k\}$. Moreover, as C_{i-1} is a frontier and diam $(C_i) \leq d(p, C_i)$, one of Cases (2.1.1) and (2.1.2) applies. In any case, this implies that α_i is a P-node. Therefore all nodes in the path from p to the root are P-nodes. As this is true for any $p \in X$, all internal nodes of $\mathcal{T}_{PQ}(X)$ are P-nodes, thus by Proposition 3.13 (X, d) is ultrametric. \Box

8. CONCLUSION

Our paper establishes a cryptomorphism between the PQ-tree \mathcal{T}_{PQ} and the mmodule-tree \mathcal{T}_M of a Robinson space (X, d). We show how to derive \mathcal{T}_M from \mathcal{T}_{PQ} and, vice-versa, how to construct \mathcal{T}_{PQ} from \mathcal{T}_M . We also present optimal $O(|X|^2)$ time algorithms for constructing the \mathcal{T}_{PQ} (without ordering the children of Q-nodes) and \mathcal{T}_M . Our proofs and algorithms use two technical ingredients: the δ -graph $G_{\overline{\delta}}$ of (X, d) with the properties of its connected components and the dendrogram $\mathcal{T}_{\widehat{d}}$ of the ultrametric subdominant \widehat{d} of (X, d). We also show how to construct in $O(|X|^2)$ the PQ-tree \mathcal{T}_{PQ} with the correct ordering of the children of Q-nodes from the copoint partitions and frontiers of (X, d); this algorithm is based on the concept of universal *p*-proximity order and the construction from this order of a compatibility order presented in our previous paper [3].

Our $O(|X|^2)$ time algorithm for constructing the PQ-tree \mathcal{T}_{PQ} of a Robinson space (X, d) is simpler than the algorithm of [13] which also constructs \mathcal{T}_{PQ} in $O(|X|^2)$ time in order to enumerate all compatible orders of (X, d). At the difference of [13], our algorithm does not use the quite complex algorithm of Booth and Lueker [2] as a subroutine. On the other hand, our top-to-bottom $O(|X|^2)$ time algorithm for constructing the mmodule tree \mathcal{T}_M is more involved than the algorithm of [7]. Nevertheless, it uses some surprising links between the trees \mathcal{T}_{PQ} and \mathcal{T}_M on the one hand and the dendrogram $\mathcal{T}_{\hat{d}}$ on the other hand.

Acknowledgements

This research was supported in part by ANR project DISTANCIA (ANR-17-CE40-0015) and has received funding from Excellence Initiative of Aix-Marseille - A*MIDEX (Archimedes Institute AMX-19-IET-009), a French "Investissements d'Avenir" Programme.

References

- J. E. ATKINS, E. G. BOMAN, AND B. HENDRICKSON, A spectral algorithm for seriation and the consecutive ones problem, SIAM J. Comput., 28 (1998), pp. 297–310.
- [2] K. S. BOOTH AND G. S. LUEKER, Testing for the consecutive ones property, interval graphs, and graph planarity using PQ-tree algorithms, J. Comput. Syst. Sci., 13 (1976), pp. 335–379.
- [3] M. CARMONA, V. CHEPOI, G. NAVES, AND P. PRÉA, Modules in robinson spaces, 2023. submitted.
- [4] F. CRITCHLEY AND B. FICHET, The partial order by inclusion of the principal classes of dissimilarity on a finite set, and some of their basic properties, in Classification and Dissimilarity Analysis, Springer, 1994, pp. 5–65.
- [5] E. DIDAY, Orders and overlapping clusters in pyramids., in Multidimensional Data Analysis, J. e. a. de Leeuw, ed., DSWO Press, Leiden, 1986.
- [6] C. DURAND AND B. FICHET, One-to-one correspondences in pyramidal representation: A unified approach., in Conf. of IFCS, 1987, pp. 85–90.
- [7] A. EHRENFEUCHT, H. N. GABOW, R. M. MCCONNELL, AND S. SULLIVAN, An O(n²) divide-and-conquer algorithm for the prime tree decomposition of two-structures and modular decomposition of graphs, J. Algorithms, 16 (1994), pp. 283–294.
- [8] B. EVERITT, Cluster analysis, Wiley, 2011.
- D. R. FULKERSON, Flow networks and combinatorial operations research, The American Mathematical Monthly, 73 (1966), pp. 115–138.
- [10] J. GOWER AND G. ROSS, Minimum spanning trees and single linkage cluster analysis, Journal of the Royal Statistical Society, Series C, 18 (1969), pp. 54–64.
- [11] G. P. HUET, The zipper, J. Funct. Program., 7 (1997), pp. 549–554.
- [12] B. MIRKIN AND S. RODIN, Graphs and Genes, Springer, 1984.
- [13] P. PRÉA AND D. FORTIN, An optimal algorithm to recognize Robinsonian dissimilarities, J. Classif., 31 (2014), pp. 351–385.
- [14] W. S. ROBINSON, A method for chronologically ordering archaeological deposits, Amer. Antiq., 16 (1951), pp. 293– 301.
- [15] A. SCHRIJVER, Combinatorial optimization: polyhedra and efficiency, vol. 24, Springer, 2003.
- [16] C. SEMPLE AND M. STEEL, *Phylogenetics*, Oxford University Press, Oxford, 2003.
- [17] M. SESTON, Dissimilarités de Robinson: algorithmes de reconnaissance et d'approximation, PhD thesis, Université de la Méditerranée, Aix-Marseille 2, 2008.

9. Appendices

9.1. Construction of the subdominant ultrametrics. In this subsection we show how to construct the dendrogram $\mathcal{T}_{\hat{d}}$ of the ultrametric space (X, \hat{d}) ; recall that \hat{d} is the subdominant ultrametric, i.e., the largest ultrametric such that $\hat{d}(x, y) \leq d(x, y)$ for any $x, y \in X$. We can construct $\mathcal{T}_{\hat{d}}$ in the following iterative way (which seems us to be new): when using Prim's algorithm to compute the minimum spanning tree T of (X, d), one can build $\mathcal{T}_{\hat{d}}$ by inserting each vertex in $\mathcal{T}_{\hat{d}}$ at the moment when it is visited, leading to Algorithm 7. ALGORITHM 7. Computes the dendrogram $\mathcal{T}_{\hat{d}}$ of the subdominant ultrametric of a dissimilarity space (X, d).

dendrogram(X, d)

Input: A dissimilarity space (X, d)**Output:** The dendrogram $\mathcal{T}_{\hat{d}}$ of the subdominant ultrametric \hat{d} of (X, d)1: let $s \in X$ 2: let $\mathcal{T}_{\widehat{d}}$:= Leaf s 3: let $p(u) := +\infty$ for all $u \in X \setminus \{s\}$ 4: propagate(p, s) 5: while there is an unvisited vertex do let u be an unvisited vertex with p(u) minimum 6: u is now visited 7: $\mathcal{T}_{\hat{d}} \leftarrow \mathsf{insert}(u, p(u), \mathcal{T}_{\hat{d}}) \\ \mathsf{propagate}(p, u)$ 8: 9: 10: return $\mathcal{T}_{\hat{d}}$ propagate(p, u)

11: for $v \in X$ do

12: **if** v is unvisited **then** 13: $p(v) \leftarrow \min\{p(v), d(u, v)\}$

 $insert(u, \rho, T)$

Input: A dissimilarity space (X, d) (implicit), a dendrogram T on $S \subseteq X$ obtained at some step of dendrogram(X, d), $u \in X \setminus S$ minimizing $\min_{x \in S} d(u, x)$, and $\rho := \min\{d(u, x) : x \in S\}$ **Output:** A dendrogram on $S \cup \{u\}$

14: match T with

15: case Leaf x:

16: **return** Node(ρ , [Leaf u, Leaf x])

17: case Node(ρ' , children) when $\rho' < \rho$:

18: **return** Node(ρ , [Leaf u, T])

- 19: case Node(ρ' , children) when $\rho' = \rho$:
- 20: **return** Node(ρ , Leaf u : *children*)
- 21: case Node(ρ' , child : children) when $\rho' > \rho$:
- 22: **return** Node(ρ' , insert($u, \rho, child$) : children)

This algorithm has a pretty visualization that we explain before giving a formal proof. It builds a diagram where each point is a column, sorted left-to-right in visiting order (in the diagram, the order of the leaves is mirrored from that of the tree). Each point u casts a vertical line upward, that bends by a right angle at height p(u) to join the rest of the diagram (the vertical line from the source s does not bend). This is illustrated in Figure 7, where the diagram for the dissimilarity from Figure 2 is given. This diagram is topologically equivalent to the dendrogram, given in Figure 8. The insert procedure traverses down the leftmost branch of the tree, until finding the correct height at which the new leaf is added.

In order to analyse the algorithm, recall that $\hat{d}(x, y)$ is the minimum over all (x, y)-paths of the maximum weight of the edges of that path. This is known as the *bottleneck shortest path*, for which a good characterization is well-known (see [15, Theorem 8.17] for instance). In our context, that good characterization is:



FIGURE 7. The dissimilarity matrix from Figure 2 on the left, the diagram built to illustrate Algorithm 7 on the right. The rows and columns of the matrix are shuffled to avoid masking some of the work of the algorithm.

Theorem 9.1 ([9]). Let (X, d) be a dissimilarity space and \hat{d} be its ultrametric subdominant. Then for all distinct $x, y \in X$,

$$\widehat{d}(x,y) = \min\{\max_{uv \in P} d(u,v) : P \text{ is an } (x,y)\text{-path}\} = \max\{\min_{u \in S, v \in X \setminus S} d(u,v) : S \subset X, x \in S, y \notin S\}.$$

Let the points be sorted in visiting order, x < y means that x is visited before y. We let $p^*: X \to \mathbb{R}_{\geq 0}$ denote the final values of p, taking $p^*(s) = +\infty$. We prove by induction that at the end of each iteration, for all visited $x, y, \hat{d}(x, y)$ is the weight of the lowest common ancestor of x and y in $\mathcal{T}_{\hat{d}}$. Also let $S_v := \{x \in X : v < x\}$ be the set of points unvisited after the iteration in which u = v.

Claim 9.2. Let $v \in X$. For each $x \in S_v$ and $y \in X \setminus S_v$, $d(x, y) \ge p^*(v)$.

Proof. Consider the iteration for which u = v. Then by choice of v, p(v) is minimum, in particular $p(v) \le p(y) \le d(x, y)$. As v is now visited, $p(v) = p^*(v)$, and the claim follows.

We consider an iteration of the main loop in dendrogram, when vertex u is visited; let $u \in X \setminus \{s\}$. Let w be the maximum vertex (in visiting order) with w < u and $p(w) > p^*(u)$ (the column for w is the one to which u is attached).

Claim 9.3. There exists $v \in X$ with $w \le v < u$ and $d(u, v) = p^{\star}(u)$.

Proof. There exists $v \in X$ such that $d(u, v) = p^*(u)$ by definition of p and v < u. Suppose by contradiction that $v \le w$, then during the iteration when w is visited, $p(u) = p^*(u) < p^*(w)$, contradicting the choice of w during that iteration.

Claim 9.4. For all $x \in X$ with $w \le x < u$, $\widehat{d}(x, u) = p^{\star}(u)$.

Proof. By Claim 9.2 and Theorem 9.1, $\hat{d}(u, x) \ge p^{\star}(u)$. Let v be the vertex from Claim 9.3. Then $\hat{d}(u, x) \le \max\{\hat{d}(u, v), \hat{d}(v, x)\} = \max\{p^{\star}(u), \hat{d}(v, x)\}$. By induction, $\hat{d}(v, x)$ is the height of the lowest common ancestor of v and x, that cannot be more than $p^{\star}(u)$ as by construction the part of the diagram between w and u is below $p^{\star}(u)$. The claim follows.

Claim 9.5. If $w \neq s$, then for all $x \in X$ with x < w, we have $\hat{d}(x, u) = \hat{d}(x, w)$.

Proof. There exists $z \leq w$ with $p^{\star}(z) = \hat{d}(x,w)$ by construction of p. Then by Claim 9.2, $\min_{t < z \leq y} d(t,y) = p^{\star}(z)$, thus by Theorem 9.1, $\hat{d}(x,u) \geq p^{\star}(z) = \hat{d}(x,w)$. On the other hand, $\hat{d}(x,u) \leq \max\{\hat{d}(x,w), \hat{d}(w,u)\} = \hat{d}(x,w)$, proving the claim. Together, Claims 9.4 and 9.5 proves that $\mathcal{T}_{\hat{d}}$ is correctly computed. As for the complexity, observe that dendrogram, when removing the lines about $\mathcal{T}_{\hat{d}}$, is exactly Prim's algorithm to compute a minimum spanning tree (except that we compute neither the tree nor the predecessor of each vertex in the tree). Moreover the time spent to build $\mathcal{T}_{\hat{d}}$ is $O(|X|^2)$, as each of the |X| insertions requires at most O(|X|) operations (that part could be optimized to O(|X|) by using a zipper [11], thus avoiding going back to the root at each insertion). Therefore we have proved:

Proposition 9.6. Let (X,d) be a dissimilarity space. Then dendrogram(X,d) computes $\mathcal{T}_{\hat{d}}(X)$ in time $O(|X|^2)$.



FIGURE 8. The dendrogram associated to Figure 7, with the tree representation on the left (actually the mirror of the tree returned by Algorithm 7), and the more traditional dendrogram representation on the right.

9.2. Stable partition algorithm. In this subsection, we present the algorithm which refines any partition to a stable partition.

Lemma 9.7. Let (X, d) be a dissimilarity space, $S \subseteq X$, and \mathcal{P} a partition of S. Then the partition stablePartition(\mathcal{P}) consists of maximal by inclusion mmodules of S contained in a class of \mathcal{P} .

Proof. Let $M \in \text{stablePartition}(\mathcal{P})$. By correction of Algorithm 8, M is an mmodule, and since $\text{stablePartition}(\mathcal{P})$ is a refinement of \mathcal{P} , there is $P \in \mathcal{P}$ such that $M \subseteq P$. Conversely, let M be a maximal mmodule of S contained in some class of \mathcal{P} . Since for any $z \in S \setminus M$ and any $x, y \in M$, we have d(x, z) = d(y, z), one can check that Algorithm 8 cannot separate x from y, that is there is a set $P \in \text{stablePartition}(\mathcal{P})$ such that $M \subseteq P$. By maximality of M, we get M = P, concluding the proof of the lemma.

ALGORITHM 8. Computes the refinement of a partition of (X, d) into a stable partition.

stablePartition(\mathcal{P})

Input: a dissimilarity space (X, d) (implicit), a partition $\mathcal{P} := \{S_1, \ldots, S_k\}$ of X. **Output:** a partition \mathcal{P}' of X that refines \mathcal{P} and such that each part $M \in \mathcal{P}'$ is an mmodule. 1: for $i \in \{1, \ldots, k\}$ do 2: | yield from refinePart $(S_i, X \setminus S_i)$

2. $_$ yield from termer at (D_i, Z_i)

refinePart(B, Z(B))

Input: a dissimilarity space (X, d) (implicit), a class $B \subseteq X$ and a set $Z(B) \subseteq X \setminus B$. **Output:** a partition $\{B_1, B_2, \ldots, B_k\}$ of B.

2: if $Z(B) = \emptyset$ then 3: $\lfloor \text{ return } \{B\}$ 4: let $q \in Z(B)$, \triangleright choose q to be the first element of Z(B)5: let $\{B_1, \ldots, B_m\}$ = refine(q, S) \triangleright ignore the order of the B_is 6: for $i \in \{1, \ldots, m\}$ do 7: $\lfloor \text{ yield from refinePart}(B_i, \text{ concatenate}(B_1, \ldots, B_{i-1}, B_{i+1}, \ldots, B_m, Z(B) \setminus \{q\}))$

refine(q, S)

Input: a dissimilarity space (X, d) (implicit), a point $q \in X$, a subset $S \subseteq X$.

Output: an ordered partition of S, by increasing distances from q.

- 9: let T be an empty balanced binary tree, with keys in \mathbb{N}
- 10: for $x \in S$ do
- 11: **if** \neg containsKey(T, d(q, x)) then
- 12: insert(T, d(q, x), [])
- 13: $\lfloor \text{ insert}(T, d(q, x), x \cdot \text{get}(T, d(q, x))) \rfloor$
- 14: return values(T)